The building and antennas in the background are the short-wave broadcast facilities for radio station WWV which broadcasts time and frequency information to the United States. The van in the foreground is a mobile satellite communication terminal used by the Time and Frequency Division for experiments on accurate time transfer. One objective of this work is the development of a highly accurate satellite time service.

The NIST High Accuracy Cryogenic Radiometer (HACR) ties optical power measurements to electrical power measurements, based on the NIST standard volt and ohm. Each power source causes a temperature rise on a receiving cavity in the center, which is precisely measured and balanced. Cryogenic operation, which is not a part of traditional electrical substitution radiometry, substantially reduces uncertainties and systematic errors. The Radiometric Physics Division relies on the HACR to derive measurement scales in radiometry and photometry.

The lifetime of the free neutron is measured by "trapping" decay protons in an electromagnetic Penning trap. The figure shows a design study of the trap electrode structure used in the NIST neutron lifetime determination. The measurement of the neutron lifetime has implications for cosmology, astrophysics, and particle physics. Techniques resulting from this measurement will also provide new standards for neutron dosimetry and for analytical chemistry. (Ionizing Radiation Division)

The molecular structure of the ethylene-ketene weakly bound complex is shown as derived from microwave spectroscopy (viewed along the C=C bond of ethylene). The geometry shows that the heavy atoms of the two molecules are crossed at 90 degrees, as predicted by organic chemists for the cycloaddition reaction which produces cyclobutane. (Molecular Spectroscopy Division)

Scanning Electron Microscopy with Polarization Analysis (SEMPA) magnetization images show the domains in a clean Fe single crystal whisker (bottom panel), where the white and black regions denote magnetization to the right and left respectively. The top panel shows the magnetization in a 2 nm thick Fe film separated from the Fe whisker of the bottom panel by an evaporated wedge of Cr which varies linearly in thickness as shown on the bottom scale. The exchange coupling starts off ferromagnetic at small Cr thickness, then changes to antiferromagnetic (magnetization antiparallel to that of the whisker substrate), as the thickness increases and undergoes several oscillations in this manner with a period of 1.4 to 1.7 nm, equivalent to the thickness of 10 to 12 Cr layers. (Electron and Optical Physics Division)

Triple axis diffraction tracing of an x-ray optic multilayer structure. The structure consists of 20 bi-layers of molybdenum and silicon with a 2d spacing of 13.2 nanometers. (Quantum Metrology Division)

The NIST Reference Cell is pictured. Powered at a radio frequency of 13.56 MHz, this source generates a plasma similar to that used in semiconductor etching devices. Several laboratories throughout the United States are cooperating in reference measurements, including emission and laser spectroscopy, energy-analyzed mass spectrometry and electric probes, to study its properties. (Atomic Physics Division)

Elevation view of the major components—throwing chamber, interferometer, and superspring—of the FG5 instrument for ultrahigh precision absolute gravity measurements. This NIST-developed technology is being transferred to Axis Instruments for engineering and manufacture. (Quantum Physics Division)
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February 24-25, 1992

Katharine B. Gebbie
Director
Physics Laboratory

February 1992

U.S. DEPARTMENT OF COMMERCE
Rockwell A. Schnabel,
Acting Secretary
Technology Administration
Robert M. White, Under Secretary
National Institute of Standards and Technology
John W. Lyons, Director
ABSTRACT

This report summarizes research projects, measurement method development, calibration and testing, and data evaluation activities that were carried out during calendar year 1991 in the NIST Physics Laboratory. These activities fall in the areas of electron and optical physics, atomic physics, molecular physics, radiometric physics, quantum metrology, ionizing radiation, time and frequency, quantum physics, and fundamental constants.

Key Words: atomic physics; calibrations; data evaluation; electron physics; fundamental constants; ionizing radiation; measurement methods; molecular physics; optical physics, optical radiation; quantum metrology; quantum physics; standard reference materials, time and frequency
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INTRODUCTION

This report is a summary of the technical activities of the National Institute of Standards and Technology (NIST) Physics Laboratory for the period January 1991 to December 1991. The Laboratory is one of nine major operating units of the National Institute of Standards and Technology. The mission of the Physics Laboratory is to advance science and technology by: pursuing fundamental research in the physical sciences; developing new physical standards, measurement methods, and data; conducting an aggressive dissemination program; and collaborating with industry to commercialize our inventions and discoveries.

The Laboratory is vertically integrated, spanning the full range of programs from tests of fundamental postulates of physics through generic technology to the more immediate needs of industry and commerce. Its constituencies are broadly distributed throughout academia, government, and industry.

As part of a major NIST reorganization, the Laboratory was formed from the former Center for Atomic, Molecular, and Optical Physics and the former Center for Radiation Research and began official operation on February 10, 1991.

The Physics Laboratory focuses its long-term research on atomic, molecular, optical, and radiation physics. It develops new physical standards, measurement methods and reference data, and promulgates these standards, methods, and data by providing measurement services, conducting workshops, publishing research results, and collaborating with industry, universities, and other agencies of government.

Specifically, the Laboratory establishes spectroscopic methods and standards for infrared, visible, ultraviolet, x-ray, and gamma-ray radiation; investigates the structure and dynamics of atoms and molecules, singly and in aggregate; develops and disseminates national standards for time and frequency and for the measurement of optical and ionizing radiation by means of calibrations, measurement quality assurance, and standard reference materials.

The Laboratory generates, evaluates, and compiles atomic, molecular, optical, and ionizing radiation data in response to national needs, develops and operates major radiation sources as user facilities, and maintains appropriate collaborations with other Laboratories in NIST, the Nation, and throughout the world. It conducts a major cooperative research program with the University of Colorado through the Joint Institute for Laboratory Astrophysics. The Laboratory’s programs support the research community and industry in such areas as communication, defense, energy, environment, space, health, electro-optics, electronics, radiation, and transportation.

The Physics Laboratory consists of eight Divisions.

- Electron and Optical Physics Division. Provides the central national basis for the measurement of far ultraviolet and soft x-ray radiation; conducts theoretical and experimental research with electron, laser, ultraviolet, and soft x-ray radiation for measurement applications in fields such as atomic and molecular science, multiphoton processes, radiation chemistry, space and atmospheric science, microelectronics, electron spectroscopy, electron microscopy, surface magnetism, and solid state and materials science; determines the fundamental mechanisms by which electrons and photons transfer energy to gaseous and condensed matter; develops advanced electron- and photon-based techniques for the measurement of atomic and molecular properties of matter, for the determination of atomic and magnetic microstructure, and for the measurement and utilization of ultraviolet, soft x-ray, and electron radiation; develops and disseminates ultraviolet, soft x-ray and electron standards, measurement services, and data for industry, universities, and government; and develops and operates well-characterized sources of electrons and photons including the NIST synchrotron ultraviolet radiation
facility (SURF II), a scanning tunneling microscope, and two scanning electron microscopes with unique magnetic imaging capabilities.

- **Atomic Physics Division.** Carries out basic theoretical and experimental research into the spectroscopic and radiative properties of atoms and highly ionized species to provide measurement and data support for national needs in such areas as fusion plasma diagnostics, processing of materials by plasmas, spectrochemistry, and laser development; develops well-defined atomic radiation sources as radiometric or wavelength standards to meet national measurement needs; studies the physics of laser cooling and electromagnetic trapping of neutral atoms and ions; develops new measurement techniques and methods for spectral analysis and for the measurement of plasma properties; and collects, compiles, critically evaluates, and supplements spectroscopic data bases to meet major national demands for such data.

- **Molecular Physics Division.** Determines spectroscopic properties of molecules, radicals, and their ions from experimental measurements of their spectra; applies advanced theoretical concepts to the analysis of spectra and to the use of spectroscopic data for the determination of molecular properties such as dissociation energies, potential functions, dipole moments, line shapes, and structures; develops advanced experimental techniques and instrumentation for obtaining, measuring, and interpreting molecular spectra; establishes secondary frequency standards; collects, compiles, and critically evaluates spectroscopic data and associated physical properties, and supplies data necessary for the calculation of thermodynamic functions; applies molecular spectroscopic techniques to the solution of measurement problems in areas such as the environment, energy and laser technologies, chemical kinetics, and materials science research; and develops theoretical descriptions of collisional, radiative, and nonradiative processes for applications to spectroscopic phenomena, atomic collisions, and state-selected kinetics.

- **Radiometric Physics Division.** Provides national measurement standards and support services for ultraviolet, visible and infrared radiation to meet major national needs in such areas as health and safety, the lighting, photographic, and xerographic industries, solar measurements, and national defense; provides standards dissemination and measurement quality assurance services leading to accurate and uniform measurements of optical radiation throughout the Nation; conducts research in optical radiation, pyrometry, photometry, and quantum radiometry to provide competence necessary to improve the accuracy and extend the range of optical radiation measurements and develop standards and methods for both source and detector based radiometry; and develops standards and calibration procedures for spectroradiometers, spectrophotometers, electrooptical radiometric devices, and reflectance and transmittance measurements.

- **Quantum Metrology Division.** Engages in a program of research characterized by strong coupling between advances in measurement technology and basic physics; addresses problems in the determination of fundamental physical constants and interacts with others in the Physics Laboratory and other Laboratories in NIST where work in fundamental quantities occurs; contributes to the extension and refinement of the electromagnetic scale and devises tests of basic symmetries and invariances; and maintains continuing efforts in several discipline areas including fundamental neutron physics, x-ray spectroscopy of atoms, molecules and simple solids, spectra of laboratory and astrophysical plasmas, and application of high accuracy measurements to the study of calculable spectra of basic scientific interest.

- **Ionizing Radiation Division.** Provides primary national standards, dosimetry methods, measurement services, and basic data for application of ionizing radiation (x-rays, gamma rays, electrons, neutrons, and radioactivity, etc.) to radiation protection of workers and the general public, radiation therapy and diagnosis, nuclear medicine, radiography, industrial radiation processing, nuclear power, national defense, space science, and environmental protection; conducts theoretical and experimental research on the fundamental physical interactions of ionizing radiation with matter; develops an understanding of basic mechanisms involved in radiation-induced chemical transformations and the parameters that influence the yields of short-lived intermediates, final chemical products, and biological effects; develops improved methods for radiation measurement, dosimetry, and radiography; develops improved primary radiation standards, and produces highly accurate standard reference data for ionizing radiation or radioactive materials; provides standard reference materials, calibrations, and measurement
quality assurance services, to users such as hospitals, industry, states, and other federal agencies; and develops and operates well-charac-
terized sources and beams of electrons, photons, and neutrons for primary radiation standards, calibrations, research on radiation interactions, and measurement methods development.

- **Time and Frequency Division.** (Boulder) Maintains, develops, and improves the national standards for time and frequency and the time scales based on these standards; carries out research in areas of importance to the further fundamental improvement of frequency standards and their applications, focusing on microwave and laser devices, atomic and molecular resonances, and the measurement of fundamental physical phenomena and constants; adapts time and frequency standard devices and concepts to special scientific and technological demands; develops time and frequency measurement methods in the radiofrequency, microwave, Infrared, and visible radiation regions; coordinates the national time and frequency standards, time scales, and measurement methods nationally and internationally in conjunction with the United States Naval Observatory; operates time and frequency dissemination services, such as radio stations and broadcasts, for the purpose of traceability to the national standards of time and frequency; coordinates these services nationally and internationally; evaluates existing services in terms of present and future user needs and implements improvements as appropriate; assists present and potential users to apply NIST time and frequency services effectively to the solution of their particular problems; provides publications and consultations, and conducts seminars and demonstrations relating to NIST time and frequency dissemination facilities and services; and performs research and development on new dissemination techniques and, as appropriate, implements improved services based on these studies.

- **Quantum Physics Division.** (Boulder) Engages in long-term, high-risk research in quantum physics and related areas such as atomic and molecular collisions, spectroscopy and radiative interactions, chemical physics, optical and laser physics, gravitational physics, geophysical measurements, radiative transfer, and solar physics; performs basic, highly accurate measurements and theoretical analyses in these areas essential to the foundations of the Nation's science and technology; develops the laser as a refined measurement tool; applies state-of-the-art methods to measurements and tests of the fundamental postulates and natural constants of physics; engages in research in atomic, molecular, and chemical physics leading to the determination of key techniques and data essential to understanding, predicting, and controlling the properties of excited and ionized gases and the pathways of chemical processes; improves the theory and instrumentation required for measurements of astrophysical and geophysical quantities such as the cosmic distance scale, earth's gravity, and terrestrial distances; maintains, through its association with the Joint Institute for Laboratory Astrophysics (JILA) at the University of Colorado and JILA's Visiting Fellows Program, active contact with and expertise in advanced research in physics; and makes its scientific knowledge available to many other areas of NIST and to industry through publications, visits, and exchange of personnel.

**ORGANIZATION OF REPORT**

This technical activities report is organized in nine sections, one for the Physics Laboratory Office which includes the Fundamental Constants Data Center, and one each for the eight Divisions. For each Division the report consists of brief statements of the Division's mission and organization, followed by a discussion of current directions, highlights of the year's accomplishments, and a discussion of future opportunities.

Following the technical activities section are a series of Appendices which list: publications; Invited talks; committee participation and leadership; workshops, conferences, and symposia organized; journal editorships; industrial interactions; other agency research and consulting; calibration services and standard reference materials; and a list of acronyms used in this report. Each appendix is grouped by Division; if a Division is not listed in a particular appendix it means that they had nothing to report in this category.

To obtain more information about particular work, the reader should address the individual scientists or their Division office, c/o Physics Laboratory, B160 Physics Building, National Institute of Standards and Technology, Gaithersburg, Maryland 20899.
FUNDAMENTAL CONSTANTS
DATA CENTER
B. N. Taylor

MISSION

- to provide an international information center on the fundamental physical constants (FC) and closely related precision measurements (PM);
- to analyze the consistency of measured values of the constants in order to test fundamental physical theory and to obtain sets of recommended values of the constants for international use;
- to administer the NIST Precision Measurement Grant (PMG) Program;
- to provide the editorship of the Journal of Research of the National Institute of Standards and Technology;
- to serve as the NIST-authorized organization for the Interpretation of the International System of Units (SI) in the United States.

CURRENT DIRECTIONS

- Measurement Uncertainty. Take advantage of the expertise of the Fundamental Constants Data Center (FCDC) in analyzing measurement data to contribute to an international effort under the auspices of ISO (International Organization for Standardization) to generate a guide on expressing measurement uncertainty that will be followed worldwide.

- Information Center. Update and improve the organization of the FCDC's extensive collection of reprints and other material relating to the FC-PM field in order to improve the FCDC's responsiveness to inquiries and its ability to carry out the next CODATA (Committee on Data for Science and Technology) least-squares adjustment of the constants, to be completed sometime in 1995, that will provide a new set of recommended values of the constants for international use.

- 1995 Constants Adjustment. Make initial preparations, such as surveying relevant work underway in laboratories throughout the world, for the 1995 constants adjustment.

- Precision Measurement Grants. Implement policies that will ensure that the PMG program continues to attract proposals of the highest quality and provides maximum benefit to NIST.

- NIST Journal of Research. Implement policies that will ensure that the NIST Journal of Research continues to be a widely read, highly respected, scientific publication and an attractive vehicle for NIST scientists to use to report the results of their research in measurement.

- SI Units. Generate publications related to the SI and disseminate them widely in order to meet the information needs of the increased number of users of the SI arising from the Federal government's planned 1992 conversion to the SI.

HIGHLIGHTS

- Guide on the Expression of Uncertainty. The FCDC assumed principle responsibility, in collaboration with C. E. Kuyatt, also of the Physics Laboratory, for drafting a Guide titled "Expression of Uncertainty In Measurement." This Guide is being prepared under the auspices of ISO, Technical Advisory Group 4 (TAG 4) in particular, at the request of the International Committee for Weights and Measures (CIPM). It will be published jointly by ISO, IEC (International Electrotechnical Commission), OIML (International Organization for Legal Metrology), and BIPM (International Bureau of Weights and Measures) for worldwide use in metrology at all levels of accuracy and in a wide range of fields. A first draft was completed in March 1991 and subsequently discussed at a meeting of the ad hoc Drafting Group of Working Group 3 (WG 3) of TAG 4, which Is the Working Group actually preparing the Guide. A second draft was completed in August 1991 and discussed with the ad hoc Drafting Group in October. A third draft, and it is hoped the final draft, was completed in December 1991 and will be discussed at a meeting of WG 3 in its entirety in January 1992. It is expected that the resulting final version of the Guide will be submitted to TAG 4 for their review during the first half of 1992.

- SI Units. The FCDC prepared and published two important NIST special publications (SP)
designed to increase the use of the SI in the United States. The first was NIST SP 330, 1991 edition, a booklet that is the U.S.A. edition of the English-language translation of the sixth edition of Le Système International d'Unités (SI), the definitive reference on the foundation and fundamental principles of the SI published in 1991 by the BIPM in the French language on behalf of the CIPM and the General Conference on Weights and Measures (CGPM). The second was NIST SP 814, a booklet that reprints the December 1990 Federal Register notice published by the FCDC restating the Department of Commerce's interpretation of the SI for the United States; the January 1991 Federal Register notice issued by the Office of the Secretary of the Department of Commerce that revises the Code of Federal Regulations to remove the voluntary aspect of the conversion to the metric system by Federal agencies; and Executive Order 12770 issued in July 1991 by the President of the United States that provides Presidential authority and direction for the use of the metric system of measurement by Federal departments and agencies in their programs.

- **Precision Measurement Grants.** The FCDC awarded, on behalf of NIST, new Precision Measurement Grants to Daniel J. Heinzen, University of Texas at Austin, and Carol E. Tanner, University of Notre Dame. The grants are in the amount of $30,000 per year, renewable for two additional years. Heinzen's project, "Quantum Limited Cooling with Stored Ions," has the ultimate goal of increasing the accuracy of mass ratio and electron and positron g-factor measurements to the unprecedented parts in $10^{11}$-$10^{12}$ range by extending recently developed quantum limited cooling and detection techniques. Tanner's project, "Absolute Calibration of Atomic Parity Nonconservation Measurements," will provide data that will allow the detailed interpretation of new atomic parity nonconservation experiments in cesium, experiments that, because of their high accuracy and low interaction energy, will probe the standard model of the weak interaction at a level that can test it critically and search for new physical effects.

**FUTURE OPPORTUNITIES**

The main focus of the FCDC's work in 1992 will be the completion and wide distribution of the ISO/IEC/OIML/BIPM Guide, "Expression of Uncertainty in Measurement." Nevertheless, preparations for the next CODATA least-squares adjustment of the constants will continue through active participation in the planned 1992 meeting of the CODATA Task Group on Fundamental Constants. The efforts of the FCDC will increasingly be devoted to this adjustment in 1993 and beyond until its completion sometime in 1995.
MISSION

The Electron and Optical Physics Division is broadly chartered to advance the capabilities for absolute measurement of electron and photon interactions with matter, and to diffuse such capabilities into industry, academia, and other branches of Government. In pursuit of this mission, it maintains an array of research, measurement, and calibration activities. In particular, the Division

- provides the central national basis for absolute radiometry in the far ultraviolet and soft x-ray regions of the electromagnetic spectrum, which together span the photon energy range of 5 eV to 250 eV. This basis is maintained through a combination of ionization chambers, calibrated transfer standard detectors, and an electron storage ring, the SURF-II Synchrotron Ultraviolet Radiation Facility, which provides a dedicated source of radiation over this spectral range. SURF-II also supports a range of research activities by members of the Division, of other NIST organizational units, and external research groups.

- maintains specialized electron microscopy facilities for Scanning Electron Microscopy with Polarization Analysis (SEMPA), and Scanning Tunneling Microscopy (STM). The SEMPA facility provides unique capabilities for the study of surface magnetism, and has resulted in a wide range of collaborative research involving the magnetic recording industry. The STM facility is used for studies of surface electronic structure, particularly that associated with adsorbed atoms.

- performs basic theoretical and experimental research in atomic, molecular, surface, and condensed matter physics in support of its basic mission objectives.

ORGANIZATION

The Division has about 34 full-time equivalent members of staff, and during the past year had the equivalent of 10 Guest Researchers working full-time during visits of three or more months. It consists of three groups: the Photon Physics Group, working primarily on soft x-ray optics and spectroscopy and laser spectroscopy; the Far Ultraviolet Physics group, which operates SURF-II and performs calibrations; and the Electron Physics group, which is engaged in various types of electron microscopy, electron-atom scattering, and theoretical condensed-matter physics.

CURRENT DIRECTIONS

The work of the Division falls into three main categories. In descending order of the resources dedicated to them, these are: basic research and measurement methodology; operation of the SURF-II facility; and absolute radiometry and calibration services.

- Basic Research and Measurement Methodology. The Division pursues basic research on electron and photon interactions with matter, with its principal emphases being the elucidation of electronic structure of atoms, molecules, and condensed matter, and the electronic and magnetic structure of surfaces. The specific projects now active are: multiphoton ionization of atoms (Photon Physics); soft x-ray fluorescence spectroscopy (Photon Physics); high-resolution VUV spectroscopy of atoms and molecules (Photon and Far UV Physics); soft x-ray optics (Photon and Far UV Physics); electron-atom scattering (Electron Physics); scanning tunneling microscopy (Electron Physics); scanning electron microscopy with polarization analysis (Electron Physics); and theoretical physics (Electron Physics and Division Office). Development of advanced instrumentation and novel measurement techniques is a central focus of all of our experimental efforts, and our principal apparatus has largely been designed and built in-house. Maintenance of this development capability is a high priority, for three reasons: it provides the key competitive scientific advantage enjoyed by our research programs; it has been extremely fruitful as a platform for technology transfer to industry and other laboratories; and its products
enhance calibration and measurement services efforts, both in the Division and elsewhere in NIST. We maintain active research collaborations with industry, particularly in the areas of SEMPA, soft x-ray optics, and multiphoton ionization.

- Operation of the SURF-II Synchrotron Ultra-violet Radiation Facility. Operation of SURF-II is one of the Division’s major responsibilities. SURF-II provides the basis for our efforts in absolute radiometry, and is also an important vehicle for general scientific work. Although SURF-II is a mature instrument that cannot match the performance of the latest generation of storage rings, it is still highly competitive for many applications in the region of photon energies below 200 eV. The main thrusts of our efforts at SURF-II are in improving basic machine performance and providing facilities enhancements for users. In the past year we have attained record operating currents; have greatly expanded the office and preparation space available to SURF-II users; have installed ethernet communications throughout; and have begun work on an expansion of the beam hall, which should increase the usable beam line space by about 50%. Support of SURF-II users from outside the Division is a high priority. The main steps taken in this direction were the commissioning of the High-Resolution Spectrometer on BL-3, which is used at present by groups from the University of the District of Columbia, Howard University, and the Naval Postgraduate School; and a refurbishment of BL-5, which was used by a group from the University of Oregon.

- Absolute Radiometry and Calibration Services. We pursue two types of work in this area: the development and dissemination of transfer standards in the VUV and soft x-ray spectral regions; and custom calibration of particular spectrometers, detectors, and other x-ray optical systems. Our transfer standard activities have flourished in the past year, due to the introduction of new semiconductor photodiodes, and the commissioning of a new dual monochromator system for absolute calibration of windowed photodiodes. The principal facility for custom calibrations is BL-2 at SURF-II. It has been responsible for calibrating virtually all VUV instrumentation flown on U.S. spacecraft. Our main customer for this work is NASA, which has long supported BL-2 operations, and significantly increased its financial commitment during the past year. Soft x-ray optics are calibrated on a reflectometry facility on BL-8. A major contract to expand this facility was awarded by DARPA in the past year, as part of its x-ray lithography development program.

**HIGHLIGHTS**

Highlights of technical activities performed within the past year include:

- **Magnetic Coupling in Multilayer Materials.** The SEMPA apparatus has been used to discover very dramatic variation of magnetic coupling present in iron-chromium-iron sandwich structures. Our earlier investigations of the magnetic structure of ultra-thin ferromagnetic films were extended to study the magnetic coupling in multilayer films. We have been particularly successful in precisely measuring the magnetic coupling between Fe films separated by Cr spacer films of varying thickness. The coupling in these films had been previously shown to oscillate between ferromagnetic and antiferromagnetic with a period of about 2 nm or 15 monolayers. By growing very high quality films, we discovered that the coupling actually oscillates with a period of two monolayers. In other words, the Fe film goes from being ferromagnetically to antiferromagnetically coupled as the Cr spacer thickness changes by only one monolayer. We have found that when atomically well-ordered Fe/Cr/Fe sandwiches are grown these oscillations can persist for up to 50 monolayers of Cr. The multilayers were grown in situ using a Fe single crystal whisker substrate, with the Cr exposure varied along the length of the Fe whisker to produce a Cr wedge. This enabled us to measure the coupling as a continuous function of the Cr spacing. In addition, to the pure ferromagnetic or antiferromagnetic coupling at certain Cr thicknesses, we also observed intermediate coupling in which the magnetization in the Fe film was roughly ninety degrees with respect to the substrate magnetization. We are currently trying to understand this interesting biquadratic coupling effect, and are beginning to measure the coupling using other non-magnetic spacers. (R.J. Celotta, M.H. Kelley, D.T. Pierce, J. Unguris)

- **Alternative Physical Mechanisms for High-Temperature Superconductivity.** There is at present no established theory of high Tc superconductivity in the oxides. It has recently been suggested that a simple modification of the usual BCS theory might be able to account for both the large values of Tc and the small values of the isotope coefficient a in the superconduct-
ing oxides. The physical basis for this modification is found in the density-of-states peaks suggested by band structure calculations. The usual BCS-type expressions for $T_c$ and $\alpha$ are modified if the Fermi energy lies near a singularity in the density of states. Very recently it was shown that this approach is consistent with the anomalous behavior of $\alpha$ as a function of doping $x$ in La$_2$Sr$_2$CuO$_4$. A quantitative study of the consequences of introducing broadening into the density of states has been carried out. Three sources of broadening were considered: inhomogeneities, three-dimensional effects, and inelastic electron scattering. The first two sources were represented by a constant energy and the third by a broadening proportional to temperature. We showed that for materials such as YBaCuO the presence of a logarithmic singularity in the density of states is not sufficient to explain the very small isotope coefficient even in the absence of broadening. For LaSrCuO it was found that for values of the broadening consistent with band structure calculations, the theory fails to explain the measured properties. (D.R. Penn; M.L. Cohen, T.W. Barbee III, Univ. California)

- **Complete Experimental Determination of Scattering Amplitudes for Electron Collisions with Na.** A long-standing concern of the Electron Physics Group is to investigate the interaction of spin-polarized electrons with free atoms in as complete a manner as possible, with the expectation that the resulting information will lead to a much more solid understanding of the complex processes at work in spin-polarized electron interactions. We pursue this goal with experiments in which a beam of spin-polarized electrons is scattered by an atom in a specific quantum state produced by optical pumping. By spin, angular, and energy analysis of the scattered electron we therefore obtain detailed information on the state of the system before and after the collision, and are therefore able to make comparison with theory without averaging over unresolved variables. This year we have studied both elastic and inelastic scattering by Na at a number of collision energies. Elastic results were obtained at the very low incident energies of 1.0 and 1.6 eV. These energies are below the threshold for excitation of the 3P state in sodium, and therefore they provide an exacting comparison for theoretical calculations in a region where the calculations can be expected to be good. Elastic and inelastic results were also obtained at energies of 4.1, 10, 20 and 40 eV, effectively spanning the energy range of interest to electron scattering theoreticians. In addition, we have been able to combine our results with complementary measurements done by others to generate a "complete" experimental determination of the magnitude and relative phase of the elastic scattering amplitudes. (M.H. Kelley, J.J. McClelland; R. Scholten, Flinders Univ.)

- **Scanning Tunneling Microscopy of Atoms Adsorbed on Metal Surfaces.** The goals of the scanning tunneling microscopy (STM) program are to investigate the novel properties of matter that occur in nanometer size structures, and to develop advanced methods which further the application of scanned electron probe techniques. At present our focus is on semiconductor and magnetic materials, along with the development of a synergistic marriage between the two with epitaxially grown magnetic films on semiconductor substrates. The newer of our two STM microscopes was used to obtain an unprecedented vertical sensitivity of 1 picometer. This enables us to routinely resolve individual atoms on metal surfaces, an achievement which only a few laboratories in the world can claim because of the very low signal levels on metal surfaces. Results of particular interest have been obtained for Fe on Au surfaces. In this work we have shown how one material (Au) can stabilize an artificial structure of another (Fe in the fcc configuration) when the Fe is grown epitaxially on the Au (111) surface. This represents a phase of Fe that does not naturally occur at room temperature (where iron is bcc), and shows how new magnetic phases can be "atomically" engineered and measured. We are currently continuing this work in growing iron on iron to understand the fundamental process in metal epitaxy in order to better understand how to engineer new materials with tailored magnetic properties. (R.J. Celotta, R.A. Dragoset, D.T. Pierce, and J.A. Strosclio)

- **Theory of Resonant Tunneling Junctions.** The behavior of resonant tunneling heterojunctions has been the subject of much study since the pioneering work of Tsu and Esaki on superlattices. This type of heterojunction exhibits useful characteristics for electronic applications such as oscillators or switching devices due to its negative differential resistance and rapid charge transfer in a microwave field. Therefore, we studied the behavior of resonant junctions subjected to photon radiation. Theoretical work on resonant tunneling junctions in the presence of a photon field has generally been carried out within the framework first introduced by Tien.
and Gordon. They suggested that in the presence of a photon field an energy level, \( E \), develops side bands at \( E \pm n\hbar \nu \) where \( n \) is an integer. This allows a tunneling current not only from the state at energy \( E \) but also at energies corresponding to the side bands. The model admits a simple analytical solution. This picture is in sharp contrast to the way in which photon absorption in solids takes place; as an excitation of an electron from one state to a different one that is separated from it in energy by \( \hbar \nu \). We have suggested that a model in which an electron is photoexcited to another state and then tunnels through the barrier may be applicable to some of the experiments on tunneling junctions. Our theory takes the same form in the weak field limit as that of Tien and Gordon and we have derived an expression for the relative size of the tunneling currents. (D.R. Penn, M.D. Stiles; P. Apell, Chalmers Univ.)

- **Analysis of BEEM Spectra to Elucidate the Properties of Buried Interfaces.** Ballistic-Electron Emission Microscopy (BEEM) is a technique based on Scanning Tunneling Microscopy (STM) that is used to investigate buried interfaces. The STM tip is used to inject electrons into a metal overlayer which has been grown on a semiconductor substrate. Measuring the current as a function of the voltage at which the electrons are injected gives a direct measurement of the transmission properties of the buried interface. In collaboration with AT&T Bell Laboratories the first *ab initio* calculations of BEEM spectra have been carried out, for interfaces between silicon and both cobalt and nickel disilicide. These materials have been proposed for use in metal-base transistors, a novel type of device that depends crucially on the transport across its interfaces. A measurement of the BEEM spectrum for cobalt disilicide done independently, which could not be understood using previous models, was found to agree quite well with the calculation. The agreement showed that this was the first BEEM measurement that was sensitive to two aspects of the transport that were explicitly included in the calculations. It was the first to show a clear signature of the band structure of the metal and the first to show the conservation of crystal momentum parallel to the interface for transport across an interface. The comparison of calculated and measured spectra for both interfaces should allow better understanding of BEEM as a tool for studying buried interfaces. (M.D. Stiles; D. Hamann, AT&T Bell Laboratories)

- **Marked Expansion of XUV Optics Characterization Facility.** The XUV optics characterization facility on BL-8 at SURF-II is the only dedicated national facility for performing reflectivity measurements on normal-incidence XUV multilayer optics. Commensurate with the growing general scientific interest in this field, the number of characterizations performed this year exhibited a dramatic increase; over seventy independent multilayer characterizations were made, vs. thirty last year. In addition, some other special-purpose measurements were undertaken. The most noteworthy of these involved the determination of the absolute diffraction efficiency of a special transmission grating that will be incorporated in a rocket-launched solar spectrometer by a group from Stanford University. This grating, a free standing array of 100 nm thick, 300 nm tall gold wires spaced 200 nm apart, is a recent accomplishment of microfabrication technology produced at MIT. (R.N. Watts and C.S. Tarrio)

- **DARPA Funds National X-Ray Optics Characterization Facility at SURF-II.** The Defense Advanced Research Projects Agency (DARPA) funded a major proposal involving the Photon Physics and Far-Ultraviolet Physics Groups, the Precision Engineering Division, and the Quantum Metrology Division. The main thrust of this proposal is the construction of a new beam line at SURF-II for dedicated x-ray optics characterization; complementary research on multilayer components utilizing profilometry and hard x-ray diffractometry is also supported by this program. The basic design of the new beam line has been completed, and its major components are now being procured. It will provide us the capability for the testing of much larger optics than can be handled on the current facility, and for the measurement of additional parameters whose determination is essential for improving the performance of x-ray optical components. We envisage this facility as providing a major step towards the development of a full-fledged "optical-bench" capability in the soft x-ray spectral region. (D.L. Ederer, T.B. Lucatorto, R.P. Madden, and R.N. Watts)

- **Cooperative Research and Development Agreement (CRDA) Initiated in Optics for X-ray Lithography.** The Photon Physics Group has entered into a CRDA with Hampshire Instruments, Inc. (Rochester, NY) to assist them in their development of collimating optics for an x-ray lithographic system. NIST has provided...
consultation on the feasibility of various approaches to collimating x-rays and will provide a characterization of a multilayer coated optic being fabricated for that purpose. This is the second CRDA currently in effect in the Division; the other involves a collaboration with Eastern Analytical, Inc. (College Park, MD), using multiphoton resonance ionization to enrich low-abundance stable isotopes in calcium samples for biomedical applications. (T.B. Lucatorto)

- **AC Stark Effect Measured in Ca.** Significant disagreement exists between experiment and theory on the magnitude of the AC Stark shift on high lying Rydberg levels. Theory predicts a shift equal to the so-called ponderomotive potential, which is the average kinetic energy imparted to a free electron by an oscillating electric field. Recent measurements elsewhere had shown shifts less than this value; in particular, detailed measurements in Xe were found to yield about one-half of the predicted value. Our measurements on the closely spaced 4s8d, 4s9s, 4s10s, and 3d5s levels of Ca find the shift to be equal to the ponderomotive value for all but the 3d5s level. The difference is attributed to the strong coupling of the 3d5s level to an autoionizing level in the continuum. (T.B. Lucatorto; J.B. Kim, Korean Science and Engineering Foundation)

- **Generation of VUV Radiation for Measurement of Lamb Shift in He.** A Ti:Sapphire laser has been constructed and first results have been obtained on the generation of 120.285 nm radiation for Doppler free spectroscopy of the 1s2 1S-1s2s 1S transition in He. Preliminary measurements show conversion efficiencies of about 5 X 10^-8. This is comparable to what has been achieved by other workers in the field, and is sufficient to perform the spectroscopy on He. We expect that with the addition of injection seeding and further refinements to the Ti:Sapphire laser, this efficiency will improve substantially. (T.B. Lucatorto and T. O'Brien)

- **Associative Ionization of Ultracold Sodium.** We have observed complicated structure in the dependence on detuning from atomic resonance of the associative ionization rate of Na atoms confined in a laser trap. These experiments demonstrate a new class of laser-controlled chemical reactions. Because the thermal energy (~1 mK) is of the same order of magnitude as the light shifts of the atomic levels, the reaction can be dramatically affected by altering the parameters of the laser field. In addition, the extremely slow velocity of approach allows access to molecular states unresolvable at higher energies. (P.D. Lett)

- **Sequential vs. Simultaneous Ionization of Atoms by an Ultra-strong Laser Field.** There is much uncertainty over the basic mechanism of multiple ionization of atoms in strong laser fields. We have solved numerically the time-dependent Schroedinger equation for helium in a model radiation field, using the Connection Machine at the University of Maryland Institute for Advanced Computer Studies. Visualization of the two-electron wave function has enabled us to view this process in detail. We have found that at low laser intensities, the two electrons leave the atom in sequential order, as expected. However, there appears to be a relatively sharp threshold in laser intensity (of the order of 3 x 10^{16} W cm^{-2} at the frequency of the ArF laser), at which both electrons are stripped from the atom in the early stages of the laser pulse. Even for such strong fields, significant effects of electron correlation are manifest: at threshold, the electrons depart predominantly on opposite sides of the nucleus. (S. Blodgett-Ford; C.W. Clark; J.S. Parker, Univ. Maryland)

- **New Record Currents Achieved at SURF-II.** On October 22nd, 1991, a new record beam current of 325.6 mA was attained. The previous maximum beam current record of 303 mA occurred in March, 1989. In addition, a record monthly average beam current of 244.8 mA was achieved for the month of November, 1991; this average as of mid-December 1991 was in excess of 250 mA. The improvement in ramped current appears to be due primarily to repairs made as a result of two system failures: RF breakdown of the microtron accelerator cavity in May 1991, and a capacitor failure in the power supply for the microtron modulator in October 1991. After repairing the cavity, and replacing the power supply with one of a slightly higher voltage rating, the operations group was able to experiment with a variety of operating parameters, which have led to the results mentioned above. All this suggests that beam current performance might be considerably improved by a redesign of the modulator system to increase the magnetron voltage. This possibility will be explored in the coming year. (A. Hamilton, L.R. Hughey, and A. Raptakes)

- **SURF-II Calibrated Instruments Launched from the Space Shuttle.** In September 1991, the Upper Atmosphere Research Satellite (UARS)
was successfully launched from the space shuttle Discovery. Aboard were two instruments which were calibrated at the Spectrometer Calibration Facility (BL-2) on SURF-II. UARS will perform the first systematic, comprehensive study of the stratosphere, and will furnish important new data on the mesosphere and thermosphere. The two instruments, SUSIM (Naval Research Laboratory) and SOLSTICE (University of Colorado) will monitor solar ultraviolet light in the range 115 to 430 nm with about 0.1 nm resolution. Data from these instruments will provide a record of the long-term variation of the solar ultraviolet spectrum. One of the uses of these measurements is for determining the net effect of ultraviolet radiation on the amount and distribution of ozone in the stratosphere. Fifteen instruments and gratings were calibrated by five user groups at the Spectrometer Calibration Facility during CY91. Facility users included NASA/Goddard Space Flight Center, Naval Research Laboratory, Laboratory for Atmospheric and Space Physics/University of Colorado, CRI Incorporated, and National Institute of Standards and Technology. (M.L. Furst and R. Graves)

• SURF High-Resolution VUV Spectrometer Commissioned. The 6.65 m High-Resolution Spectrometer at SURF II was officially commissioned in October 1991, after 15 months of reconstruction and alignment. Earlier, opportunities for enhancing the spectrometer’s performance were identified, and numerous repairs and improvements were made in the spectrometer, its illumination system, and the data acquisition equipment. This year, the spectrometer was aligned and focused, and has been operating at a resolution of about 100,000 in the first order. This appears to be grating-figure limited, and a factor of two or three improvement could be obtained by a replacement grating or, by working in higher orders. The research problems that are now being studied are in N₂ and Ar. In N₂ we are able to resolve individual rotational lines which are not shown in other published results. In addition, our light intensity is high enough that we can scan a substantial portion of the spectrum, quickly, with a reasonable signal-to-noise ratio. The study in N₂ centers on the determination of the cross section of N₂ at wavelengths of emission lines of O⁺ that are important diagnostic lines for determining the height of the ionosphere. In argon, resonance locations and shapes are being obtained in the vicinity of the 3s3p⁶np ¹P₁ autoionizing resonance series. (N. C. Das, D.L. Ederer, M.L. Furst, D.C. Humm, L.R. Hughey, and R.P. Madden; J.D.E. Fortna, H.D. Morgan, and M.M. Seyoum, Univ. of the District of Columbia; A. Asfaw, Howard Univ.; D. Cleary, Naval Postgraduate School)

• Far UV Detector Calibrations. Specially selected far ultraviolet radiometric detectors have been calibrated and made available to those in the scientific community concerned with establishing the ability to do absolute radiometry in the 5-254 nm spectral region. 33 such calibrations were carried out in 1991. Two classes of detectors were required to cover the above region: a windowless photoemissive photodiode for the 5-122 nm portion of the region, and a magnesium fluoride-windowed photoemissive photodiode for the 116-254 nm portion. The new high-efficiency low cost silicon detector, which was the subject of an R&D 100 award for 1990, has now been made available as an alternate NIST transfer standard in the 5-50 nm region. It offers greatly improved sensitivity, long term stability, and significantly reduced sensitivity to surface contaminants. Promising new detectors with potential applications in the far UV have been studied during 1991. These were Schottky-type photodiodes using gallium phosphide or gallium arsenide phosphide, with a thin gold film on the outer surfaces. Our studies have identified some improvements over silicon technology, and some areas which need further study and perhaps alternate processing. (L.R. Canfield and R. Vest)

HIGHLIGHTS OF EXTERNAL USER RESEARCH ON SURF-II

• Photoemission Studies with the Display Analyzer (BL-1). During the past year the Ellipsoidal Mirror Analyzer was installed on BL-1 at SURF. Initial testing was completed and the first experiments on clean Ru(001) were performed. This analyzer is one of only a few in the world which allow the acquisition of a two dimensional image of the photoemission from solids and solid surfaces. Using this analyzer, it is possible to simultaneously collect a very large number of electron emission angles in parallel, greatly enhancing the ability to perform angle resolved photoemission experiments. Images acquired for clean Ru(001) at a variety of binding energies in the valence bands have shown distinctly different symmetries which can then be related to the symmetry of the states at the binding energy. Images obtained at the Fermi surface have been
interpreted in terms of the known Fermi surface of Ru and this method has been proposed as an alternative to de Hass-van Alphen or positron annihilation techniques as a method for obtaining detailed information on the Fermi surface of solids or, perhaps more importantly, solid surfaces. Preliminary adsorption studies of O/Ru(001) were also performed, showing that the different O states formed during chemisorption give signature profiles which may yield information on the nature of surface bonding. (R.L. Kurtz, S.W. Robey, L.T. Hudson, and R.V. Smilgys, Div. 837; R.S. Stockbauer, Louisiana State Univ.)

**Relaxation Effects in Potassium Halides (BL-5).** A new 1 m normal-incidence VUV spectrometer was tested on BL-5, and a resolution of 50 meV at photon energies of around 20 eV was attained. This instrument was used to study reflection features of potassium halides in the vicinity of the $E_{\text{III}}$ edges, with the intention of comparing reflection and (previously obtained) fluorescence emission data from the same samples on the same instrument. In both measurements, we find two strong features, located between 19 eV and 22 eV, which are believed to be $\Gamma$ and $X$ excitons. Both features are shifted by about 0.9 eV between the reflection and emission spectra. We believe this may be explained by a Franck-Condon shift due to lattice relaxation. Detailed analysis of the data is in progress. (Z. Tang, Z. Xu, and S. Kevan, Univ. Oregon)

**Photoemission Investigations of Oxide Materials (BL-8).** Using the Surface Science chamber on BL-8 at SURF II, we have performed the first valence and core-level photoemission measurements upon vacuum-fractured, single-crystal barium titanate. These results resolve contradictory reports in the literature which have employed other methods of sample surface preparation. Resonant photoemission was used to probe the covalent coupling between titanium and oxygen in the cubic and tetragonal phases of this ionic compound. Photoelectron spectra of the Ti 2p and O 1s core levels reveal the valence of these two ions to be TiO$_2$-like. Valence, core, satellite, and Auger transitions have also been assigned and tabulated. We have learned that when clean, vacuum-fractured surfaces of BaTiO$_3$ are analyzed using ultraviolet and x-ray photoelectron spectroscopy (UPS and XPS), more than one set of barium core levels is observed. The UPS spectra are found to change when the surface is sputtered with ions, while little change is noted in XPS. Sputtering of the surface also causes band bending and the creation of mid-band-gap surface states of Ti 3d character. Upon comparison of Ba 4d line shapes taken in UPS and XPS, the lower binding energy features are assigned to barium with the twelve-fold oxygen coordination representative of the bulk stoichiometry; the higher binding energy components originate from undercoordinated barium at the sample surface. Such information is of interest in the context of high-temperature superconductors which contain barium where similarly split Ba core levels are observed and have been a source of controversy. (L.T. Hudson, R.L. Kurtz, S.W. Robey, and R.V. Smilgys, Div. 837; R.S. Stockbauer Louisiana State Univ.)

**FUTURE DIRECTIONS**

The main strength of this Division is in the development of original measurement capabilities. Some of these capabilities mature into practical devices that are disseminated outside NIST: the most notable recent examples are the high-current SEMPA microscope developed jointly with Physical Electronics, and the semiconductor photodiodes produced in collaboration with Universal Detector Technology. Others remain in-house, such as the scanning tunneling microscope and the parallel VUV spectrometer system; such technologies are usually transferred to the external technical community via publications and collaborative research efforts. Our calibration work, exemplified by BL-2 at SURF-II, is based on original beam line construction linked to our own synchrotron radiation source. Theoretical work within the Division tends to be fairly closely linked to measurement applications; some pertinent examples are the work on the Coulomb blockade in tunnel junctions, ballistic electron emission microscopy, and multiphoton ionization mass spectrometry. Although the particular scientific topics that we study are often similar to those investigated in academic institutions or industrial laboratories, we are driven by a different motivation: the advancement of basic physical measurement technology. For example, the determination of the Lamb shift of the 2S state of helium, now under way in the Photon Physics Group, could easily be justified in terms of its intrinsic, permanent scientific value. However, we tend to view it more in terms of an opportunity to define a clear-cut goal for the generation of coherent
radiation in the VUV spectral region, which will have wide-ranging applications.

This philosophy underpins the avenues we shall pursue in the near future, which include:

- **Comprehensive Characterization of X-Ray Optical Components and Systems.** As noted above, we currently maintain a dedicated facility, unique in the nation, for reflectivity measurements on multilayer optics at wavelengths between 6 and 50 nm. We shall build upon this capability, acquiring first the ability to make more comprehensive reflectance, transmittance, and scattering measurements of a wider range of optical components, and second, the ability to characterize the x-ray optical performance of composite systems. Collaboration with the Quantum Metrology Division, which maintains unique capabilities for independent physical characterization of multilayer structures, and the Precision Engineering Division, which specializes in surface figure and finish measurements, can give NIST a leading effort in this field. The competitive pressures to maintain this lead will intensify as new synchrotron radiation sources come on line, and as industrial laboratory interest in the field increases.

- **Physical measurement basis of nanotechnology.** Nanotechnology, or the engineering of materials properties at the atomic level, exhibits a wide gap between its intoxicating speculative possibilities and its sobering actual practice. The ability to manipulate individual atoms on surfaces with an STM tip has recently been demonstrated in specific systems, but we are still very far from being able to create useful devices. Recent work in the Electron Physics Group has demonstrated both the capabilities for creating novel structures of atoms adsorbed on room-temperature samples, and the difficulties of doing so in a controlled or predictable manner. A main focus of our continuing effort in STM will therefore focus on developing a physical measurement basis for nanotechnology, focussing on quantized electronic states of nanostructures, studies of single-electron tunneling devices, and near-ballistic electron transport in mesoscopic devices. Techniques that could be pursued include the development of a dual tip STM and a scanning optical near-field microscope.

- **A unified chain of radiometric measurements.** Responsibility for absolute radiometry in the infrared, visible, ultraviolet, and vacuum ultraviolet spectral regions is partitioned among several Divisions in the Physics Laboratory, and is exercised by a variety of different methodologies. Although intercomparison of alternative techniques in regions of overlap does not reveal glaring inconsistencies, we feel it should be a long-range institutional goal to develop a unified basis for absolute radiometry that spans the entire optical spectrum. The technical feasibility of this goal has recently been enhanced by the development of the absolute cryogenic radiometer in the Radiometric Physics Division. We believe that the linking of this radiometer with the SURF-II radiation source offers the potential for achieving a primary national standard which would provide absolute radiometric accuracies of 0.1% at wavelengths above 200 nm and 1.0% in the vacuum ultraviolet and soft x-ray region. This would represent an improvement of more than an order of magnitude over existing approaches in these spectral regions, and it would be achieved in the context of a unified set of procedures covering the entire spectral range, which does not exist at present. Active collaboration with the Radiometric Physics Division will be pursued towards this goal.

- **The Next Decade.** We perceive a general trend that will likely govern the evolution of the Division's work over the next decade. The background of most of our senior staff is in atomic and molecular physics, which has historically provided the principal methodologies for absolute determination of electron and photon interactions with matter at energies below 1 keV. The practice of these methodologies has, however, led us gradually to find our key concerns to lie more in the areas of surface and condensed matter physics. For example, the Division's interest in polarized electron technology was motivated to a significant degree by its potential for extending the scope of electron-atom scattering experiments, which were a major part of the Electron Physics Group's efforts 10 years ago. This potential was indeed realized, and continues to be exploited, but it also gave rise to opportunities for leading-edge work in the characterization of magnetic surfaces. This latter subject has been one of the main areas of growth in the Group during the past five years. Similarly, work on localized core-excited states of atoms, which was the principal scientific activity of the Photon Physics group in the early 1980's, has been found to be of substantial interest in the condensed matter physics community; the major research initiatives taken by us in this area in the past few years have focussed on condensed matter systems. As present
indicators of this trend, we note that in FY91: the Division began a 5-year Competence Project on soft x-ray optics, the goal of which is the characterization of multilayer optical systems; it accounted for all work in the Physics Laboratory supported by the High-Temperature Superconductivity Budget Initiative; and it provided the technical champions for the Magnetics Budget Initiative. Although the Division continues to maintain strong efforts in atomic and molecular physics, we believe that involvement surface and condensed matter physics will increase. With the departure of the Surface Science Division from the Physics Laboratory in 1991, Division 841 has become the principal actor in these fields within the Laboratory. ☠
MISSION

The Atomic Physics Division carries out a broad range of experimental and theoretical research in atomic physics, including the atomic radiation of plasmas. The Division:
- carries out basic theoretical and experimental research into the spectroscopic and radiative properties of atoms and highly ionized species;
- provides measurement and data support for specific needs in such areas as fusion plasma diagnostics, processing of materials by plasmas, spectrochemistry and laser development;
- develops well-defined atomic radiation sources as radiometric or wavelength standards;
- studies the physics of laser cooling and electromagnetic trapping of neutral atoms and ions; and
- critically evaluates and compiles spectroscopic data bases on wavelengths, energy levels, transition probabilities, and line widths and shifts.

These activities support many areas of science and technology. For example, there is strong demand for the detailed understanding of atomic processes in technical plasmas, both for modeling purposes and diagnostics. This has arisen from the widely applied plasma etching process for semiconductors as well as from surface cleaning by plasmas and materials deposition by plasma sputtering techniques. The understanding of these processes on the atomistic level is the key to optimizing operating conditions and to achieving competitive advantages. Furthermore, process monitoring and modeling in plasma chemistry, in spectrochemistry and medical applications is possible on a fundamental level only with reliable atomic radiation and collision data.

Urgent demands for spectroscopic data exist in VUV and X-ray laser physics. Transition energies and radiative decay rates of highly stripped ions are essential in the search for and the modeling of potential new laser systems. VUV and X-ray laser research continue to be important in defense work as well as for biological and biomedical studies.

Research on magnetic fusion energy has become very sophisticated and is increasingly directed towards optimizing fundamental physics questions. Thus, the atomic data we produce for highly stripped, heavy ions are essential for evaluating the effects of impurities on the plasma energy balance and for modeling ion transport. They are also needed for plasma diagnostics such as the measurement of ion temperatures. The area of highly stripped ions is also the natural laboratory in the fundamental quest for the ultimate atomic structure theory that properly considers all relativistic and QED effects.

Finally, our vacuum ultraviolet radiometry work with plasma sources provides miniaturized calibrated radiation source packages for radiometric calibrations on board spacecraft. Several applications have already occurred, most recently for the Hubble Space Telescope instrumentation.

ORGANIZATION

The Division is organized into four technical groups—atomic spectroscopy, atomic theory, plasma radiation, and laser cooling—and in each group several research projects are pursued. Some of these involve collaborations with other groups, either within the Division, with other divisions of the Physics Laboratory or with outside groups. The Division has currently 17 professional staff members, 3 Postdocs, and 9 long-term (>3 months) guest scientists.

CURRENT DIRECTIONS

Our principal current work areas are briefly as follows:
- Atomic Data Production. We are producing a large variety of atomic structure and collision data through innovative experimental and theoretical approaches, concentrating on highly ionized atoms as well as neutral helium.
- **Physics of Laser Cooling.** We study the basic physics of laser cooling and electromagnetic trapping of neutral atoms, and the interaction of atoms and radiation in order to develop applications of these studies to new classes of physical measurements, such as high resolution spectroscopy and atomic clocks, and Bose-Einstein condensation.

- **Plasma Spectroscopy.** The Division is also engaged in plasma spectroscopy, i.e., the use of spectral radiation as a non-intrusive diagnostic of technical plasmas (RF cells) and research on the effects of plasma environments on atomic radiation, mainly spectral line broadening.

- **Test of Pauli Exclusion Principle.** In a fundamental atomic physics experiment, we have a test under way for small violations of the Pauli Exclusion Principle in helium, utilizing a very sensitive photon-burst spectrometer.

- **Data Compilations.** Two data centers located in the Division critically evaluate and compile atomic energy levels, wavelengths, transition probabilities, and line shape parameters.

- **VUV Source Radiometry.** Finally, well-defined atomic radiation sources are developed, improved and maintained as VUV radiometric and wavelength standards, and special calibration services are provided.

### HIGHLIGHTS

- **Reference Wavelengths for the Far Ultraviolet--an Atlas of the Platinum/Neon Spectrum.** During the past several years we used one of our 10.7-m vacuum spectrographs to measure the spectrum of a platinum/neon lamp for wavelength calibration of the Goddard High-Resolution Spectrograph (GHR S) of the Hubble Space Telescope--the Space Telescope has on-board platinum lamps for this purpose. The calibration codes for GHS incorporate our measurements, which gave wavelengths for some 3000 lines (1032–4100 Å) with an average uncertainty of ±0.002 Å. We have also made scans of the platinum/neon spectrum using photon-counting detection and obtained relative intensities accurate to about 20%. These data plus new energy level data comprise a new atlas of the spectrum showing some 5600 lines. In addition to the calibrations of the GHR S and Faint Object Spectrograph of the Hubble Space Telescope, our platinum-lamp measurements are being used for calibrating other satellite- and rocket-borne spectrometers and for ultraviolet wave-length calibration in laboratory spectroscopy. They are also essential for interpretation of recent GHR S spectra of certain stars having surprisingly large abundances of platinum in their atmospheres. (J. Reader, C. Sansonetti)

- **High-Accuracy Test of Quantum Electrodynamics in Helium.** Rapid advances in theoretical calculations for two-electron atomic systems have created the need for improved experimental data to test quantum electrodynamical contributions (Lamb shifts) to the binding energies of such systems. We have recently completed high-precision laser measurements to determine the helium 2S binding energy with an estimated accuracy of 2.2 parts in 10^10, providing a stringent new test of the theory.

  About one year ago we reported that the calculated Lamb shift for the helium 2S binding energy was in error by more than 90 MHz based on our measurement of the 2S - 3P transition. This result has been confirmed with higher accuracy by a group at Yale University. In both of these experiments, however, calculated binding energies for higher nD states were used in determining the 2S energy.

  We have now completed observations of the long series of transitions 2S - nP (n = 7-74) by using a frequency doubled laser to excite metastable helium atoms produced in a collimated beam. Our precise measurements of Rydberg states over this large range of n permit us to determine the 2S binding energy directly from the behavior of the series without recourse to any theoretical calculation. The newly determined binding energy

\[
32033.228855(7) \text{ cm}^{-1}
\]

is the most accurate purely empirical determination of the binding energy of any system. Its accuracy is sufficient to test the quantum electrodynamic contributions to better than one part in 10^4.

Prompted by the recent improvements in the experimental data, John Morgan at the University of Delaware has developed improved theoretical methods for calculating the two-electron Bethe logarithm, the greatest source of uncertainty in the calculated Lamb shift. His new results have removed the previous 90 MHz discrepancy between theory and experiment and now agree to sub-MHz accuracy with our experimental data (Fig. 1). (C. Sansonetti, J. Gillaspy)
Fig. 1. Experimental and theoretical progress in determining the He 2S binding energy. All points are plotted with respect to Drake's 1990 theoretical prediction. The recent theoretical value by Morgan is shown in the closeup view. Its error bar represents the uncertainty of calculated contributions to the binding energy. The uncertainty of uncalculated contributions is estimated to be about 1 MHz (shaded region in the plot).

- Highly Ionized Spectra Observed with Tokamaks and Laser-Produced Plasmas. In a NIST/University of Texas Collaboration, we achieved higher electron temperatures at the TEXT tokamak at Austin and consequently more highly stripped ions by operating the tokamak with a neon plasma. For this series of experiments with neon we injected very heavy elements (Hf, W, and Au). In a new experiment with the single beam Glass Development Laser (GDL) at the University of Rochester highly-stripped Li-like, Na-like, Cu-like, Co-like, and Fe-like ions were observed. With a new well-defined geometry of observation, experimental wavelengths of increased reliability are indicated from preliminary measurements. Excellent spectra, including newly observed \( n = 3 - 4 \) transitions, were obtained for Fe XXIV. (J. Sugar, J. Reader)

- Atomic Spectroscopic Database and New Data Compilations. The Data Centers on Atomic Energy Levels and Atomic Transition probabilities (the latter located in the Atomic Theory Group) are building a computer-readable spectroscopic database intended eventually to cover all atoms and atomic ions for which data are available. The database includes wavelengths, energy levels, and transition probabilities; our bibliographic files of references will be keyed to the data. The system allows sorting and retrieval according to spectrum, wavelength region, etc., and covers all wavelengths from about 1 Å to
the mm region. We have loaded into the database our evaluated energy level data for 571 spectra, as well as transition probabilities for about 200 spectra. Strong interest in and financial support for such a comprehensive spectroscopic database exists in the space astronomy and fusion energy research communities. Our most recent additions of newly evaluated data include: (a) energy levels for all germanium spectra; (b) wavelengths and energy-level classifications for the 13 aluminum spectra and 58 high-ionization spectra of vanadium, chromium, and cobalt; and (c) transition probability data for C, N and O through all stages of ionization. (W. Martin, W. Wiese)

- Precise f-values for Lithium. In the past, uncertainties in the range of 20-50% were commonly encountered in the determination of transition probabilities, or f-values, whereas some other atomic properties have fared much better, e.g., wavelengths have been measured with accuracies of ppm almost since the inception of atomic spectroscopy. Recently, however, fast-beam laser excitation lifetime measurements of selected resonance lines have improved the experimental accuracy several orders of magnitude, claiming uncertainties of a few percent to better than 1%; for the lithium atom the uncertainty is stated to be 0.2%.

One of the distinctive characteristics of this field is the fact that theory and experiment stand, in general, on an equal footing. In view of the simplicity of the lithium atom, we mounted an effort to calculate fully correlated, variational configuration-interaction wave functions for the ground and 2p states of lithium with the aim of pushing the theoretical calculation of the f-value to the same level of precision. Our result disagrees, however, by about 1% with the high-precision measurement, while we agree with four other recent calculations of comparable accuracy within 0.1%, which suggests that the experimental error bounds have probably been set without accounting properly for all systematic errors. (A. Weiss)

- Quantum Electrodynamic Effects in Atomic Structure. We have improved fundamental atomic structure theory by including effects of quantum electrodynamics (QED) in the predictions of atomic energy levels, with an emphasis on highly-ionized atoms. Two milestones in this program have been achieved recently: The first, which is a result of a long-term effort to improve the computational techniques of bound-state QED, is the precise calculation of the Coulomb self-energy correction for highly-excited states over a wide range of the nuclear charge Z. This correction is the dominant QED effect in most atoms. The other milestone is the first complete calculation of the effect of electron screening on the self-energy. This effect takes into account the change in the self-energy caused by the presence of more than one bound electron through an effective potential produced by the charge distribution of the other electrons. This demonstration calculation has been applied to the theoretical determination of the Lamb shift in lithium-like uranium for comparison to the measured value recently obtained by a group at Lawrence Berkeley Laboratory. The two results are in slight disagreement. (P. Mohr)

- Resonance Transitions of Alkali-Like Ions. Theoretical estimates of the energies for the resonance transitions of Li-like (2s \rightarrow 2p), Na-like (3s \rightarrow 3p) and Cu-like (4s \rightarrow 4p) ions have been compared with available experimental data to identify systematic differences between theory and experiment. An example of such a comparison is shown in Fig. 2. The theoretical values are combinations of relativistic many-body perturbation results by Johnson et al. and estimates of quantum electromagnetic (QED) corrections by our group. The difference between theory and experiment in Fig. 2 is almost independent of the nuclear charge Z for Z < 60. For Z > 60, the difference for the experimental data obtained from (high density) laser-produced plasmas tends to grow with Z, while the difference for the experimental data from (low density) plasmas produced in tokamaks seems to extend the same pattern observed for Z < 60.
If the steep departure of the experimental data for $Z > 70$ is verified, then the theory must be missing some significant relativistic and/or QED corrections. On the other hand, if the trend seen above $Z = 70$ turns out to be an experimental artifact, then a large volume of experimental data on highly charged ions produced by powerful lasers (Nova in Livermore and Omega in Rochester) must be reexamined for possible systematic problems. New experiments of this type have just been carried out by members of our Atomic Spectroscopy Group using the TEXT tokamak at the University of Texas in Austin and the GDL laser at the University of Rochester to obtain additional data for comparison with theory. (Y.-K. Kim)

- **Advances in Characterization of GEC RF Reference Cell.** For devices that utilize plasmas to process materials, such as semiconductor etchers, the norm to monitor the actual processing has been to measure the applied voltage or power, the gas pressure, its constituency and flow rate. It has been observed that this is not sufficient to guarantee the day-to-day reproducibility of the desired process or to match one "identical" process machine to another. Since the requirements on these process machines are becoming more and more demanding, due to the decrease in feature size in semiconductors and the increase in throughput, it is necessary to find a set of process control measurements that will suit these demands.

  Radio frequency (rf) plasmas are being utilized in many of the applications in materials processing. It becomes critical for further progress to understand in detail how the plasma is actually performing the process as designed.

  Therefore, our Division has undertaken experiments to investigate various measurement techniques as diagnostic approaches utilizing the Gaseous Electronics Conference (GEC) RF Reference Cell. This device was chosen as the experimental platform because its plasma is similar to that of a process machine, and its electrical characteristics are being thoroughly studied at many laboratories throughout the U.S. Time and space resolved spectroscopy was chosen as our principal method to measure the optical emission from the plasma. This method is non-intrusive and has proven to be a successful diagnostic method for the investigation of plasma conditions, especially the population of excited states of atoms and ions. Since it is the ions in a plasma that are primarily responsible for the etching process, it is essential to know the details of their populations. Optical emission measurements look promising for monitoring production-line semiconductor processing machines. (J. Roberts)

- **Radiometry for Semiconductor Photolithography.** This project was initiated to help solve a serious problem in the semiconductor industry. Photolithography, the use of light to make patterns on semiconductor wafers, plays an important part in integrated circuit processing. In this manufacturing process, extremely bright ultraviolet light sources are used to irradiate the semiconductor wafers through masks to control the etching of fine patterns. A serious problem has been to control the amount of ultraviolet radiation; the UV meters used to measure the radiation dose have until now not been able to monitor the dose with sufficient accuracy. As a result, the UV dose has been controlled by observing the results of etching as the dose is varied, and selecting that which gives the best results. This trial-and-error method is very time consuming, however. Also, the efficiencies of different manufacturing instruments are unable to be accurately compared.

  We therefore calibrated and characterized two types of commercial radiometers for SEMATECH. The tests performed by us include calibrations relative to standard detectors and sources. Also tested were the effects of several parameters such as temperature, angle of irradiation, and radiation dose on the response of the radiometers. Our results indicate problems with geometrical factors in the measurements, calibration methods, and temperature control.

  As a result of our work, specific problems have been identified, and should be easily overcome with proper calibration and use of the UV meters. This will allow better monitoring of the ultraviolet light in semiconductor lithography, leading to more reliability in manufacturing of semiconductor components and improved production yields. This was a joint project with the Radiometric Physics Division.

  Additional work included the development and calibration of a spectroradiometer for photolithography. This instrument was designed to measure UV exposure for the same general purpose as the meters described above, but for a different semiconductor manufacturing system. This was also a joint project with the Radiometric Physics Division. (M. Bridges, J. Roberts)

- **Precision Test of the Pauli Exclusion Principle.** In order to search for rare atomic states predict-
ed to violate the Pauli exclusion principle (or more generally, the symmetrization postulate), we have constructed a High Efficiency Resonance Fluorescence System (HERFS). The extremely high signal-to-noise ratio of HERFS makes it possible to study a variety of very weak signals which would otherwise be obscured in conventional experiments. HERFS is able to detect one in every ten photons emitted by a fluorescing atom, while simultaneously rejecting unwanted background light from all sources, including the excitation laser, without resort to spectral filters; the HERFS incident light rejection factor is $5 \times 10^{19}$, the highest ever reported for a system with such a high detection efficiency.

We have used HERFS on an atomic beam of metastable helium to rule out the existence of states which violate the exclusion-principle at levels approaching the part-per-million regime. Below this level, the rare states can become fundamentally obscured by spectral tails from the natural widths of nearby lines. In order to go beyond this limit, we make use of the quantum amplification inherent in cycling transitions to boost our overall atom detection efficiency to 100%. HERFS can then produce a fast (nsec resolution) temporal record of the fluorescence behavior of individual atoms in the atomic beam. By feeding the raw data from HERFS into a bank of electronics which form a real-time nonlinear digital filter, we are able to extract subnatural linewidth spectra using the photon-burst technique. At the same time, we achieve additional background rejection from the nonlinear temporal filtering; we now reach noise levels of only one or two false counts per minute. We have determined that these false counts arise from cosmic rays. A two-stage coincidence configuration is planned in order to reject these false counts. We have successfully applied the photon-burst technique to Ytterbium (Fig. 3); however, current efforts in helium are being hampered by the unexplained lack of cycling in the $2^{3}S-3^{0}P$ transition. (D. Kelleher, J. Gillaspy)

- **Cesium Atomic Fountain Clock.** In collaboration with the laser cooling group at Ecole Normale Superieure in Paris, we have demonstrated a Ramsey resonance in a Zacharias-type atomic fountain. In the mid-1950’s Zacharias proposed that atoms launched vertically through a microwave cavity, so that they fell again through the same cavity, could interact twice with the microwaves in the manner of Ramsey’s separated oscillatory fields. This could produce a very precise frequency standard because of the long time between interactions. Using the technique of sub-Doppler laser cooling discovered a few years ago in our labs, it became possible to do such an experiment, and ours was the first demonstration with cesium (the atom on which time is currently defined) and the first in the Zacharias configuration. The importance of that configuration is that the double passage results in a cancellation of important systematic errors (see Fig. 4, facing page). The experiments, performed in Paris, gave an observation time, and thus a resonance linewidth, about 25 times better than the best conventional cesium atom beam clocks. (W. Phillips)

- **Universal Temperature Behavior for Laser Cooling.** The new theories of laser cooling, which explain the sub-Doppler temperatures first observed in our lab, predict that the temperature should depend on the ratio of laser intensity to detuning from resonance ($I/\delta$). This was confirmed for Cs atoms. We have now measured the same dependence for Rb atoms, with the surprising result that the coefficient relating thermal energy to $I/\delta$ is identical to that for Cs (when properly normalized to the linewidth and transition strength). Furthermore, the two isotopes of Rb have the same coefficient. What changes among all these species is the total angular momentum F in the ground state. We had thought that the F value would affect the temperature,
and calculations for a different polarization configuration had predicted that the temperature would vary with \( E \). Instead, we see a universal behavior and we are now trying to understand the reason theoretically. (C. Westbrook)

- **Laser Trapping Without Heating.** Dipole force traps for atoms use the stimulated-emission forces applied by a laser beam. While in principle this need not lead to any heating of the trapped atoms, in practice it does because the laser frequency is tuned near an atomic resonance and the spontaneously emitted photons cause heating. We are now using laser beams powerful enough that they can be tuned so far from resonance that only very few spontaneous emissions take place. The process is aided by having extremely cold atoms so that the trap need not be very deep. We have demonstrated the far-off-resonance-trap (FORT) in a regime where the light shift caused by the trap is so small that it does not interfere with cooling (a problem in all previous dipole traps). We plan to explore the regime where the heating is very small as well. (S. Rolston)

**FUTURE DIRECTIONS**

- **Atomic Data Production.** We shall continue the production of high-accuracy atomic structure data on two fronts: (a) We shall explore experimentally and theoretically the structure of very highly stripped atomic ions where relativistic and QED effects are significant. We expect to have an electron beam ion trap (EBIT) facility operational during 1992 for soft X-ray and extreme UV observations of very highly stripped ions. (b) We shall also continue to use major national plasma facilities (TEXT Tokamak and the Rochester GDL Laser). On the theoretical side, we have developed sophisticated fully relativistic atomic structure programs which have all major QED corrections built in, and we plan to test these against observed data and identify systematic trends.

- **Laser Spectroscopy.** We shall also continue our high accuracy laser-spectroscopy observations for few-electron neutral atoms. These measurements test the advanced QED calculations that have been recently developed at several institutions.

- **Critical Atomic Data Compilations.** Our critical data compilation work is proceeding vigorously on tabulations of spectroscopy data for light elements of atomic numbers 1 through 20 and on the establishment of a comprehensive spectroscopic database. Our new tabulations will contain significantly more accurate as well as much more comprehensive data than the current NIST tables which have been the standard reference data works since the 1960s.

- **Laser Cooling.** In our laser cooling work we shall do further experimental and theoretical work to establish if there are universal relationships determining the temperatures. Also, we shall further improve atomic fountains as the next generation atomic clocks, in collaboration with the Time and Frequency Division. In closely related activities, we shall study laser cooling in magnetic fields to optimize the application of magneto-optic traps, and we want to explore such elements of atom optics as laser-mirror reflectors.

- **Precision Tests.** Other high precision atomic physics work will concern basic improvements on QED theory to improve fundamental atomic constants and the continuation of our tests for possible small violations of the Pauli Exclusion Principle.

- **Plasma Diagnostics.** In our diagnostic work on technical plasmas we will pursue non-perturbing approaches which utilize atomic radiation to probe these low temperature discharges. Since the spatial and temporal variations in the plas-
ma are instantaneously reflected in the atomic radiation, it can be readily utilized for time and space resolved analysis of the plasma conditions, especially for determining the important concentrations of excited ions and atoms.

- VUV Source Radiometry. In the area of VUV radiometry with plasma sources we are working on several improvements in our present array of sources and possibly also the addition of a new source. We see a continuing strong interest in this work by the solar physics, upper atmosphere and space astronomy communities.
MOLECULAR PHYSICS DIVISION

MISSION
The Molecular Physics Division uses advanced spectroscopic measurement methods in the time and frequency domain and modern computational techniques to attack fundamental and applied molecular problems in physics, chemistry, and the interdisciplinary area between them. The Division provides:

- critically evaluated reference spectroscopic data on molecular species of importance in environmental and climatic concerns, chemical reaction mechanisms, and planetary and interstellar chemistry,
- experimental data and theoretical models for determining and predicting fundamental properties, energetics and internal dynamics of stable molecules, molecular complexes, and reactive species (ions and radicals),
- state-of-the-art data and models on ultrafast molecular processes, intramolecular dynamics, energy transfer in dilute and condensed phase systems, and molecule-surface interactions, and
- advanced theoretical models of atomic collision and molecular dissociation phenomena, especially as influenced by intense laser fields or by ultra low temperature.

Though the problems currently attacked bear the mark of fundamental investigations, all of them are pursued either in direct response to the needs of other government agencies, industry, or as long-term research projects to establish experimental or theoretical databases for newly emerging technologies, as well as to meet the contemporary challenges implied in the mission statement of NIST, newly reformulated in the Omnibus Trade Bill of 1988.

ORGANIZATION
The Molecular Physics Division employs approximately 20 scientists organized into three groups having different technical directions. The groups are High Resolution Spectroscopy, Molecular Dynamics, and Molecular Theory. Each has a group leader responsible for the technical activities of the group. The division has an active program of collaborative research with guest researchers from other institutions, with 10 guests who visited for one month or longer. Projects involving molecular dynamics at surfaces is done in collaboration with Drs. R.R. Cavanagh, L.J. Richter, and S.L. Buntin of the Surface and Microanalysis Division of the Chemical Science and Technology Laboratory.

CURRENT DIRECTIONS

- **High Resolution Molecular Spectroscopy.** Work in the High Resolution Spectroscopy group involves experimental and theoretical application of molecular spectroscopy for characterizing gas phase molecules, primarily in the infrared and microwave spectral regions, and the development and application of new experimental techniques for high resolution spectroscopy. The emphasis of these studies is in the applications of this expertise to problems in structural chemistry, atmospheric chemistry, chemical analysis, radio astronomy, characterization of novel molecular species, e.g., complexes, ions, or radicals, and spectral data evaluation.

- **Microwave and Infrared Spectra.** The High Resolution Group employs experimental microwave and infrared spectral methods on stable molecules and weakly-bound molecular complexes to determine chemical structures, potential energy surfaces, internal motions, reaction coordinate geometry, and reaction mechanisms. Theoretical studies of internal motions provide Hamiltonians required for modeling large-amplitude tunneling motions. Experimental laser measurement and analysis of properties affecting line-broadening for modeling atmospheric observations are provided to support the NASA Upper Atmosphere Program relating to chemical cycles identified in ozone destruction. Infrared spectral measurements of important atmospheric constituents in chemically reactive cycles are obtained for interpretation of atmospheric measurements. Detection and spectroscopic characterization of intermediates in chemical reactions provide the basis for identifying them in other
environments, e.g., plasmas, combustion chemistry, chemical vapor deposition (CVD) processes and interstellar clouds. These species are the carriers of a wide variety of important chemical processes; without their participation, the reaction would stop. Because many of them react extremely rapidly, specialized techniques such as matrix isolation sampling and Fourier transform microwave spectroscopy must be used in order to detect them.

- **Critically Evaluated Molecular Data.** Critically evaluated data on rotational, vibrational, and electronic energy levels of selected types of molecule (e.g., free radicals, molecular ions, interstellar species) are developed for use by the scientific and industrial communities. The data evaluation efforts are supported by the Standard Reference Data program and disseminated through publications in J. Phys. Chem. Ref. Data.

- **Interaction of Carriers with Molecules on Surfaces.** Catalysis, corrosion, chemical vapor deposition, photoetching, and semiconductor device operation may all depend on the interaction of carriers (electrons and holes) with molecules on surfaces. The Molecular Dynamics group is doing quantum-state-resolved laser pump-probe experiments to elucidate the mechanisms by which hot carriers couple to adsorbates, influencing surface chemistry. The different mechanisms (hot bulk electrons, hot surface state holes, and adsorbate-localized electronic excitation) have been found, respectively, for laser-induced desorption of NO from Pt(111), NO from Si(111), and CO from MO(CO)$_6$ on Si(111). These mechanisms, first proven by the NIST experiments, should have broad applicability to the chemistry and dynamics of molecules on metals and semiconductors.

- **Vibrational Energy Transfer.** Catalysis on metals and chemical vapor deposition on semiconductors are related to vibrational energy transfer (VET) between a molecule and a surface. VET rates influence sticking, desorption, surface mobility, reactivity, and surface vibrational spectroscopies. Sub-picosecond laser infrared pump/probe experiments obtained the first time and frequency resolved spectra of vibrationally excited molecules on a surface, specifically ordered monolayers of CO(v = 1) chemisorbed on a Pt(111) surface. The VET decay time (2 ps) and damping mechanism (electron/hole pair formation in the Pt metal) were established, as were the inadequacies of available theories.

- **Pump/Probe Studies of Dimer Molecules.** Statistical theories are frequently used to model important chemical reactions, e.g., in the atmosphere or in combustion. However, our recent time-resolved and quantum-state-resolved laser pump/probe studies of weakly bound (van der Waals) dimer molecules like NO•NO and NO•HF proved these reactions are dramatically nonstatistical. Dissociation rates depend critically on which reactant bond is excited, not the total energy in the molecule. How the available energy appears in products (i.e., as electronic, vibrational, rotational, or kinetic energy) is extremely specific. For example, there is essentially no kinetic energy release in the reaction HF(v = 1)•NO → HF + NO, and the HF and NO are formed in a single rotational level, although hundreds of levels are energetically possible. These new results challenge theorists to develop adequate potential energy surfaces and methods of treating the dynamics of these elementary reactions.

- **Theory of Cooled and Trapped Atoms.** The Molecular Theory Group has established a theoretical program to develop predictive theoretical models for understanding and interpreting the novel physics of collisions of laser cooled and trapped atoms at temperatures below 1 mK. This supports the NIST program in use of laser cooled atoms for improved time and frequency standards. State-of-the-art numerical implementations of quantum wavefunction methods are used to do calculations. Analytic approximations based on these are used to interpret the results. A completely new theory based on quantum density matrices and optical Bloch equations is being developed to treat new features of these unusual collisions.

- **Modeling of Fast Dissociation and Ionization.** The dissociation and ionization of molecules by short extremely intense pulses of laser light has been studied at several laboratories outside of NIST. Theoretical models are being developed to interpret such experiments and to make predictions which can be tested by new experiments. New phenomena such as bond softening and trapping of vibrational populations are predicted when a molecule is irradiated by pulses of intense light. Expertise in applying time-dependent quantum wavefunction methods is being developed in order to attack these problems.
Physical Understanding of Molecular Dynamics. Although quantum wavefunction calculations can be used to give the right results for a variety of atomic and molecular dynamical and spectroscopic phenomena, complex numerical calculations often do not unmask simple underlying physical pictures. For this reason tools are being developed for analyzing and projecting physical insight from the analytical structure of multichannel quantum scattering wavefunctions. These methods are being applied successfully to problems in molecular dissociation, aligned atom collisions, spectral line shapes, and ultracold collisions.

HIGHLIGHTS

- Reaction Mechanisms Probed Using van der Waals Complexes. Direct examination of reactant orientation along the reaction coordinate (distance between reactants during collision) and the structure of the transition state has been experimentally examined only for the simplest reactions due to the transient nature of this process. F.J. Lovas and R.D. Suenram, in collaboration with J.Z. Gillies and C.W. Gillies, have determined the reaction coordinate and geometry of the transition state of cycloaddition reactions by characterizing the reaction adduct and cyclic product geometry. The method provides a way to observe reactants at large interaction distances (2-4 Å) where the weak intermolecular electrostatic forces orient the two molecules before the reaction occurs and prior to the transition state interaction distance.

In most cases our knowledge of chemical reaction mechanisms at the molecular level is based on detailed reaction product analysis and modeling by molecular-orbital theory. For example, state-to-state collision dynamics of a few elementary reactions have been studied extensively by mapping the energy distribution in the products of photo-dissociation reactions, e.g., the hot hydrogen atom reaction with carbon dioxide (H$^+$ + CO$_2$ → OH + CO).

The study of more general classes of organic reactions which involve complicated reactants, e.g., Diels-Alder and other cycloaddition reactions, are not amenable to such product energy distribution analyses. Several cycloaddition reactions, common in many synthetic processes, have been studied by rotational spectroscopy of the weakly-bound complexes to determine the structure of the adduct. Initially, the adducts O$_3$-ethylene and O$_3$-acetylene, 1,3-dipolar cycloaddition reaction components, were examined and the structure of the complex was found to be on the reaction coordinate in which a two center bond forms the cyclic product.

This year another example of this cycloaddition reaction, HCNO with HCCH, was studied and a planar two-center bonded geometry was determined, as predicted from orbital theory. They also studied the reaction between ketene and ethylene, a 2π + 2π cycloaddition reaction and obtained a structure with the heavy atom frame crossed at about 90°, also consistent with molecular orbital theory. While the method appears to have broader applicability, a more severe test will be steric effects due to substituents added to the reactant species.

- Vibrational Dynamics of CO(v = 1) on Pt(111) Studied by Ultrafast Infrared Laser Spectroscopy. Catalysis on metals and chemical vapor deposition on semiconductors are related to vibrational energy transfer (VET) between a molecule and a surface. VET rates influence sticking, desorption, surface mobility, reactivity, and surface vibrational spectroscopies. NIST researchers R.R. Cavanagh, M.P. Casassa, E.J. Hellwell, and J.C. Stephenson performed sub-picosecond laser infrared (IR) pump/probe experiments to obtain the first time- and frequency-resolved spectra of vibrationally excited molecules on a surface. In the first experiments, CO chemisorbed on a Pt(111) surface was studied. This is the absorbate/substrate system best characterized by conventional surface science methods.

There are two CO binding sites on Pt(111), bridge sites (ν$_{CO}$ = 1860 cm$^{-1}$) and top sites (ν$_{CO}$ = 2106 cm$^{-1}$) with binding energies of about 11,000 cm$^{-1}$. A particularly stable adlayer structure, C(4×2), forms at a half-monolayer coverage, with equal occupancy of each site. Tunable IR pulses of duration t$_p$ = 0.7ps are generated as the difference frequency between two tunable visible dye lasers. Tuned resonant with the top-site CO v = 0 → v = 1 band, the pump pulse excites a significant fraction (<30 %) of the top site CO bonds. The probe pulse, delayed a period of time t$_p$ after the pump, bounces off the sample (prepared and characterized in an ultra high vacuum apparatus) and is dispersed in a monochromator. The IR absorption spectrum of the adlayer is obtained versus t$_p$ with time resolution < 1ps and spectral resolution < 1 cm$^{-1}$.

The transient IR absorption spectra showed several surprising features. There was a large pump-induced change in absorption for t$_p$ < 0
(pump follows probe), which naïvely violates causality. However, the negative time transients are explained qualitatively as perturbed free induction decays which occur when \( t_D < T_2 \), the sample dephasing time. For \( t_D > 0 \) the pump caused \( \text{CO}(v = 1) \) absorption band to shift to lower frequency, broaden, increase in intensity, and become asymmetric. There is no theory which accounts for all these spectral changes. The shift in laser frequency is the result of anharmonicity of the CO stretching mode. The spectra return to the initial, nonexcited, narrow Lorentzian profile with a time constant of \( T_1 = 2 \text{ ps} \). These time-dependent spectral changes are independent of pump laser intensity, surface temperature (150 < \( T_S < 300 \text{ K} \)), and CO coverage (0.1 < \( \theta < 0.5 \)), including complete removal of all bridge site CO.

We believe the mechanism responsible for the fast decay of \( \text{CO}(v = 1) \) population is damping by electron/hole pair formation in Pt (other mechanisms like top-bridge \( v\text{-}v \) transfer or to multophonon relaxation can be excluded). To test this idea, the experiment is now being run in "reverse," using non-resonant pump pulses to create Pt electron-hole pairs, and using transient IR probe spectroscopy to monitor hot-carrier-induced population of the \( \text{CO}(v = 1) \) band. These experiments show that new theories are urgently needed for vibrational spectroscopy and dynamics of molecules on metal surfaces. These new time-resolved methods of studying molecules on surfaces will have wide applicability.

- **Optically Driven Surface Reactions: Laser Probes of Surface Dynamics.** This represents a joint program with staff in the surface dynamics group in the Chemical Sciences and Technology Laboratory (D.S. King; S.A. Buntin, R.R. Cavanagh, L.J. Richter) to investigate novel, non-thermal reaction mechanisms occurring at gas-surface interfaces. Surfaces of metal, semiconductor and insulator materials are investigated. In studies of the desorption dynamics of NO from the 7X7 reconstruction of Si(111) under the influence of light, varied in wavelength from the infrared to the ultraviolet, the role of surface electronic states in mediating chemistry at semiconductor interfaces was conclusively demonstrated. Unambiguous assignment of the reaction mechanism required our state resolved studies of the desorbed NO species performed for a range of surface preparations, doping levels and irradiation wavelengths in conjunction with inverse photoemission and scanning tunneling microscopy results from other labs. Optical excitation creates a surface rest-atom localized hole, and subsequent charge transfer occurs between this excited surface state and an adjacent, adatom-bound NO species. Desorption proceeds from this new, NO-localized excited state.

There is great interest in the direct photochemistry of metal carbonyls on semiconductor substrates, since this provides a viable model for low temperature processing. We have developed the capability to perform time and state resolved diagnostics on CO species for this purpose. Preliminary experiments investigated the dissociation dynamics of \( \text{Mo(CO)}_6 \), as an isolated molecule in the gas phase. These experiments demonstrated the detection sensitivity for CO and provided a benchmark for determining the role that the surface will play in the ensuing reaction(s). State of the art single external reflection absorption FTIR has been adapted to the ultrahigh vacuum chamber used in these surface experiments to characterized the nature of the initial \( \text{Mo(CO)}_6/\text{Si(111)} \) adlayer and to characterize the photolysis products left behind on the surface. These studies have shown that \( \text{Mo(CO)}_6 \) forms islands on Si rather than forming an evenly dispersed layer, even at very low coverage. Following irradiation (for example at 266 nm) the IR absorptions characteristic of \( \text{Mo(CO)}_6 \) decrease in intensity while new features characteristic of \( \text{Mo(CO)}_5 \) grow in intensity. Unlike the isolated molecule reaction, where every excited \( \text{Mo(CO)}_6 \) fragment sequentially loses 2 or 3 CO ligands, on the surface the primary fragment, \( \text{Mo(CO)}_5 \) is rapidly quenched. The state and velocity resolved data for the desorbed \( \text{CO} \) species indicates there are two sources of this CO. High energy CO species, characterized by rotational degree of freedom and translational temperatures around 500 K, is from the direct fragmentation of the adsorbed \( \text{Mo(CO)}_6 \); low energy CO species (characterized by temperatures around the 100 K surface temperature) probably result from initial trajectories towards the surface. Both characteristic temperatures are significantly different from that characterizing the isolated molecule fragments. Additional experiments are in progress to further characterized these surface mediated dynamics.

- **Collisions of Ultracold Atoms.** Rapid advances in laboratory techniques for laser cooling and trapping of neutral atoms at temperatures below 1 mK offer many new opportunities to science and technology, including greatly improved time and frequency standards. Collisions of laser
cooled and trapped atoms exhibit new and unusual physics which must be understood in order to make optimal use of this technology, since collisions can cause loss of atoms from a trap or interfere with precise frequency measurements. Paul Julienne, Frederick Mies, and Robert Heather of the Molecular Theory Group have done pioneering research in the unique physics of these collisions at temperatures below 1 mK, supported in part by a NIST Competence Program and in part by the Office of Naval Research.

Cold collisions in the absence of light are affected by the onset of special quantum effects. Cold collisions of laser excited atoms are sensitive to the interatomic potentials at extremely long range and exhibit a new low temperature effect, the suppression of an excited state collision rate due to radiative decay during the long time of the collision. New theoretical methods based on density matrix rather than wavefunction calculations are being developed which treat dissipation during a collision.

Approximate calculations demonstrate good agreement with experimental data on Cs atom collisions at 300 K and 300 μK for rate coefficients of fine structure changing collisions which heat the Cs atoms and eject them from a shallow magneto-optical trap. The predicted rates of similar processes for other alkali species show a wide variation in magnitude and mechanism among alkali species. These predictions will be tested by forthcoming experiments.

Calculations on the associative ionization process measured at NIST in Na atom traps qualitatively explain the observations and suggest a new kind of photoassociation spectroscopy for probing molecular bound states very close to a dissociation limit. This work has been carried out in collaboration with Jacques Vigue at Ecole Normale Superieure, Paris, and Andrew Smith and Keith Burnett at Oxford University, England.

- Coincident Fragment Observations in Unimolecular Decomposition Reactions. Observations of chemical transformations at an atomic level elucidate the forces acting in molecules undergoing reaction. Such observations have profound importance for understanding chemistry, or developing new chemical processes, since the underlying forces determine the rates and products of chemical reactions.

We have measured internal energies and recoil velocities with unprecedented resolution for fragments produced in unimolecular decom-

position reactions. The measurements reveal the relationship (or correlations) between the orientations and energies of geminate fragments, and thus provide a detailed picture of the mechanics of the dissociation event. Two reactions studied are dissociation of the nitric oxide dimer and the NO-HF cluster,

\[
(\text{NO})_2(\text{X}^1\text{A}_1) \rightarrow \text{NO}_2(\text{X}^2\Pi_g) + \text{NO}_2(\text{X}^2\Pi_g) \\
\Delta H = 2 \text{ kcal/mol},
\]

\[
\text{NO-HF} \rightarrow \text{NO} + \text{HF} \quad \Delta H \approx 1 \text{ kcal/mol},
\]

excited to specific metastable vibrational states using infrared lasers. The NO fragment states and recoil velocities were determined by measuring their Doppler-shifted laser-induced fluorescence (LIF) spectra.

The NO dimer is interesting because the \( \text{2}\Pi \) electron configuration of NO gives rise to 16 electronic states in \( \text{NO}_2 \). Certain of these have been supposed to participate in the collisional quenching of \( \text{NO}(v=1) \), which is unusually facile. Another peculiarity is the dramatic mode specificity observed for decomposition of vibrationally excited \( \text{NO}_2 \). We found that dissociation times vary in an unpredictable fashion from 20ps to 800ps for four different combinations of the NO stretching motions. This anomalous behavior is at odds with standard theories of unimolecular decomposition, and also has been attributed to the additional electronic states.

Prior to our experiments there had been no determination of which excited electronic surfaces (if any) are actually involved in the vibrational dynamics of NO. We find that dissociation proceeds via a single vibrational channel with \( \Delta v = 1 \), consistent with energy-gap laws for vibrational energy transfer. Most (87 %) of the remaining available energy appears in fragment translation. The minimal fragment rotation is accounted for by projection the parent zero-point vibrational motion onto the fragment rotations. The cofragment rotations, \( J_a \) and \( J_b \), are not correlated.

The NO cofragment spin-orbit states, which specify the motion of electrons in the fragments, are highly correlated. We can distinguish between four channels, \( (\Omega_a, \Omega_b) = (1/2, 1/2), (1/2, 3/2), (3/2, 1/2), \) and \( (3/2, 3/2) \), because these result in slightly different fragment velocities. The specific correlation observed depends upon the vibrational motion which is initially excited in the dimer. For example, the \( v=2 \) combination state dissociates mainly via the (1/2,3/2) chan-
nel, while the dimer $^1A_1$ ground state correlates adiabatically to (1/2, 1/2). This proves that nonadiabatic transitions occur during the dissociation.

The dissociation of NO-HF, observed following excitation of the HF stretching motion in the cluster, proceeds with vastly different dynamics than (NO)$_2$. In contrast to (NO)$_2$, we observed two vibrational dissociation channels, NO($v = 1$) + HF($J = 2$) and NO($v = 0$) + HF($J = 9$), with similar probability. The fact that two such dissimilar channels have equal importance is quite surprising. Also unlike (NO)$_2$, little of the available energy is carried by fragment translation, and the rotational energy release is highly specific, with only one HF rotational level formed in each channel.

Until recently, it has generally been assumed that forces acting in vibrationally energized molecules would scramble quantum states of the separating fragments, producing no particular product state correlations, with no dependence upon initial vibrational motion. Our results contradict that intuition. These chemical coincidence experiments challenge our understanding of unimolecular decomposition and should lead to greater insight into chemical processes.

### Spectroscopy of Atmospheric Molecules

A.S. Pine, G.T. Fraser and W.J. Lafferty have provided state-of-the art spectral measurements to the NASA Upper Atmosphere Research Program. Doppler-limited and sub-Doppler spectra have been recorded of several heavy atmospheric species including acids, alcohols, aromatics and fluorocarbons in order to interpret their spectra and predict their atmospheric properties. This year, room temperature spectra of nitric acid and sulphur dioxide were recorded with a difference-frequency laser system and higher resolution and much lower temperatures were achieved in molecular-beam studies of methanol, nitric acid, benzene, cyclopropane, CHF$_2$Cl, and CH$_3$CF$_3$ with a color-center laser in the 3 $\mu$m region and with a newly developed CO$_2$-sideband laser in the 10 $\mu$m region.

In a second project, an extensive study of all the fundamentals as well as a number of overtone bands of the free radical, ClO$_2$, one of the species involved in the stratospheric ozone destruction cycle, is nearly complete and provides line assignments, band intensities, and Herman-Wallis parameters. This study was done in collaboration with J.B. Burkholder and C.J. Howard (NOAA, Boulder) and with J. Ortigoso and R. Escribano (CSIC, Madrid).

In addition, also in collaboration with the NOAA group, we are in process of assigning the $v_4$ band of HOCl.

Accurate modeling of collisional lineshapes is critical for interpreting atmospheric measurements. The laboratory study of collisional lineshapes, with emphasis on the phenomenon of line mixing in heavily overlapped spectra, has provided new insights on models in use. We have recorded three combination and hot-band Q branches in HCN from the well-resolved Doppler limit at low pressures to the blended contours at atmospheric pressures using a tunable difference-frequency laser spectrometer. At low pressures, the broadening coefficients as a function of rotational quantum number $J$ are independent of vibrational level and can be modelled successfully using an energy-corrected-sudden (ECS) approximation scaling law, but not with simpler empirical energy-gap fitting laws. Line mixing, which is manifest as a non-additive superposition of Lorentzian lines, strongly affects the blended contours at higher pressures, and indicates that the coupling between lines is some 64% of the collisional broadening. The decoupling presumably arises from collisional energy transfer to the other member of the J-type doublet not observed in the Q-branch transitions of these II-$\Sigma$ bands. We have also studied self- $N_2$, $O_2$, $H_2$, Ar and He broadening of the Q branch of the $v_3$ band of methane, and the data are currently under analysis.

### Infrared Spectra of Molecular Ions

In collaboration with guest workers D. Forney and W. Thompson, M.E. Jacox has obtained the infrared spectra of several small molecular ions trapped in solid neon. The CH-stretching absorption of the acetylene cation was detected only 1.6 cm$^{-1}$ from the gas-phase band center. Very recent experiments have resulted in the first observation of the absorption spectrum of the HCN$^+$ molecular cation. The CN$^-$ anion, which had not previously been observed in an inert, non-interactive environment, was also detected in these experiments. HCN$^+$ was found to photoisomerize to the more stable HNC$^*$ structure, for which no spectroscopic data were previously available, and two of the three vibrational fundamentals of HNC$^*$ were identified.

### Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules

An upgrade of NIST VEEL---Standard Reference Database #26, a computer-searchable database designed for use with personal computers, has
been completed by M.E. Jacox. Critically evaluated data for the ground- and excited-state vibrational fundamentals and the electronic band origins of some 1270 molecules are included in the upgrade, which is more than 20% larger than the original version. Users may search by molecule, by wavenumber range, or by wavelength range.

* Vibrational Trapping and Suppression of Dissociation in Intense Laser Fields. A significant problem in exploiting short-pulse high intensity laser technology for such phenomena as harmonic generation of far UV lasers is the rapid depletion of atom or molecule populations in the leading edge of the pulse. For example, starting from some initial stable state of a diatomic molecule and given a sufficiently intense pulsed laser we might expect that the intensity in the rising edge of the pulse could be sufficient to completely dissociate the molecule well before the peak intensity is reached. Indeed calculations of multiphoton dissociation for the following process,

\[ H_2(1s\sigma_g^+ v) + n\hbar\omega \rightarrow H^+ + H \]

in intense short pulsed laser fields for a variety of wavelengths and a wide range of initial vibrational states \( v \), by F.H. Mies and A. Giusti-Suzor (Univ. of Paris), confirm that the low \( v \) levels achieve 100% dissociation in the leading edge of the pulse. Hence no bound state population ever experiences the peak intensity much less survive to the end of the pulse. Comparable leading edge saturation effects have been postulated for photoionization and have obfuscated the observation of the strong-field effects associated with the peak intensity.

However, for all \( v \) above some specified value, which is well prescribed by the particular photon energy \( \hbar\omega \), all higher \( v \) reveal a remarkable survival of the bound state population in this intense field. Thus, for high \( v \) there is an onset of stabilization, and significant (5-50%) population remains in bound vibrational states throughout the entire pulse. The dissociation is incomplete, and a coherent distribution of excited vibrational states is left behind at the conclusion of the pulse. This survival effect can be attributed to the trapping of portions of the initial vibrational wavepacket in transient laser-induced potential wells. Although calculations are only presented for hydrogen molecular ions, we expect dissociative stabilization to be quite general. In addition this trapping mechanism might offer some new insight into the stabilization of atoms in intense fields.

**FUTURE DIRECTIONS & OPPORTUNITIES**

- **Catalytic Processes.** One example of widely employed industrial catalytic processes is conversion of methanol to gasoline (MTG) over a solid zeolite (acidic) catalyst. While the MTG process is not competitive with crude oil processing, it could become competitive with oil as a source of fuel if the yield, branching ratio and cost can be improved through a better understanding of the reaction mechanism. Although the reaction mechanism has generated considerable interest, much controversy still remains over the particular steps which lead to the formation of the first C-C bond. One problem in studying catalytic processes experimentally is the difficulty of obtaining reliable information on interactions within the zeolite matrix. Suenram, Fraser and Lovas propose constructing model gas-phase systems which closely mimic the solid-phase MTG reaction environment to overcome these difficulties. The high sensitivity and species selectivity of pulsed-supersonic-nozzle fourier-transform microwave techniques will be used to determine structures and internal motions of these gas-phase "reaction" complexes. Surface-bound methanol will be simulated by binding various protonic acids, e.g., HF, HCl, or H\(_2\)O, to the O atom of methanol. Further interactions of these dimeric species, mimicking "surface bound" methanol, will be examined by adding known or postulated intermediates in the MTG process, e.g., CH\(_3\)OH, CH\(_3\)OCH\(_3\), or CO. Such studies could provide a detailed picture of the orientation and atomic site of interaction along the entrance channel to reaction, and in favorable cases, give information about the transition state for reaction.

- **Photochemistry of Dimers.** With partial funding from the AFOSR High Energy Density Materials Program, the Molecular Dynamics Group will do time- and quantum-state-resolved studies of the photochemistry of chemical reactions with reagents initially oriented as van der Waals dimers. An example is O\(_2\)•H\(_2\) + hv \rightarrow O•O+H\(_2\) \rightarrow OH + O + H, where all the products are detected by laser induced fluorescence or multiphoton ionization spectroscopy. The time evolution of the products can be monitored with 100 fs time resolution ("femtochemistry"). The internal states, kinetic energy, and angular distribution of the products will be determined. Potential
energy surfaces and calculations of the lifetimes of O(D)*H₂ = H₂O⁺ type complexes are now becoming available and fruitful comparison of theory and experiment is expected.

- **Fast Processes in Semiconductor Systems.** As the packing density of devices on integrated circuit chips becomes higher, and operating speeds faster, interfaces between active materials, insulators, and interconnects affect device performance, as carrier dynamics are more strongly influenced by scattering from interfaces. To obtain information about very fast processes, a laser technique sensitive to interface-as opposed to bulk-properties is needed. The Molecular Dynamics Group will develop the technique of femtosecond laser sum frequency generation (SFG) to study Si interfaces. At the interface between Si and CaF₂ (a promising practical epitaxial insulator for 3-d IC's) we will excite bulk carriers in the Si substrate, while using SFG to probe excitation and decay rates of surface electronic states associated with Ca-Si bonds. At interfaces between Si and the conducting layer CoSi₂ (a low dispersion interconnect for high speed IC's) SFG spectroscopy will be tried as a contactless probe of ultrafast circuit characteristics in the Schottky barrier region (one laser resonant with barrier height) following junction current injection with a fs laser pulse. This research is planned jointly with a group at IBM-Yorktown.

- **Development of Theoretical Methods.** The studies on ultracold collisions will continue along the directions already begun, emphasizing the control of collision rates by external field manipulation. New theoretical methods will be investigated for treating collisions coupled to a dissipative bath, including development of optical Bloch equation and quantum Monte Carlo methods. The role of hyperfine structure in ground and excited state collisions will be treated. Pressure shifts in ultraprecise atomic clocks need to be studied. New experiments will be proposed to test the developing theory. Until recently much of the theoretical effort in understanding the physics of intense laser interactions with matter has exploited time-independent techniques to solve coupled equations for the matter-field interactions. An extremely attractive alternative approach to calculate the properties of atoms and molecules in intense fields is to introduce explicitly the time-dependence of the laser into the calculations, and directly integrate the coupled time-dependent Schroedinger equation for the interacting system. New techniques and state-of-the-art time-dependent codes are being implemented, and extensive applications of these codes to multiphoton phenomena of small molecules induced by intense short-pulsed lasers will be made. Continued development of analytic methods for interpreting and analyzing multichannel scattering wavefunctions should lead to powerful new tools for understanding collisions and half-collisions. These methods factor quantum transition amplitudes into contributions from different zones of interatomic interaction, and establish the interconnections between zones. One application will be to study the velocity dependence of atomic collision rates from conventional to ultracold collision energies.

- **Collisional Relaxation Processes.** In ongoing studies of collisional lineshapes for modelling atmospheric spectra, Pine has found that the phenomenon of line mixing or collisional interference provides new information about collisional energy transfer not available from line broadening measurements alone. He has observed in O branches of linear molecules that RR collisions dominate the broadening but that significant decoupling exists due to cross-relaxation to other unspecified levels, presumably the vibrational parity (l-doublet) partners. Such collisional relaxation processes will be explored directly in the time domain by transient state-to-state pulsed-pump, cw-probe laser double-resonance techniques. A new high-energy, transform-limited-pulse Nd:YAG laser system is being acquired for both simulated Raman and nonlinear-optical infrared generation for high-resolution pumping of individual rovibrational levels of molecules. A color-center laser will be used as a probe. In a second project, the collision induced absorption in O₂ and N₂ will be examined by Lafferty. Construction of a coolable multiple path White cell is a critical element of this effort, and the cell has been completed and optically aligned. This cell is coupled into the BOMEM FTS instrument via a set of evacuated transfer optics. Since this absorption is very weak and proportional to the square of the pressure, the cell has been designed to withstand 20 atmospheres of pressure, to be coolable to -80 C, and have a maximum path length of 104 meters.

- **Measurement of Rapid Chemical Reactions.** M. Jacox plans to develop and exploit a technique for characterizing the products of the reaction of O⁺ and F⁻ with simple molecules. Among the most rapid chemical reactions which exist are those of O⁺ and F⁻, which have a large probability of occurring on a single collision with
a molecule. These reactions are important in high energy environments such as those encountered in plasmas.

- **High-Resolution Measurements of Atmospheric Molecules.** Diode laser and microwave spectrometers are being coupled with a slit-jet nozzle expansion by J. Domenech, G.T. Fraser, and R.D. Suenram to undertake high-resolution studies of atmospheric molecules. \( \text{H}_2\text{SO}_4 \) will be investigated to understand its formation from the \( \text{SO}_3\cdot\text{H}_2\text{O} \) adduct by exciting high frequency vibrations near the expected peak of the barrier separating adduct and molecule. The non-polar \( \text{(NO}_2)_2 \) will be examined to determine the structure and barrier to internal rotation. Zeeman experiments will attempt to reveal nearby repulsive triplet excited states.

- **Vibrational State Couplings at Intermediate Levels.** A pulsed Ti:Sapphire laser will be combined with a super-conducting bolometer and mass spectrometer by B. Pate and G.T. Fraser to investigate the \( v = 3 \) and 4 overtones of hydride stretches and \( \text{(HF)}_3 \). The spectra will provide information about the vibrational state couplings at intermediate levels to contrast with the seminal studies of Pate, Scoles, and Lehmann (Princeton) in the \( v = 1 \) and 2 region. For \( \text{(HF)}_2 \) we plan to examine the vibrational dependence of the vibrational predissociation and tunneling splittings. The later will test dipole-dipole coupling models for the partial quenching of tunneling in the excited vibrational states. The \( v = 4 \) experiments on the dimer will look for evidence of hydrogen scrambling as predicted by recent calculations.
RADIOMETRIC PHYSICS DIVISION

MISSION
The Radiometric Physics Division of the Physics Laboratory is the primary unit within NIST for carrying out the basic mission of promoting accurate, meaningful, and compatible optical radiation measurements in the ultraviolet, visible, and infrared spectral regions. The Division:
- develops, improves, and maintains the national standards for radiation thermometry, spectroradiometry, photometry, and spectrophotometry;
- disseminates these standards by providing measurement services to customers requiring calibrations of the highest accuracy;
- conducts fundamental and applied research to develop the scientific basis for future measurement services in optical radiometry.

To accomplish these goals in a responsive manner, the Division staff works closely with other government agencies in developing programs to meet the specific agency needs. The Division maintains a broad range of fundamental and applied research programs, calibration services, and Standard Reference Material (SRM) production to meet the technical needs of the community and to provide leadership in identifying future needs. Additionally, the Division staff is active in professional societies and participates in the activities of the Council on Optical Radiation Measurements (CORM) and the International Commission on Illumination (CIE). CORM and CIE are technical organizations that include a strong industrial constituency. These organizations provide the Division insight on the needs of American industry which are necessary to meet the requirements of quality manufacturing. Meeting some of the goals requested will assist American industry in maintaining a competitive posture in the world market.

ORGANIZATION
The Division employs approximately 30 scientists, engineers, and technicians, and maintains a balanced mix of research, development, and measurement services. It is organized into four groups and operates under a project structure with collaborations across group lines. Each of the projects has an assigned leader who is responsible for planning and accomplishing the technical objectives of the project. The project teams in the Division interact and work jointly on various tasks, sharing resources to achieve common goals. For example, the staff of the Detector Applications Project in Group 844.05 work with the staff of most other projects in the Division to supply calibrated detectors for particular radiometric purposes. The project structure is sufficiently fluid to allow for redirection of resources to accomplish newly identified program goals and has proven to be a useful management tool for tracking progress and assigning responsibility.

CURRENT DIRECTIONS
- High Accuracy Cryogenic Radiometry. The Division has recently placed into service an absolute High Accuracy Cryogenic Radiometer (HACR) as the base for a radiometric chain to maintain scales of spectral radiance and irradiance and in scales of absolute detector responsivity. A second, high sensitivity cryogenic radiometer serves as the measurement basis for the Low Background Infrared (LBIR) calibration facility. This facility performs calibrations and serves as the foundation for research and development for technology applications in space and other areas.
where high sensitive infrared sensors are used. The HACR instrument is used in conjunction with laser light sources to calibrate transfer standard detectors which can be used throughout the Division in radiometric application. The HACR has an intrinsic accuracy of 0.01% or better and serves as the basis for improving and calibrating the NIST radiometric scales.

- **Absolute Spectrophotometry.** Three absolute spectrophotometric instruments serve as the primary method for maintaining scales of transmittance, reflectance and optical density. They are: the reference transmittance spectrophotometer, the reference reflectance spectrophotometer, and the inverse fourth densitometer. These instruments operate in the 200-2500 nm wavelength range and provide calibrated samples as references for secondary instruments used for routine service calibrations. The intrinsic accuracy of the transmittance and reflectance reference instruments is a part per ten thousand and a part per thousand respectively of the appropriate units. In addition to calibration services, SRM materials are prepared for distribution to industrial and scientific customers. New instruments for hemispherical reflectance and Bidirectional Scattering Distribution Function (BSDF) measurements are under development.

- **Temperature Scales.** The Division has the institutional responsibility for maintaining temperature scales above the freezing point of silver (1234.96 K) utilizing techniques of optical pyrometry. The pyrometry scale is based upon the spectral radiance scale and hence is inferred from the absolute detector scale based upon the HACR. A wide range of black body sources are maintained for calibration purposes. The Division pursues a vigorous program in thermal source research and design to provide the highest quality measurement assurance for our customers needing temperature scale calibration for a variety of industrial and scientific purposes.

- **Detector-Based Photometry.** Photometry, the science of measuring light with the response function of an "average" human observer, is an activity that has been made integral to the detector characterization efforts in the Division. The unit of luminous intensity, the candela, is maintained on a set of well characterized, appropriately filtered detectors. This provides a direct link between the HACR and the SI unit the candela and provides an alternate method of transferring this unit to calibration customers.

Heretofore, the candela unit was disseminated by supplying calibrated lamps to customers for a fee. While this practice will be continued, depending upon lamp availability, we can offer photometric detector characterization to customers as a more direct and perhaps more stable calibration procedure.

- **Radiometric Research.** The Division maintains research efforts in low level radiometry, biological applications, optical properties of cryogenically cooled materials, black body physics, and in new areas of spectrophotometry such as BSDF measurements.

**HIGHLIGHTS**

- **High Accuracy Cryogenic Radiometer.** American industry has defined requirements for higher accuracy radiometric measurements. The new requirements are designed to assist manufacturers in achieving quality production processes as an ingredient in insuring better product quality. The needs for radiometric measurement improvement have been documented in the 5th CORM report and include requests for better spectral radiance and irradiance standards as well as better detector standards. One step in achieving some of the measurement improvements sought by the CORM membership is to improve the fundamental radiometric basis by improving, in a fundamental way, the NIST radiometric scales. To this end, a new instrument was developed in conjunction with the National Physical Laboratory (NPL) in the UK and installed in a NIST Radiometric Physics Division laboratory. The cryogenic radiometer operates at around 5 K. The low temperature operation provides a simplification of correcting for the loss mechanisms compared to conventional room-temperature electrical substitution radiometry. Additionally, there is a gain in sensitivity due to decreased heat capacity of the receiver at the cryogenic temperatures. The HACR instrument was commissioned this year and a series of measurements on silicon trap detectors have been concluded. The trap detectors are constructed by an arrangement of three silicon detectors which, due to reflection to additional detector surfaces, gather all the light incident upon them. The known internal quantum efficiency of the silicon then provides a detector of determined spectral responsivity. A program has been initiated to develop appropriate transfer standard detectors which can be
referred to the radiometric scale established by the HACR.

The absolute accuracy of the HACR has been established to be on the order of 0.01%. Techniques to incorporate this new level of accuracy into the radiometric chain are being devised and a research and development program is being devised to improve the practical usefulness of the instrument by improving its response time and sensitivity. A first implementation of the improved accuracy will be in establishing the detector spectral response scales based upon the HACR. This should be done this fiscal year and will be the first step in improving the accuracy of the NIST spectral radiance and irradiance scales. Development is underway to extend the wavelength region which the HACR operates. The instrument is used by comparing the intensity of a stabilized laser beam and hence the wavelength range depends upon the availability of laser lines and characterizing optical windows. Ms. Jeanne Houston is responsible for the operation of the instrument and maintains interactions with other laboratories developing cryogenic radiometers.

- Detector Based Candela. The CORM 5th report gives as one of its top priorities the need for improved radiometric and photometric standards. In addition, the availability of high-quality standard lamps is not sufficient to meet the nation's needs. NIST is offering leadership in alternate technology that may eventually better serve the nation's scientific and technical establishment for the support of high quality photometric measurements.

Photometry involves the study of the apparent brightness of a source as seen by an "average" observer. Traditionally, standardization in photometry was driven by primary light sources. Candles were used at first, and beginning in 1948, ovens (blackbody radiators) operating at the freezing point of platinum were used. More recently, standardization at NIST followed from measurements of a gold-point blackbody. The spectral irradiance of these blackbodies are known to follow the Planck equation.

The SI base unit for photometry, the candela, has recently been realized at NIST using absolute detectors rather than absolute sources. This change in the candela realization allows luminous intensity calibrations of standard lamps to an accuracy of 0.65%, a factor of two improvement. A group of eight reference photometers has been constructed using silicon photodiodes, matched with filters to mimic the CIE spectral luminous efficiency function for photopic vision. Photopic response assumes an average human visual response function and weights the intensity observed accordingly. The standard photometers are calibrated for spectral response traceable to the NIST high-accuracy cryogenic radiometer. A new automated measurement bench for routine calibrations of luminous intensity, luminous flux, and color temperature has also been completed. In the future, NIST can provide improved standards and services for the nation's photometric measurement needs.

- SEMATECH Collaboration. SEMATECH is a nonprofit public/private partnership consisting of fourteen U.S. semiconductor manufacturers and the federal government, formed to sponsor and conduct research in semiconductor manufacturing. Its mission is to provide for America the capability of leadership in semiconductor manufacturing. The objective of SEMATECH is to achieve parity with, and overtake Japan in semiconductor manufacturing by 1994.

The semiconductor industry has experienced difficulty in making reliable and accurate mea-
surement of the ultraviolet radiation used in exposing masks for semiconductor photolithographic processing. The industry is pushing photolithography toward shorter wavelengths to reduce feature size and increase chip densities. Currently, most US processing uses blue light, but an increasingly large fraction of photolithography uses near-uv radiation at 365 nm. Initial survey studies by NIST indicated that the measurement devices commonly used in the industry could give results differing by 20% or more. The measurement problems increase as the industry moves further into the uv, which would adversely affect the quality control of the production of integrated circuits and the competitiveness of US semiconductor manufacturers, worldwide.

The Radiometric Physics Division, in collaboration with the Atomic Physics Division, has completed two joint development contracts with SEMATECH to establish calibration procedures for uv intensity measurements. The first contract addressed the issues in near-uv radiation measurements. NIST provided characterization and calibrations of commercial I-line (365 nm) radiometers currently used in semiconductor photolithography systems.

The second contract focused on deep-uv radiation measurements near 250 nm. NIST provided a prototype deep-uv spectroradiometer which could be incorporated directly into the design of photolithography manufacturing systems. NIST demonstrated the feasibility of routine absolute uv radiation measurements in the 200-300 nm wavelength range, directly at the silicon wafer plane, to 1% overall accuracy.

Accurate uv exposure measurements traceable to NIST standards are now available, which will allow the US semiconductor manufacturing industry to be more competitive. A direct benefit of the program was to demonstrate that US producers of semiconductor manufacturing equipment are competitive with similar foreign systems. The improved uv measuring capability will favorably impact other areas such as ozone depletion monitoring and ascertaining the health effects of uv radiation on the skin.

- **CCPR Spectral Irradiance Intercomparison.** An international intercomparison, which was organized by the CCPR of the BIPM to assess thirteen national laboratories' ability to measure spectral irradiance from 250-2400 nm, has been completed. This study will give guidance to the international community in establishing measurement accuracy in a variety of radiometric areas. The various national laboratories use different methods and techniques for establishing their spectral irradiance scale. Spectral irradiance is the most common radiometric quantity in use worldwide, and hence its accuracy is reflected in many other derived measurements. This work documented the present status of radiometric measurements in the world and serves as a true indicator of the uncertainty in spectral irradiance measurements. The measurements at NIST, which served as the central laboratory are completed and the comparison and analysis of the data from the other laboratories is finished. The results (Fig. 3) show that the national laboratories agree to ±10% in the uv and infrared and about ±1% in the visible. These uncertainties are very close to the uncertainties of the 1975 spectral irradiance intercomparison. The data was analyzed to look for indication of a difference between laboratories which realize their scales with a source base compared to a detector base, with the result of no difference suggested by the data. This work serves as a benchmark, representing the present status of radiometric measurements in the world. The final paper on the intercomparison was completed in May 1991 and was published in the NIST Journal of Research in December 1991.

- **Freezing Point Blackbodies.** Newark Air Force Base is the primary calibration laboratory for the Air Force and the DOD leader in high temperature optical temperature measurements. These measurements are playing critical roles in the defense of our country. Freezing-point blackbodies are used as primary standards to calibrate a variety of radiometers used to measure rocket plumes and target signatures, and to find hostile targets. Freezing-point blackbodies can provide the low uncertainties that are required. Newark is also a primary laboratory for high temperature measurements that other government organizations such as NASA and the Navy frequently use. Temperature measurements are emerging as an important tool needed for the development of high technology. Many of these new technologies require temperature uncertainties of approximately 0.1 °C and a minimal resolvable temperature (MRT) of less than 10 mK. The blackbodies that NIST delivered to Newark 20 years ago have deteriorated from use. Therefore a project has been established to build and characterize a new set of blackbodies that are interchangeable with NIST blackbodies. This program is in keeping with a national measure-
ment system for critical governmental use. A set of blackbodies that cover the temperature region from 400 to 1100 °C have been built, characterized and delivered. The set included gold, silver, aluminum, salt, and zinc blackbodies plus two heat-pipe furnaces. A cesium heat-pipe furnace was used for the temperature range 400-600 °C. The second furnace was a sodium heat-pipe furnace that covered the temperature range 600-1000 °C.

- NASA’s Earth Observing System (EOS). The goal of the EOS science mission is to advance the understanding of the Earth on the global scale by developing a deeper comprehension of its components, the interaction among them, and how the Earth system is changing. To quantify changes in the Earth system, EOS will provide systematic, continuing observation from low Earth orbit for a minimum of 15 years. The division has agreed to participate in a long-range measurement and calibration support program with NASA during the development and deployment of various systems on EOS satellites. A number of radiometric challenges exist to ensure calibration of a variety of instruments. The first platform will have about five different instruments that measure the same quantities using different methods. NIST’s first challenge is to develop measurement techniques that can ensure that all instruments have the same calibration and that the results have a common base. Each instrument on the platform will have a completely different optical design. This measurement is further complicated by the fact that all instrument will be working in proximity to each other which allows cross-talk between the instruments. The Radiometric Physics Division can contribute significantly and will solve some of NASA and NOAA problems concerning validation of data. NIST is working with GE, the NASA contractor, to compare the instruments on each platform. The second part of the program is to validate the measurements of two portable radiometers. One of these instruments is being developed at University of Arizona and the second radiometer is being developed at NPL in Japan.

Grand-Mean Percent Differences from NIST of All Participants’ Spectral Irradiance Measurements

Fig. 3. Final results of international spectral irradiance intercomparison.
LBIR User Workshop Held. The national need to establish a primary standard reference for calibrating infrared sensors lead to the establishment, in 1989, of the Low Background Infrared Radiation (LBIR) facility at NIST. The facility serves a variety of users from industry and government laboratories by providing calibrations of blackbody sources and serving as a resource to develop calibration technology. As part of continuing service to the user community, the second LBIR user workshop was hosted by the Division with participation from the user community and the sponsoring governmental organizations. The one-day meeting was attended by nearly 40 people. Thirteen talks were given by users, invited speakers, and NIST LBIR staff.

The presentations included a strong appeal for NIST to enlarge its role in IR calibrations and to establish a long term program to insure the continuity of measurement support in this critical area of technology. A number of user presentations were reports on the results of blackbody calibrations that were recently completed at the facility. A consensus was developed on the methodology of uncertainty analysis and the reporting of results. The workshop was followed by a User Board meeting. The User Board was set up by the user community to interact with NIST and to give technical guidance concerning the capabilities that NIST should acquire to best serve the LBIR community. The User Board is composed of representatives from Department of Defense laboratories, private industry, and University laboratories.

The calibration and support requirements are constantly evolving due to technical advances in the field. To meet these new requirements, future capabilities identified for NIST were:

- Spectral capability at the LBIR facility to calibrate low-background IR detectors and to spectrally calibrate sources.
- A transfer standard spectral radiometer that could be used to calibrate IR sensor test chambers in industry.

NIST staff have started building the spectral capability by designing a new IR monochromator system that will operate at the cryogenic temperatures.

Proceedings of the workshop were mailed to the users and workshop attendees.

LBIR Spectral Instrumentation. The LBIR facility is being equipped with an enhanced spectral measuring capability. This capability is required by the major customers of the LBIR facility for a variety of calibration requirements on space-based systems. This includes the ability to measure the spectral responsivity of low background sensors and the necessity to spectrally characterize the sources used in calibrations systems. The instrumentation required to furnish the spectral capability at the LBIR facility is an IR monochromator, IR sources, and a standard detector to measure the low level spectrally dispersed radiation. Dr. Raju Datla has completed the design of a cryogenic compatible IR monochromator which will provide three distinct capabilities:

- Spectral calibration of cryogenic IR sources such as blackbodies.
- Spectral calibration of detectors such as Blocked Impurity Band (BIB) detectors and Solid State Photomultipliers (SSPM).
- Characterization and calibration of optical components such as filters and other attenuators for LBIR applications.

The monochromator is a grating device with a KRS-5 prism predisperser (Fig. 4). The predisperser will eliminate higher orders and will reduce the optical scatter which contributes to the background in the instrument. The instrument will cover the spectral range of 2 to 30 micrometers with a resolving power of 50. The contract to build the instrument has been awarded.

A superconducting, kinetic-inductance absolute cryogenic radiometer will be used as a standard detector with the spectral instrument. It is being fabricated at the NIST Boulder laboratories by Dr. Donald McDonald and Dr. Joseph Sauvageau. This detector utilizes the kinetic inductance of a superconducting element as the temperature sensor. The noise floor of its temperature sensor was measured to be 0.7 picowatts in a prototype detector, which would be 150 times less than the Johnson noise of a germanium resistance thermometer similarly applied. This detector will be capable of measuring spectrally resolved radiation from cryogenic IR sources below one nanowatt with an uncertainty of 1%.

Two low-background IR sources have been developed. Dr. Steven Lorentz has developed a lead-salt laser based IR source, with multiple lasers to provide known radiation from 2 to 25 micrometers. The laser diode source, which operates at 20 K inside the LBIR chamber, will be useful as a source for detector spectral response characterization, optical materials spec-
central characterization, and the evaluation of the IR monochromator. Mr. Steve Ebner has overseen the design and construction of a low-background blackbody source. This source will operate from 100 K to 450 K, and is equipped with 6 apertures from 50 micrometers to 2 millimeters, a filter wheel which will accommodate 8 filters, and a chopper wheel. This source will serve as a general purpose source for many activities with the spectral instrument, including detector calibration and optical materials characterization.

- **Laser Heterodyne Densitometry.** Neutral density (ND) filters are important components in optical systems employing high sensitivity sensors and in the systems used for their calibration. They are used to attenuate the radiation necessary for calibration. Calibrated attenuators are required to determine the dynamic range of the sensors. The advent of very sensitive detectors such as Blocked Impurity Band (BIB) devices in the infrared made it necessary to develop attenuators of ND 4 and larger for infrared optical calibration systems used to characterize them. The traditional method of measuring attenuation using a spectrophotometer is found to be not sensitive enough to measure attenuations above ND 3 with expected uncertainties of less than 5%. This is due to the difficulty of establishing detector linearity and in eliminating scattered radiation in the spectrophotometric instrument. NIST researchers developed the heterodyne technique to measure optical attenuation of neutral density filters using laser sources. The system is free of noise due to background radiation and does not depend strongly upon the linearity of a detection device. ND filters over the range of ND 4 to ND 12 have been measured with an uncertainty of 2-5% in the infrared using this technique. The technique, first demonstrated for the visible region, has been extended to the infrared at 10.6 micrometers. Dr. Alan Migdall demonstrated the measurement over a dynamic range of 12 decades at 10.6 micrometers for room temperature samples. Tests have begun to verify the ultimate accuracy of the method in the IR. These tests will include studying the temperature dependencies of the filter samples (4.2 to 300 K) using a filter cryostat.

- **International Intercomparison of Spectral Transmittance.** Commercial spectrophotometers for measuring spectral transmittance have become more precise but not always more accurate. Therefore, it has become necessary for national standardizing laboratories to build reference instruments that are well characterized, accurate, and precise. Only recently, other national standardizing laboratories have completed such reference spectrophotometers. Mr. Kenneth
Eckerle took the initiative and NIST was the reference laboratory for an international intercomparison of spectral transmittance scales of four national standardizing laboratories: NIST, Gaithersburg, MD (USA); INM, Paris, France; NRC, Ottawa, Ontario (Canada); and VNIIOFI, Moscow (USSR). This intercomparison was accomplished using NIST developed neutral glass filters with transmittances ranging from approximately 0.92 to 0.001. Aging the filters for a longer period of time produced no conclusive evidence of improvement over a previous interchange between NIST and three different national standardizing laboratories. The agreement ranges from 0.01% to 0.3% depending on the laboratory and the filter used (Fig. 5). The differences between NIST and the individual laboratory are generally smaller than the estimated uncertainties (99.97% confidence level). The sample-induced error contributed 40% or more of the total uncertainty except for a few cases as found in the previous comparison. Since this interchange is very similar to a previous one, it is an ongoing effort to obtain international standardization.

- NIST Research on Diffuse Reflectance Factor Used for ASTM Standard. Recently, the American Society For Testing and Materials (ASTM) issued a standard practice ASTM E259-91 entitled Preparation of Pressed Powder White Reflectance Factor Transfer Standards for Hemispherical Geometry. NIST results of research and development on reflection properties of pressed polytetrafluoroethylene (PTFE) powder were used in this standard.

The reflection properties of pressed PTFE powder have been under investigation by the Radiometric Physics Division for the past several years. This material has a great potential, both as a standard of diffuse reflectance factor and as a coating for integrating spheres for applications in reflectance spectrophotometry and other signal-averaging devices. It possesses certain physical and optical properties that make it ideal for use in these applications. Techniques were developed for preparing reflection standards and coating integrating spheres with the pressed powder. The effects of powder density and thickness on its reflectance were studied, and possible problems with fluorescence that are due to the presence of contaminants in the powder were investigated. The absolute reflectance (6°/hemispherical reflectance factor relative to a perfect diffuser) was calibrated for the spectral range of 200-2500 nm. The directional/hemispherical reflectance factor relative to 6°/hemispherical reflectance factor was measured for several wavelengths in the ultraviolet and visible spectrum and for angles of incidence between 5 and 75°. The bidirectional reflectance factor was investigated for 300, 600, and 1500 nm at angles of incidence of -10, -30, -50, and -70° and at viewing angles at 10° intervals from -80 to +80°. This research was done by Dr. Jack Hsia and Mrs. Yvonne Barnes.
Infrared Spectrophotometry. Accurate knowledge of the optical properties of materials in the infrared spectral region is impeded by a lack of available SRMs, as well as a lack of accurate and reliable commercial measurement equipment. A program to develop absolute techniques and measurement equipment, as well as SRMs, for IR spectrophotometry is underway.

During the past year, Mr. Kenneth Eckerle and Mr. Tie-Ming Wang have developed the methodology and instrumentation for absolute regular (specular) reflectance and regular transmittance measurement in the IR. The reflectance measurement method combines a standard "v-w" geometry with auto-collimation using a high resolution telescope for the very precise alignment capability required to achieve high measurement accuracy. The transmittance measurement method features the use of collimated light for more accurate measurement of the transmittance at a specified incidence angle.

For measurement of materials which scatter light diffusely to any degree, detection instrumentation which collects light over the hemisphere above a sample is required. Methods for measurement of directional-hemispherical (diffuse) reflectance and diffuse transmittance, which are being developed, include both those employing a hemi-ellipsoidal collecting mirror and those using an integrating sphere. Dr. Leonard Hanssen, working in collaboration with Dr. Keith Snail of the Naval Research Laboratory, has designed a hemi-ellipsoidal collecting mirror device which incorporates non-imaging optical technology to significantly improve the measurement accuracy over previous designs (Fig. 6). It will be used with both Fourier transform and grating monochromator spectrophotometers.

Also, through Monte Carlo simulation, Dr. Hanssen is studying the performance of absolute methods utilizing integrating spheres. One of the impediments to construction of an ideal integrat-

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Fig. 6. Hemi-ellipsoid/CPC reflectometer design. The sample and compound parabolic concentrator (CPC) are placed at the two foci of the hemi-ellipsoid. Incoming light scattered by the sample at one focus is collected by the CPC at the other.
ing sphere is the lack of perfectly diffuse interior wall coatings, especially in the ir. A preliminary examination of the effects of deviation from a perfect diffuse wall coating indicate that the resulting measurement error, using typical infrared parameters, is relatively small and manageable. After completion of the absolute methods study, the most promising method will be selected for implementation in the laboratory.

**FUTURE OPPORTUNITIES & DIRECTIONS**

- **Need for Improved Radiometry.** Environmental and health concerns about the penetration of uv radiation into the biosphere due to ozone depletion has renewed emphasis on the necessity for accurate and reliable uv radiometry. NIST is in a unique position within the government to offer long term measurement support for USDA, NASA, and other agencies. Requirements for defining health effects and determining energy efficiency of building and outdoor lighting also drive the need for improved radiometry in the uv and visible.

- **Infrared Characterization Facilities.** The growing interest in space-based observation for both civilian and defense purposes and emerging industrial application demand development of infrared spectral radiometric calibration and characterization facilities. This includes the development of detector characterization facilities for both low-background and ambient-background applications, as well as developing appropriate sources for customers whose measurement needs can best be met by providing them.

- **Optical Properties of Materials.** Optical properties of materials measured under a variety of temperature conditions, and to much better precision, are required for a number of scientific and technical applications. Space-based systems have requirements for spectral emittance and transmittance heretofore not contemplated. Details of the scattering of light from optical surfaces are important to characterize a number of sophisticated optical systems and which will require the development of new measurement techniques. NIST can help meet these challenges by developing technical expertise and furnishing calibration and measurement support.

- **Improved Radiometric Standards.** American industry has expressed the need for improved radiometric standards for a variety of technical, competitive, and production quality reasons. These needs have been documented in CORM 5th report, and projects designed to answer some of the issues have served as an impetus for several Director's Reserve proposals. The challenge remains to implement the necessary methodology and instrumentation to meet the needs of our customers.

- **Increased Range of Absolute Detectors.** Over the last several decades, absolute detectors have been developed which serve as the fundamental radiometric base. A challenge is to develop this capability for all wavelengths of interest and at the various power levels needed by the calibration customers. In terms of optical power, the demands can be over 12 decades of intensity and with many varied detectors and background circumstances. In many calibration activities, detector-based radiometry can replace traditional source-based techniques for improved accuracy. It will be a challenge for the Division to provide the technical base for this conversion where appropriate, and to provide the leadership and guidance to affect the desired results.
QUANTUM METROLOGY DIVISION

MISSION

The Quantum Metrology Division engages in a program of research characterized by strong coupling between advances in measurement technology and basic physics. In particular, the Division
- addresses problems in the determination of fundamental physical constants and interacts with others in the Physics Laboratory and other Laboratories in NIST where work in fundamental quantities occurs;
- contributes to the extension and refinement of the electromagnetic scales and devises tests of basic symmetries and invariances;
- maintains continuing efforts in several discipline areas including fundamental neutron physics, x-ray spectroscopy of atoms, molecules and simple solids, spectra of laboratory and astrophysical plasmas, and application of high accuracy measurements to the study of calculable spectra of basic scientific interest.

CURRENT DIRECTIONS

In its origin and initial directions the Division was intended to address physical problems where enhanced measurement technology appeared critical. It was focussed on fundamental constants and the evolution of certain units of measurement toward an atomic basis. (For historical reasons, it was permitted to retain a residual activity in the area of x-ray inner-shell physics.) The initial efforts were directed toward introduction of laser wavelength standards, linking infrared and visible lasers, mass, density and isotopic abundance (leading to the Avogadro constant), gravitational measurements (G), and unification of the electromagnetic scale to the gamma-ray region. These metrological efforts, with the exception of that seeking to link visible, x-ray and gamma-ray wavelengths, have either been completed or transferred to other parts of the organization.

The inner-shell physics and x-ray technology efforts are temporarily enhanced by special funding (a competence program) and by external support from NASA for calibration of flight hardware directed toward high energy astrophysics.

- Precision X-Ray and Gamma-Ray Measurements. As more fully described in the previous annual report, this work has significant impact on the determination of fundamental physical constants, the masses of elementary particles and precise tests of physical theory. The secondary standards ladder begins with an iodine stabilized HeNe laser (closely coupled to the current definition of length and, more significantly, the basis for all modern determinations of the Rydberg constant). This laser is applied to the measurement of the lattice period of a highly perfect sample of monocrystalline Si near 0.2 nm in an exercise combining x-ray and optical interferometry (the XROI experiment). Transfer of this datum to other crystal samples, including different crystal species, takes place in a precision lattice comparator (the delta-d apparatus) designed to give precise lattice parameter differences with only small sensitivity to the unfavorable aspects of x-ray line profiles. Finally, these calibrated crystals are used in several absolute angle measuring engines to determine the wavelengths of x-ray and gamma-ray secondary standards. Significant developments have transpired in all three phases of this exercise over the past year.

In addition to determination of spectroscopic standards, this program applies such standards to the measurement of calculable spectra of normal and exotic atoms both to establish values for the masses of certain elementary particles, and in other experimental venues where the objective is to provide critical tests of basic physical theory. The rather formidable measurement technology developed in this program has enjoyed a considerable range of application outside the originally intended scope as will be detailed in the following paragraphs.

The absolute angle measuring spectrometer for gamma-ray wavelengths located at the Institut Laue-Langevin (ILL) permits crystals and materials to be characterized at energies...
which are more than an order of magnitude higher (a few hundred keV to 2 MeV) than energies normally used (5 to 60 keV). Two examples of such measurements include crystal structure factor determinations and measurements of indices of refraction. In the case of structure factors, scattering processes such as Delbruck scattering and pair production which increase with increasing energy should be observable, given sufficient measurement precision. Index of refraction measurements yield values for the real part of the atomic scattering factor. At low energies anomalous contributions to the scattering factor are large and thus the detection of small additional terms predicted by theoretical calculations is difficult. At higher energies the anomalous contributions are significantly reduced making the interesting small additional terms more easily detectable.

Another application of the precision gamma-ray measurement technology has been to the determination of nuclear lifetimes and of (the not so obviously related) inter-atomic potentials in solids. Again, the combination of intense gamma-ray beams and the high resolution crystal spectrometer permit the measurement of Doppler broadening induced by gamma-ray emission. Following neutron capture, the nucleus decays by emission of a gamma-ray (primary) which causes the nucleus to recoil. A secondary gamma-ray emitted by the recoiling nucleus is Doppler broadened with the broadening being dependent upon the initial recoil velocity, the slowing down process, and the decay time of the secondary level. Nuclear lifetimes in the $10^{12}$ to $10^{16}$ sec have been measured and parameters characterizing inter-atomic potentials determined.

- **X-Ray Inner-Shell Physics (Synchrotron Radiation Studies).** The long-term effort in x-ray inner-shell physics aims to elucidate the mechanisms underlying the finer details of x-ray processes in atoms, molecules and simple solids. These mechanisms are of two-fold interest in that they reveal dynamic processes on a uniquely restricted scale of small distances and small times while, at the same time, confounding efforts to derive information about atomic and electronic arrangements based on simplified models of inner-shell processes. The objective of this program is to exploit the well-known sensitivity of x-ray spectral detail to atomic environments by means of a more fully developed appreciation of mechanistic complexity to obtain a richer understanding of the geometric and electronic structure of practically significant physical systems.

One source of widespread complexity in x-ray spectra arises from the rather copious production of multiple inner-shell vacancies on atomic sites under energetic excitation. Such multiple initial vacancy states are responsible, in large measure, for the widespread occurrence of satellite lines in x-ray emission spectra and for the appearance of structure in absorption spectra not expected on the basis of a single active electron approximation. Evidently the association of these spectroscopic features can be most readily investigated by excitation of emission spectra using monochromatic radiation tunable through the regions of single and multiple vacancy production thresholds. The implied doubly differential measurements were nearly impossible before the availability of dedicated synchrotron radiation sources such as the National Synchrotron Light Source (NSLS) at Brookhaven. It was for this reason that the Division established and operates a high performance beamline (X24A) at NSLS which has made possible a number of threshold spectroscopic studies as well as opening the way to new areas of molecular orientation, polarimetry and surface structure research. A few aspects of this work will be detailed in the following paragraphs.

Extensive effort in the last year has gone toward the development of an electron spectrometer for use on beamline X-24A. Initial experiments on atomic and molecular gases will be made early in 1992 using a cylindrical-mirror analyzer at fixed emission angle. With additional developments of instrumentation, measurements will be extended to solid-state samples under ultra-high vacuum conditions. In addition, a hemispherical analyzer will be mounted on a rotatable platform for measurements of electron angular distributions.

Measurements of x-ray induced multiple ionization of atoms and fragmentation of molecular ions will continue on beamline X-24A through collaboration with scientists from Oak Ridge National Laboratory and Argonne National Laboratory. Jon Levin, who developed this project during his post-doctoral work at Oak Ridge, has recently joined the QMD.

**Back-reflection x-ray standing wave (BRXSW) technique** has been used in several experiments on X-24A to obtain structural information about adlayers on crystalline materials. BRXSW will continue to be developed and used on X-24A, primarily through collaborative
research with scientists from other NIST divisions and outside institutions.

Considerable effort is being devoted to improvements in beamline instrumentation to enhance performance and reliability and to extend the useable energy range. Multilayer mirrors combined with large 2d-spacing (but radiation fragile) crystals are being used to extend the range below 1 keV. A novel bent-crystal/flat-crystal/torroidal mirror monochromator design will be used to extend the range above 5 keV. A beamline feedback system is being developed to maintain the monochromatized x-ray beam precisely on target. The beamline control computer, software, and auxiliary data analysis systems are being upgraded.

- **Microstructural Investigations.** A number of technical and scientific interests currently attach to the behavior of synthetic layer microstructures. To cite but two, such multilayers are important as coatings for high performance optics needed in projection x-ray lithography and x-ray microscopy. Similar structures (though with generally fewer and shorter periods) are of importance for high density information storage and for semiconductor laser and related devices. We have recently established a multi-axis x-ray system for investigating such structures using laboratory diffraction sources and making use of techniques already developed for the investigation of the quality of single crystals. This reflectometer/diffractometer system has been operational for several months and gives exceptionally high quality data even within its current 3-axis mode (see highlights). In addition, theoretical investigations are addressing the relationship of multi-layer reflection as seen in the conventional optical perspective with the dynamical theory of x-ray diffraction (see Theoretical Investigations, below). The x-ray characterization investigations carried out in this Division are closely coupled to parallel investigations of the longer wavelength performance of multi-layer mirrors as studied elsewhere in this Laboratory and the magnetic properties of multilayer structures investigated both in this Laboratory and the Chemistry Laboratory.

- **Spectroscopy of the sun and active galaxies.** We continue a long-standing association with x-ray astronomy from orbiting platforms based largely on Division resources in crystal diffraction technique built up primarily for other purposes. This involvement with spacecraft payloads provides a modest amount of added resources, interesting technical challenges and a window to an important dimension on contemporary research. In earlier times, all the crystal systems carried on the (US) Solar Maximum Mission were characterized in this laboratory and their window-functions evaluated and incorporated into a database. Similarly, crystals carried on P78-1 (the longest running solar spectrometers until the spacecraft was used as an active target in an SDI Intercept exercise) came from this laboratory. Most recently (see Highlights, below) we were responsible for several aspects of the four channel Bragg Crystal Spectrometers (BCS) currently in orbit on the Japanese satellite, YOHKOH. At the present time, we have begun (with NASA support) to characterize detectors already flown on the Shuttle (the Broad-Band X-Ray Telescope, BBXRT) in preparation for a possible preflight. We are also preparing to deal with the high resolution cryogenic bolometer detectors intended for flight on the Advanced X-ray Astronomical Facility (AXAF).

- **Theoretical Studies.** Work in this area evolves with the programs, available personnel, especially visitors, and opportunities for gaining external support. Longest standing exercises have been in the areas of atomic physics calculations of the energy levels and transition energies of atoms containing inner-shell vacancies. This is clearly in the mainstream of our efforts and was significantly advanced during the 3-year stay of Paul Indelicato, a visitor from Universite Pierre et Marie Curie (see highlights). In addition, we have had, from time to time, more fundamentally oriented theorists as staff members. The current incumbent in this area is Michael Danos, formerly of CRR. His present emphasis is on the continued development of the mathematically rigorous quantum field theory, in particular the special requirements associated with gauge theories. His present (tentative) results indicate that something like supersymmetry is needed in order for gauge QFT to exist as a rigorous theory. He has initiated other investigations on multiple photon emission and QCD dynamics in heavy ion collisions and Quantum chaos.

Theoretical studies of diffraction, reflection and penetration of x-rays and gamma-rays particularly in crystalline and periodic media have been a long-standing theme. Before his departure to Argonne, Paul Cowan was a significant contributor to diffraction theory in general, to discussions of the role of evanescent fields and the maintenance of an optical constants.
database for the x-ray region permitting prediction of crystal response functions. At the present time, two visitors are having a major impact in these and related areas. Specifically, Christopher Chantler has made a critical reassessment of the database for scattering factors from well below 1 keV to well above 1 MeV with already some rather surprising results. In addition, another visitor, Ariel Caticha, is fully engaged with the foundations of dynamical diffraction theory as applied to the study of synthetic layer microstructures. Earlier in his stay, Caticha made important contributions to the study of x-ray production occasioned by the passage of relativistic electrons through microperiodic structures.

HIGHLIGHTS

- High Resolution Gamma-Ray Spectroscopy. The Gamma-ray Induced Doppler (GRID) broadening technique and the NIST gamma-ray spectrometer were recognized by the Justus Liebig University, Giessen, Germany in the award of the 1990 Rontgen Prize. Dr. Hans Boerner of the Institut Laue-Langevin was awarded the 1990 Rontgen Prize by the Justus Liebig University, Giessen, Germany. Dr. Boerner was cited for "contributions in applications of high resolution gamma spectroscopy (namely GRID)." Dr. Borner is the staff scientist in charge of the gamma-ray spectroscopy group at the ILL and is the primary ILL contact for the NIST/ILL cooperative gamma-ray spectroscopy program. In the NIST/ILL cooperation, the ILL supplies the intense gamma-ray beams and specialized source changing facilities and NIST supplies the high resolution double flat crystal gamma-ray spectrometer. This spectrometer has a resolution approaching 10^6 and uses nearly perfect Si and Ge crystal which respond according to dynamical diffraction theory. All the GRID measurements are recorded using the NIST spectrometer which is currently the only gamma-ray spectrometer in the world capable of making GRID type measurements. GRID measurements are contributing to nuclear physics through determination of nuclear lifetimes and to solid state physics through determination of inter atomic potentials.

In the GRID technique, the Doppler broadening of secondary gamma-rays induced by the emission of primary gamma-rays is measured. A nucleus in an excited state several MeV above the ground state decays by the emission of a primary gamma-ray causing the nucleus to recoil. If the recoiling nucleus emits a second gamma-ray before stopping, the measured energy of the second gamma-ray will be Doppler shifted. The spectrometer observes a random ensemble of recoil directions and thus the measured line profile of the secondary gamma-ray shows Doppler broadening and not an asymmetric shift. The broadened profiles are a function of the crystal response function, the initial recoil velocity, the slowing down process, and the lifetime of the level under study.

The GRID method works well for lifetimes in the 10^{-12} to 10^{-16} sec range. A comparison of lifetimes of light nuclei determined by the GRID method and other methods show a generally good agreement with the GRID method being superior for lifetimes below 100 fs. In medium to heavy nuclei where other experimental techniques are not readily available, the GRID technique has been used to determine lifetimes in a deformed nucleus (^{168}Er) and a nucleus known to exhibit O(6) symmetry (^{192}Pt). Both of these measurements have contributed to long standing debates in nuclear physics.

- Atomic and Solid-State Studies on Beamline X-24A. A time-of-flight (TOF) ion spectrometer has been used on beamline X-24A by scientists from Oak Ridge National Laboratory to measure the ratio of double-to-single photonization of He far above the double-ionization threshold. This measurement tests theoretical models of electron-electron correlation in the simplest many-electron atom. The NSLS x-ray ring was operated in single-bunch or five-bunch mode during these studies to provide a pulsed x-ray beam suitable for TOF measurements. The back reflection x-ray standing wave (BRXSW) technique has been used for several experiments performed on beamline X-24A by members of the QMD in collaboration with scientists from other NIST divisions, Argonne National Laboratory, Stanford University, University of Washington, and the Naval Research Laboratory. The incident x-ray energy is tuned through the back-reflected Bragg condition associated with a particular lattice plane of a crystalline substrate. The variation of the intensity of characteristic x-ray fluorescence or Auger electrons from adsorbates or dopants is analyzed to yield information on the geometries of atomic components relative to the substrate lattice. Examples of systems studied include the orientation of Si dopants in GaAs substrates and the geometries of surface reconstructed InP, Sb absorbed on semiconductors, and rare-gas atoms physisorbed on single-crystal graphite.
A Multi-National View of the Active Sun. On August 30, 1991 a major X-ray imaging and spectroscopic spacecraft, Solar A, was launched from the Kagoshima Space Center in Sagamihara, Japan. The satellite, now dubbed Yohkoh, has begun sending back spectacular pictures of solar activity viewed with unprecedented angular resolution and spectroscopic refinement [Science, 8 November, 1991 p. 793]. Developed by the Institute of Space and Astronomical Science (ISAS), the Japanese space science agency, the spacecraft's principal instrumentation is a multi-national project involving several U.S. and U.K. institutions, including NIST, as well as Japanese research organizations, including the Tokyo Astronomical Observatory (TAO).

The high resolution soft X-ray telescope (SXT), a project of Lockheed Palo Alto Research Laboratories, is responsible for the arresting image shown in the last Science article noted above. Less spectacular in their visual impact, though no less significant, are the remarkable high resolution spectra being recorded and sent to earth from the group of four Bragg Crystal Spectrometers (BCS) on Yohkoh. These instruments, (three trained on the He-like resonance lines of S, Ca and Fe and one on H-like Fe), were developed jointly by the Naval Research Laboratory and NIST in the United States in collaboration with the Rutherford Appleton Research Laboratory and the Mullard Space Sciences Laboratory (Imperial College) in the United Kingdom. The technology needed, the result of more than two decades of development for a wide range of applications, was fully exploited in preparing the crystals now in orbit. Results already in hand indicate that the efforts were fully successful. Both the spectroscopic detail resolved and the instrumental sensitivity are in accord with expectations. Of particular note in this regard is that there is already evidence of rapid outward motion of flare material in the period of time before the flare manifests itself to the telescope.

Perfect Crystals Probe Synthetic Multilayers. A recently commissioned multi-axis X-ray diffractometer/reflectometer has begun structural investigation of the geometry of synthetic multilayer systems. Such multilayers are currently employed in VUV and soft X-ray optics for lithography, microscopy and astronomical imaging. They also appear in magnetic storage media, semiconductor lasers and organic films. In all applications, especially in the case of X-ray optics, accurate figure, layer uniformity, interfacial diffusion and micro-roughness are important performance determining parameters. To probe these parameters, we prepare X-ray beams having a high degree of collimation (< 10 arcsec), reasonable monochromaticity (0.01%) and high intensity (> 10⁶ photons per second). This combination of beam properties is realized by using perfect crystals of Si and Ge in a dispersion canceling arrangement with geometrical beam compression by asymmetric diffraction. This incident beam is reflected by the multilayer under test and reflected X-rays registered by a well-collimated detector.

Synthetic layer micro-structures produced by domestic industries, national laboratories and several overseas institutions have been examined. Some of these samples had been previously examined by other reflectometer installations including some using powerful synchrotron radiation sources. In all cases where comparisons are possible the data obtained with our diffractometer/reflectometer appear to have competitive or superior quality. Specifically, the locally obtained data show more refined angular detail and cover, in many cases, a larger dynamic range of reflectivities.

Multilayer structures intended for projection lithography are characterized both using the X-ray technique noted here and VUV reflectometry using the NIST SURF-II facility in a program proceeding with DARPA support. We are developing improved theoretical understanding of the dependence of X-ray results on the geometrical structure of the multilayer optical systems with a view toward gaining predictive capability for performance at the intended wavelength of application. We are also planning installation of two additional axes to permit study of non-specular beam profiles.

FUTURE DIRECTIONS

NIST High Precision Gamma-Ray Spectrometer. The angle measuring accuracy of this spectrometer has recently been improved by ~5 through the use of a commercial two-frequency laser heterodyne interferometer. Imperfect separation of the two frequencies in the two arms of the interferometer is the primary source of fringing nonlinearity. Additional improvements (another factor of 5) are needed in order to achieve 0.1 ppm wavelength measurements at E = 2 MeV. A new interferometry scheme using a single frequency laser and acousto-optic modula-
tion is under development to provide more accurate angle measurements.

- Systematic Study of Transuranic X-Ray Wavelengths. A precision x-ray wavelength measurement facility is being constructed in the Radiation Physics Building to measure high Z x-ray wavelengths. A 400 keV x-ray generator will be used to fluoresce high Z targets. The spectrometer is a double flat crystal spectrometer and the expected wavelength accuracy is at the ppm level. Recent theoretical calculations show good agreement between theory and experiment except in the very high Z region where QED corrections which depend upon Z and nuclear size effects are both becoming large. More accurate systematic experimental measurements are needed in this region in order to test the more refined theoretical calculations.

- Spectroscopy of Few-Electron Ions at ESR and EBIT. We have started a long-term program to measure \( Dn \geq 1 \) transitions in selected hydrogen-like and helium-like ions at the upper end of the periodic table using the heavy-ion Experimental Storage Ring (ESR) at GSI in Darmstadt, Germany. This is part of an effort to systematically check QED contributions to the transition energies in few-electron ions. This ambitious program will make use of the (projected) unique abilities of the ESR to accelerate ions up to and including uranium to high enough energies to strip away efficiently all or nearly all electrons, to decelerate the ions back to low enough velocities to minimize Doppler effects while using active electron cooling to reduce transverse velocities, and to cycle the heavy-ion beam repeatedly through a gas target to obtain usable counting rates while reducing the background from excited spectator states. The x-ray transition energies will be measured at the few ppm level using crystal spectrometers, allowing us to check the Lamb shift contributions to these transitions at the level of several tenths of a percent. An absolute calibration of the transition energies will be made by using x-ray transitions in neutral atoms as transfer standards. These transitions in turn will be measured using crystals whose spacing are known through x-ray/optical interferometry in terms of the Rydberg constant, as described above.

In order to bridge the gap in availability of one- and two-electron ions between that provided by linear accelerators, such as Argonne where we will continue existing programs, and storage rings, such as GSI where we will be starting new programs, we also plan to measure \( \Delta n \geq 1 \) transitions in selected hydrogen-like and helium-like ions in the atomic number range 30 < Z < 60 with a new Electron Beam Ion Trap (EBIT) being assembled at the NIST Gaithersburg site in the Physics Building. We will measure the transition energies with crystal spectrometers to an accuracy of several ppm, providing a check of the Lamb shift contributions to these transitions near the one percent level.

- Electron Spectrometer System Developed for Beamline X-24A. An electron spectrometer system has been developed for studies of atomic, molecular, and condensed-phase samples on the QMD's x-ray beamline X-24A. The tunability of the x-ray source will be used to selectively excite samples at core-level resonances and thresholds. Key aspects of the physics of nonradiative decay processes in core-excited systems will be characterized by the energies, intensities, and angular distributions of photo- and Auger-electrons. The vacuum system is UHV compatible, and structural studies of materials can be performed. For example, the x-ray standing wave technique can be combined with surface-sensitive Auger electron detection to determine the lattice geometries of surfaces and adsorbates.

- Polarized X-Ray Emission from Complex Molecules Using Beamline X-24A. A secondary x-ray spectrometer has been used on beamline X-24A to measure strongly polarized and anisotropic x-ray emission and strongly depolarized elastic x-ray scattering from resonantly-excited, randomly-oriented molecules. Several experiments have been performed on small molecules, and basic theoretical models have been developed. Future opportunities include the application of these techniques to more complex systems such as molecules absorbed on surfaces, molecules in solutions, and large polyatomic molecules.
MISSION
The Ionizing Radiation Division of the Physics Laboratory has the responsibility within NIST for providing national leadership in promoting accurate, meaningful, and compatible measurements of ionizing radiations (x rays, gamma rays, electrons, neutrons, energetic charged particles, and radioactivity). The Division:
- provides primary national standards, dosimetry methods, measurement services, and basic data for application of ionizing radiation to radiation protection of workers and the general public, radiation therapy and diagnosis, nuclear medicine, radiography, industrial radiation processing, nuclear electric power, national defense, space science and environmental protection;
- conducts theoretical and experimental research on the fundamental physical interactions of ionizing radiation with matter;
- develops an understanding of basic mechanisms involved in radiation-induced chemical transformations and the parameters that influence the yields of short-lived intermediates, final chemical products, and biological effects;
- develops improved methods for radiation measurement, dosimetry, and radiography;
- develops improved primary radiation standards, and produces highly accurate standard reference data for ionizing radiation and radioactive materials;
- provides standard reference materials (SRMs), calibrations, and measurement quality assurance services to users such as hospitals, industry, States and other Federal agencies; and
- develops and operates well-characterized sources and beams of electrons, photons, and neutrons for primary radiation standards, calibrations, research on radiation interactions, and development of measurement methods.

To accomplish these goals, the Division staff interacts widely in the national radiation community in all sectors including industry, State and Federal government, and universities. The Division has strong interactions in the international radiation community through scientific collaborations and committee activities. Division staff members participate in numerous professional societies and on many committees. The Division is collaborating with 18 organizations in the radiation community in the establishment of the Council on Ionizing Radiation Measurements and Standards (CIRMS).

ORGANIZATION
The Division employs about 49 scientists, engineers, technicians and secretaries. Activities include fundamental research, applied research, and a wide variety of measurements services. The group structure consists of three technical groups (Radiation Interactions and Dosimetry, Neutron Interactions and Dosimetry, and Radioactivity), together with the Office of Radiation Measurement which is our primary outreach group to the radiation user community and the secondary laboratory system.

CURRENT DIRECTIONS
- Electron Spin Resonance Dosimetry for Radiation Industry. NIST is leading the world's standards laboratories in developing electron spin resonance (ESR) techniques for measuring radiation-induced free radicals in materials. These techniques will be used in materials research (novel polymeric composites, space electronics materials) and in on-line process control for radiation processing and sterilization.
- Absorbed Dose Standards for New Modalities of Radiation Therapy. A transition has begun from radiation therapy standards based on ionization to those based on absorbed dose and NIST is playing a leading role in the development of standards for beam therapies (photons and protons), for brachytherapy (125I and 192Ir), and for radionuclide therapy (labelled monoclonal antibodies, and labelled bone seekers).
- Measurement Quality Assurance Programs for Radioactivity. The Office of Radiation Measurement (ORM) is coordinating the efforts of the
Radioactivity Group, industry and other agencies in development of new measurement quality assurance programs for commercial radioactivity standards, for radiobiological testing, and for environmental radioactivity. These programs, modelled on existing ORNL dosimetry measurement quality assurance (MQA) programs, will lead to higher quality and consistency in radioactivity measurements in the US.

- **Dosimetry for Materials Performance Assessment.** Dosimetry methods for monitoring the degradation of materials exposed to high fluxes of neutron exposures, especially in their diversity, advance NIST goals of regulatory assurance and the leveraging of industry developments in technology. This project provides some form of measurement assurance, standardization, or methods development for nearly every approach to materials dosimetry employed in the United States.

- **Investigations of Fundamental Symmetries With Low Energy Neutrons.** On-going and planned experiments will test either fundamental symmetry laws (i.e., time reversal invariance) or fundamental physical laws (i.e., the "standard" model of the electro-weak interaction). These experiments are carried out at the Cold Neutron Research Facility (CNRF) where the novel properties of "cold" neutrons can be exploited. The NIST effort in this area of fundamental physics involves a number of collaborative projects with national laboratories and universities.

- **High-Accuracy Determination of Neutron Flux.** The development and implementation of advanced methods to accurately determine low energy neutron flux will provide a primary standard for neutron dosimetry, for target assay in neutron depth profiling, and for the calibration of the NIST National Standard Neutron Source. First application of this capability will be to recalibrate apparatus used in the determination of the free neutron lifetime.

- **Radionuclide Standards for Nuclear Medicine.** The exciting application of many radionuclides as targeted therapeutic agents in nuclear medicine has brought many demands for national standards and improved decay data before the clinical research phase. These are being addressed in collaborative measurements in the division.

- **Radon Measurement Intercomparisons.** Integration of national radon standards into the worldwide atmospheric monitoring system is under-way, an intercomparison with radon gas samples distributed from NIST has evaluated the agreement among U.S. reference laboratories and several foreign reference laboratories, and radium "capsules" which quantitatively emit radon have been extensively tested in preparation for eventual distribution as SRMs.

**HIGHLIGHTS**

**Office of Radiation Measurements**

- **Federally-Owned Calibration Laboratories and Personnel Dosimetry Programs.** The first two applications for the federal lab program were received and the quality manual for one applicant was reviewed. The consensus criteria document for performance and testing of these laboratories was published as NIST SP 812 "Criteria for the Operation of Federally-Owned Secondary Calibration Laboratories (Ionizing Radiation)." Calibrated transfer ionization chambers were supplied to the testing laboratory used in the National Voluntary Laboratory Accreditation Program (NVLAP) Personnel Radiation Dosimetry program. The exposure and exposure rates for some of the laboratory's x-ray beams were intercompared with those of NIST. (J.C. Humphreys, M.D. Walker, and E. Eisenhower)

- **State-Operated and Private-Sector Calibration Laboratories.** Proficiency tests were conducted for California, Washington, South Carolina, and Illinois. Washington was tested for gamma rays, and the other three states were tested in both x rays and gamma rays. Additionally, both the IL and SC protocol and procedures manuals were reviewed due to moves to new facilities. Eberlein is the one accredited laboratory in the Health Physics Society Program; however, Victoreen is in the final stages of the accreditation process. Their protocol & procedures manual has been reviewed, and proficiency testing has been done for both x rays and gamma rays. (M.D. Walker and E. Eisenhower)

**Radiation Interactions and Dosimetry**

The Group's activities are presently divided into six projects: radiation sources and imaging research, theoretical dosimetry, medical dosimetry, worker protection dosimetry, and high-dose dosimetry.

- **Multiple Scatter Background in Compton Scatter Imaging.** Compton scatter imaging (CSI) offers an alternative method for non-invasive
imaging in medicine and industry. This is particularly true in cases where the use of transmission radiography is prohibited. CSI will provide quantitative three dimensional information on the electron density distribution of an object. An experiment was carried out to evaluate the effects of multiple scattering of incident 662 keV gamma rays in low Z (aluminum) and medium Z (brass) scatterers. The data will be compared with Monte Carlo calculations of the scattering process as a function of the scattering angle and collimator solid angle. The results will enable the design of CSI apparatus which will maximize the signal-to-noise ratio and provide optimum spatial resolution. (G. Barnea, C.E. Dick, A. Ginzburg, E. Navon, and S. Seltzer)

- **Auroral Bremsstrahlung Calculations.** Monte Carlo calculations of the bremsstrahlung flux produced by electrons slowing down in air have been done to characterize auroral bremsstrahlung phenomena. The generated information includes the electron and photon fluence distributions (differential in energy and angle) and the energy deposition as functions of altitude in the Earth’s atmosphere, from auroral electrons with initial energies from 2 keV to 20 MeV. These data will aid in the correlation of bremsstrahlung observations with measurements of ionization in atmosphere, and is important in the study of electron precipitation events associated with auroras, substorms, and magnetic storms. (S.M. Seltzer)

- **Space-Shielding Radiation Dose Calculations.** A computerized database and code package is being developed for the routine prediction of the absorbed dose from incident electrons and their secondary bremsstrahlung, and from incident protons, as functions of the thickness of aluminum shielding of structures in space. The code will rapidly perform the necessary interpolation over the database and the integration for any specified spectra of incident electrons and protons, giving the dose distribution in a variety of simple geometries in terms of rads in small detector volumes of Al, H_2O, LiF, CaF_2, Si, SiO_2, GaAs, or air. (S.M. Seltzer)

- **Dosimetry of High-Energy Photon and Electron Beams.** The American Association of Physicists in Medicine (AAPM) has set up a new task group (TG #51) with the charge to revise the protocol for calculating absorbed dose to water for photons and electrons from accelerators. NIST participates in this task group, and hosted the second meeting of TG #51 at NIST on November 2, 1991. There are major implications for NIST medical dosimetry depending on the directions taken by the group. These include A) a need to review and resolve questions about the agreement of NIST cavity chamber (ionometric) and calorimetric measurements for ^{60}Co, B) a need to complete characterization of the high-purity water calorimeter as the NIST standard for absorbed dose, and C) a need for the Medical and Industrial Radiation Facility (MIRF) at NIST to allow calibrations of chambers for the accredited dosimetry calibration laboratories. (B.M. Coursey and R. Loevinger)

- **High-Purity Water Calorimeter Development.** Cooperative investigative studies at the Physikalisch-Technische Bundesanstalt (PTB) confirmed that convection can be eliminated in an absorbed dose water calorimeter by use of a simple geometric construction. This permits the calorimeter to be operated at room temperature, which significantly simplifies the calorimeter in comparison to operating it at 4 °C. The heat defect was investigated at NIST by saturating high-purity water with high-purity hydrogen gas. Our results are in excellent agreement with theoretical calculations and measurements carried out at the National Research Council of Canada. (S.R. Domen)

- **Proton Monte Carlo Code Development.** Proton beams, because of their highly focused pattern of energy deposition, are the choice for radiation therapy in treatment of certain tumors of the central nervous system, where it is important to spare critical structures. Monte Carlo models for the calculation of proton transport are being developed for proton therapy beam energies in the range from 60 to 250 MeV. Calculations are being done of the spatial pattern of absorbed dose and proton fluence spectra under conditions of interest in proton therapy. (M.J. Berger and S.M. Seltzer)

- **Intercomparison of Orthovoltage X-Rays with the Bureau International des Poids et Mesures (BIPM).** NIST periodically intercompares instruments with the BIPM in order to maintain our links to the international measurement system. Two Shonka chambers were calibrated at NIST in March 1991 using the M-series beam codes, ranging from M60 to M300 (HVL 0.052 to 5.3 mm Cu). BIPM calibrated these two chambers at their beam codes, ranging in half-value layer (HVL) from 0.148 to 2.5 mm Cu. The agreement was 0.1% to 0.3% in the overlapping energy range. This was an improvement over the 1975
comparison when there was a difference of 0.5% for HVL > 1mm Cu. For the 1975 comparison, NIST matched the BIPM beam codes (on the basis of HVL and kV). (P.J. Lamperti)

- **Wide-Angle Free-Air Chamber (WAFAC) for 125I.** A new calibration service for 125I seeds is being developed which will use the WAFAC to measure the air kerma of individual sources in free air. The agreement between the Ritz free-air chamber and the WAFAC is within the range of agreement shown by national primary air-kerma standards when compared at the BIPM laboratory. A set of preliminary measurements has been made with No. 6702 and 6711 125I seeds from the 3M company. (R. Locvinger)

- **Workshop on the Standardization of 192Ir High-Dose-Rate Brachytherapy Sources.** From October 31 to November 1, 1991 NIST and the U.S. Nuclear Regulatory Commission co-sponsored a workshop at NIST to examine the calibration issues for the high-dose-rate (HDR) 192Ir radioactive sources used in cancer therapy. These sources have activities up to 400 gigabequerels (GBq), which is more than two orders of magnitude higher than the low-dose-rate 192Ir seeds for which NIST offers calibrations. The workshop, attended by 30 invited participants, was intended to tighten the measurement system in the United States for clinical measurements using the HDR 192Ir sources. (B.M. Coursey)

- **Gamma-Knife Dosimetry.** Improved dosimetry is required for treatment planning for Leksell Gamma Units ("Gamma-Knife") now in use in a number of hospitals in the United States. A novel method of dose mapping has been achieved by NIST, in collaboration with the University of Kentucky Medical Center, the Mayo Clinic Radiation Oncology Department, and the University of Pittsburgh Radiation Oncology Center, which involves the use of new types of radiochromic films, which provide high-resolution high-precision two-dimensional dose patterns with target and penumbra regions of cerebral phantoms, for the purpose of accurately locating the site of treatment of small, deep-seated intracranial tumors and vascular malformations. The dose mapping is made by computer-assisted laser-scanning densitometry of the film dosimeters. (W.L. McLaughlin, C.G. Soares, and J.A. Sayeg)

- **Beta-Particle Emitting Ophthalmic Applicators.** The calibration service offered for beta-particle emitting ophthalmic applicators is the only one available in the country. Twenty-four sources were calibrated in FY91 using the revised calibration procedure. Work continued on the comparison of radiochromic film dosimetry and extrapolation chamber dosimetry, and a technique was developed for calibrating curved applicators using small pieces of radiochromic film sandwiched between the source and spherical plastic eye phantoms. (C.G. Soares)

- **Radiopharmaceutical Dose Assessment.** The presently accepted dosimetry for bone-seeking radiopharmaceuticals relies on an accurate measurement of the activity administered, and calculations of the dose to the target organ (bone) as well as other organs, following the schema developed by the Medical Internal Radiation Dose (MIRD) committee. We are developing a new approach to estimating the radiation dose to bone using electron paramagnetic resonance (EPR) spectrometry. We have demonstrated that radiation-induced EPR resonances can be detected in the bone tissues of an animal treated with a radiopharmaceutical and that they are measurable in bone tissue biopsies. (M.F. Desrosiers, D. Schauer, and B.M. Coursey)

- **Radiation Accident Dosimetry.** Recent success in measuring the radiation dose using bone samples from two Salvadorian workers exposed in an accident at an industrial sterilization facility has led to further developments in accident dosimetry. Radiation-induced EPR signals produced in tooth enamel offer improved sensitivity over bone and the EPR method is now being used to assess the dose to people exposed at the Chernobyl accident. In cooperation with a Moscow Institute (through DOE) tooth enamel samples have been received for analysis. Future studies also include improvements in the measurement procedure to increase sensitivity and reduce experimental uncertainties. (M.F. Desrosiers)

- **Dosimetry for Industrial Radiation Processing.** Vital services to the multi-billion dollar a year U.S. radiation processing industry are provided through the development of measurement standard calibrations, dosimetry systems, and consultations. Such services avail to radiation sterilization industries, radiation source manufacturers, polymer processing, material and electronic testing laboratories, composites curing facilities. Considerable effort is given by NIST personnel in responding to hundreds of technical inquiries from industrial engineers and radiation facilities personnel to assist them in the design and implementation of measurement quality
assurance. (W.L. McLaughlin, M.L. Walker, J.C. Humphreys, M. Al-Sheikhly, and M. Farahani)

- **Dosimetry of High-Energy Electron Beams.** High-energy, accelerator-produced electron beams, with energies from about 4 to 12 MeV, are becoming widely employed in the radiation processing industry. The fields of applications include sterilization of medical products, the manufacture of specialty polymers and elastomers, and pest control and shelf-life extension of food products. Graphite calorimeters have been constructed that will characterize and calibrate these electron beams. Initial tests with 2.5 MeV electrons indicate that the calorimeters perform as designed with excellent sensitivity and stability. (J.C. Humphreys, W.L. McLaughlin, M.L. Walker, J.M. Puhl, and C.E. Dick)

- **Alanine Electron Spin Resonance Dosimetry.** A new dosimetry system based on radiation-induced defects in crystalline alanine (an amino acid) detected by electron spin resonance spectrometry is being developed as a future NIST calibrations service for high-dose dosimetry. When crystalline alanine is mixed with an appropriate polymer binder, the dosimeter can be fashioned into different shapes, discs, cylinders, films. The dosimeter currently used is a disc 4.8 mm in diameter and 2 mm thick; the alanine composition ranges from 80-90% with polyethylene as a binder. The reproducibility and repeatability of the dose measurements are now being evaluated. (M.F. Desrosiers, J.M. Puhl, and W.L. McLaughlin)

- **Profilerometry of Electron Accelerator Beams.** A special calibration service for the mapping of electron beams produced from electron accelerators as well as the mapping of numerous other radiation sources has been initiated. In order to map or profile an electron beam or other radiation source, radiochromic film, of sufficient size to accommodate the entire image of the source, is exposed to the fields of the source. The resultant image is then digitized by a laser-scanning densitometer (operating at 632.8 nm with 55 μm resolution) and redisplayed, using other in-house and vendor routines, into an optical density versus spatial location graph. (M.L. Walker, W.L. McLaughlin, J.C. Humphreys, J.M. Puhl, and C.E. Dick)

- **Radiation Dosimetry Using Planar Waveguide Sensors.** In a joint effort with the Analytical Sensors and Automation group we have made significant progress towards the development of a fiber-optic planar waveguide dosimeter. These waveguide dosimeters, made by either incorporating radiation-sensitive dyes in polymeric films, Ag⁺ ions into quartz substrates, or using commercially available radiochromic materials such as GAFChromatic™ [The use of trade names is for identification only and does not imply endorsement by NIST.] Dosimetry media, become colored in proportion to the amount of radiation received. By coupling light into the material such that light is propagating within the material, path lengths of several centimeters can be achieved, increasing the effective path length and thus sensitivity of the material to radiation by several orders of magnitude. (M.L. Walker; S.J. Choquette, Div. 835)

### Neutron Interactions and Dosimetry

- **The Materials Dosimetry Reference Facility (MDRF).** A new, high-intensity reference neutron field for reactor dosimetry, designed and constructed by NIST, will be operated at the University of Michigan 2-Megawatt Research Reactor. Detector development experiments and NIST-certified fast-neutron fluence irradiations are to be performed at this facility in support of neutron dosimetry for the nuclear power industry and the metallurgical-test communities. The realization of this benchmark facility is a natural extension of the long-term NIST program to develop standard neutron fields for measurement science research in materials dosimetry. This integrated irradiation facility will be used by industry and government organizations that
have major responsibilities to assess the integrity of high-risk nuclear power reactor components and more generally to establish the database that describes radiation damage in steel.

The MDRF complements existing fission neutron standard fields at NIST by providing a tenfold increase in fast-neutron fluence, a much larger irradiation volume with modest flux gradients, and a neutron spectrum rich in intermediate-energy neutrons. A variety of detector response characteristics and dosimetry interpretation methods can be investigated by means of two MDRF spectrum options.

A thorough characterization of the neutron spectrum will come from a combined interpretation of two dimensional neutron transport calculations and benchmarked reaction rate measurements and neutron fluence transfer. A special feature of the spectrum tailored with a $^{10}$B filter will be the determination of the $^{10}$B thickness by means of a neutron transmission measurement in the 2 keV filtered beam at NIST. The effective nuclear thickness obtained in this way removes all or most of the uncertainty in $^{10}$B enrichment, powder density in the thimble, and the absolute cross section scale for neutron absorption in boron.

Activation detector calibrations planned for the MDRF will serve on-going and planned steel irradiations by Materials Engineering Associates and by ORNL, pressure vessel dosimetry contracts at the Westinghouse Nuclear Technology Division, and surveillance capsule backfitting and cavity dosimetry projects at Babcock & Wilcox. Dosimetry measurement assurance requirements, to be proposed by the Nuclear Regulatory Commission, may be conveniently and inexpensively served by the MDRF. Continued development and application of Solid State Track Recorders (SSTRs), a dosimetry detector of great promise for reactor pressure vessel damage monitoring, will be substantially enhanced by the availability of the MDRF. A new generation of fission dosimeters in the form of paired uranium detectors (PUDS), sintered wires, and encapsulated beads can also be investigated and validated in the two component neutron fields of the MDRF. (J. Grundl, E.D. McGarry, and C. Eisenhauer)

- **NIST/Westinghouse Cooperative Agreement for Reactor Dosimetry Development.** Detector development and methods improvement for Westinghouse radiometric and Solid State Track Recorder (SSTR) dosimetry continues. NIST is most deeply involved in establishing reliable masses for SSTR fissionable deposits that are in the nanogram to picogram range. The SSTR dosimeters register fission product tracks in mica disks placed next to thin deposits of select fissionable material. The track density for uniformly thin fissionable deposits is proportional to fast neutron fluence. Masses of fissile and fissionable isotopes are determined to an accuracy of about 2.5% (1σ) on the basis of irradiations to known fluences in the $^{235}$U Cavity Fission Source at the NIST Reactor. (E. McGarry)

- **Neutron Transport Calculations for Slab Penetration and Iron Shell Transmission.** Results of a basic study of slab transmission and reflection by neutrons and gamma rays were published this year. Using Monte Carlo calculations, it was shown that the transmission of scattered neutrons or gamma rays from a point source through a plane slab of infinite extent to a point detector depends on the orientation of the slab but varies very little with the slab position.

The iron inelastic cross section is important for calculating fast neutron gradients in thick steel, and has become a critical issue for predicting the useful service life of power reactor pressure vessels. In preparation for a benchmark program of iron shell transmission measurements at NIST, a series of calculations of the transmission of neutrons through plane slabs of iron have been performed. It was found that published reaction rates for threshold detectors with nearly the same threshold diverged as the slab thickness was increased. This unexpected result may indicate a significant problem with energy group structures in either the transport calculation or in the detector cross sections. The endpoint of these benchmark measurements will be to assess the adequacy of recent revisions of the iron inelastic cross section.

There was a notable advance in neutron transport calculational capability at NIST this year. The two-dimensional discrete ordinates code, DORT, has been acquired and some sample problems have been run on the Cray. Likewise, all neutron and photon transport codes, including ANISN, MCNP, and the DETAN code for dosimetry analysis, have been converted from the NIST CYBER 205 computer to the new NIST Cray Y-MP Computer. (C. Eisenhauer)

- **R&D For Materials Dosimetry.** A joint project with the Westinghouse Science and Technology Center has been initiated to monitor possible radiation damage to major structural components at the Trojan Nuclear Power Reactor. Neutron fluence standards prepared in certified
fission neutron irradiations were furnished to Westinghouse to benchmark their in-house activation measurement system. The benchmarked dosimetry measurements will be used to adjust calculations at the dosimeter locations before extrapolation and prediction of radiation (damage) exposure within the support structures.

Ex-vessel cavity experiments at the Davis-Besse Power Reactor, an industry benchmark under the auspices of the B&W Reactor Owner’s Group. Included NIST-developed PUD neutron detectors along with industry furnished radiometric, SSTR, niobium, and helium-accumulation fluence monitors. The irradiation is complete and neutron fluence and spectrum results are coming in from five separate laboratories including one university and one European research center. NIST developed LiF Chip gamma dosimeters were also included in this benchmark experiment and, incidently, were also tried out at Three Mile Island.

Involvement with the Nuclear Regulatory Commission has focused recently on writing of the regulatory guide, “Calculational and Dosimetry Methods for Determining Pressure Vessel Neutron Fluence.” The guide summarizes up-to-date methodology for performing out-of-core neutron transport calculations and specifies requirements for performing and reporting reliable dosimetry measurements which are used validate the calculations. Emphasis is on in-situ surveillance, benchmarking all experimental techniques, and the use of NIST neutron fluence standards. (E.D. McGarry, D. Gilliam, and J. Grundl)

- **Measurement of Water-Sphere Neutron Leakage Spectra.** In collaboration with the Los Alamos National Laboratory and Oak Ridge National Laboratory, an experimental program has been undertaken to improve the understanding of neutron leakage from aqueous systems which are representative of situations occurring in chemical processing of fissionable isotopes. Experimental and calculated fission rates have been obtained for four fissionable isotopes – $^{235}\text{U}$, $^{239}\text{Pu}$, $^{238}\text{U}$, and $^{237}\text{Np}$ – with pure water spheres of diameters 7.62 cm and 10.16 cm. Monte Carlo calculations were done with the MCNP code using a “light water” $S(\alpha,\beta)$ scattering kernel. The calculations and experimental results are generally in good agreement, but some discrepancies are found in both the fast and thermal energy ranges. The calculations generally predict more thermal neutrons than observed, with the discrepancy larger for the thicker of the two moderators studied. (D. Gilliam)

- **Establishment of Fundamental Neutron Physics Beamline at the CNRF.** In March of 1991, the first beam was delivered through Neutron Guide 6 (NG6) at the guide hall of NIST’s Cold Neutron Research Facility to the fundamental physics experimental station. The operation of this station is a joint project with the Material Sciences and Engineering Laboratory (MSEL) and the Neutron Interactions and Dosimetry Group of the Ionizing Radiation Division. This station was one of the first experimental facilities at the CNRF to become operational and is the first of its kind in the United States. Initial measurements at NG6 concern intercomparisons between several new absolute, high-accuracy neutron flux monitors. These devices will be used to provide new primary standards for neutron dosimetry, for the assay of primary calibration targets for neutron activation analysis and depth profiling, and later, for the recalibration of the NIST National Standard Neutron Source. In addition, these systems are the basis for establishing neutron beam intensities to unprecedented accuracy as required for the determination of the neutron lifetime.

Two new devices, a $^6\text{Li}$ calorimeter and a $^{10}\text{B}$ alpha-gamma coincidence device were installed at NG6 in the summer of 1991 and are presently undergoing detailed intercomparison in identical neutron beams. This work includes the collaboration of NIST staff from MSEL as well as the Chemical Sciences and Engineering Laboratory. Outside Collaborations include Los Alamos National Laboratory, Harvard University, the Central Bureau for Nuclear Measurements (European Community), the Scottish Universities Research and Reactor Center and the Kurchatov Institute (Moscow). (G. Greene, D. Gilliam, M. Snow, S. Dewey, and M. Arif)

- **Improved Quantitative Tests of Quantum Mechanics and Special Relativity.** In collaboration with others, a novel method of analysis has been used to establish what may be viewed as a new class of tests of quantum mechanics and special relativity. In the first such test (PRL 66, 256), G.L. Greene in collaboration with E. Fischbach (Purdue) and R. Hughes (LANL) investigated the possibility that Planck’s constant might be slightly different for different particles. This work demonstrated that the existing, overconstrained set of data from which the fundamental constants are determined could
be used to set very stringent limits on such a variation of Planck's constant. It was also shown that this analysis could also be interpreted as providing the most accurate microscopic test to date of the law of conservation of angular momentum. A second analysis carried out by G. Greene and M.S. Dewey, in collaboration with E.G. Kessler, Jr. (Quantum Metrology) and E. Fischbach (Phys Rev D, 44, R2216), examined the fundamental assumption that the speed of light represents the limiting velocity at which ponderable matter may move. Again, existing data was reanalyzed to provide a strict test of special relativity. This test may be viewed as the most precise numerical test, to date, of the Einstein mass-energy relation $E = mc^2$. (G. Greene and S. Dewey)

### Reaction Cross Section Measurements

Because of large uncertainties in the value of the $^{10}$B(n,$\alpha$) cross section, an important standard in the energy region above 500 keV, a collaborative effort has been undertaken to measure this cross section using the Oak Ridge Electron Linear Accelerator (ORELA) facility at the Oak Ridge National Laboratory. Data obtained in the neutron energy range from 0.2 to 4 MeV were presented at the International Conference on Nuclear Data for Science and Technology held in Jülich, Germany in May. Results are in good agreement with the most recent Evaluated Nuclear Data File (ENDF/B) cross section evaluation for neutron energies below about 2 MeV but significant discrepancies, greater than 40%, were found at the higher energies. Generally, the $^{10}$B(n,$\alpha$) cross section has received much attention lately because of the problems its relatively poor data base has caused in the standards evaluation process for ENDF/B-VI. An interlaboratory working group endorsed by the Nuclear Energy Agency Nuclear Data Committee (NEANDC) was recently formed to coordinate these cross section improvement efforts. (R.A. Schrack, O.A. Wasson, and A.D. Carlson)

### Fission Cross Section Measurements

Neutron-induced fission cross sections for actinide nuclei, important for the U.S. nuclear data program, were measured at high neutron energies where no previous data existed. Summary reports of results were presented at the International Nuclear Data Conference held in Germany and at the NEANDC sponsored workshop held in Sweden. Measurements were performed at the fission flight path of the target-4 neutron source at the Los Alamos Meson Physics Facility and covered the neutron energy region from 1 to 400 MeV. Fissionable isotopes included in the measurements, $^{234}$U, $^{235}$U, $^{236}$U, $^{238}$U, $^{237}$Np, and $^{239}$Pu, provide an important contribution to the nuclear data base for technology and to the understanding of neutron reactions at previously unexplored neutron energy regions. (A.D. Carlson)

### Interlaboratory Measurements of Charged-Particle Production

The neutron-induced charged-particle production cross sections for oxygen are important for the determination of kerma factors for medical therapy and radiation protection, and for neutron source calibrations in manganese sulfate baths. Preliminary measurements on oxygen in the neutron energy interval from 2 to 40 MeV have been completed using a neutron time-of-flight beam line at the LAMPF accelerator facility at Los Alamos National Laboratory. After initial tests which optimized the detection system for alpha particles, particle identification and energy measurements at angles of 30, 60, 90 and 135 degrees in the laboratory system were undertaken. Preliminary analysis indicates that suitable cross section and charged particle energy spectra can be obtained in two-week running periods. (A.D. Carlson and O.A. Wasson)

### Bias Induced By Small Numbers

A new approach to a not widely understood data analysis problem involving the statistics of small numbers has been investigated. It can be of use for many types of standards measurements. The problem occurs when a cross section is obtained as the quotient of small numbers of counts from two separate experiments. A small number of counts in the denominator (i.e., less than five) always introduces large statistical uncertainty in a quotient but in addition it will induce a bias in the final result when the quotients from many runs are combined to obtain acceptable statistical uncertainty. A preferred method, if at all possible, is to first combine the numerators and denominators and then take the quotient. If the data acquisition technique does not allow the data to be combined in this way, procedures are available to greatly reduce or eliminate the induced bias. A paper describing the application in experimental cases is being developed in consultation with the Statistical Engineering Division at NIST. (R.A. Schrack)

### Radioactivity Group

#### Dissemination of National Standards of Radioactive Activity

Continuing primary functions of
the Radioactivity Group are the supplying of special SRMs anchored on the national standards of the radionuclides involved and the checking of measurement traceability of subsidiary organizations. Over 500 SRMs were distributed in the past fiscal year, and over 220 certificates of traceability were issued to federal regulatory agencies, radiopharmaceutical manufacturers, commercial suppliers of calibration sources and services, and the nuclear-power industry. Industrial steering committees guided the work of two research associates in cooperative testing programs. (D.D. Hoppes, J.M. Calhoun, F.J. Schima, and J.M.R. Hutchinson)

- Quantification of Radionuclides for Cancer Treatment. Research and development of palliative and therapeutic applications of radionuclides targeted to malignant organs require accurate knowledge of their activities radiation probabilities, and half lives in order to quantify the tissue destruction. Calibration techniques developed for 64 h ²²²T were applied to the radionuclide in glass microspheres distributed by Nordion International. The spheres are injected into the hepatic artery where they lodge in the microcapillaries and destroy liver cancer cells. A national standard was developed for ¹⁶⁶Ho, used in a bone-seeking radiopharmaceutical. Solutions were measured by liquid scintillation counting, with calculated efficiency tracing with tritium. The decay scheme shows underlined radiation probabilities and uncertainties deduced from emission rates measured for quantitative sources with well calibrated gamma-ray spectrometers, and the half life measured with a stable ionization chamber. (D.D. Hoppes, F.J. Schima, and J.M. Calhoun)

- Applications of the National Radon Standard. Several significant accomplishments have been made in the radon measurement standards program this year. These include: (1) Completion of an international measurement intercomparison involving 11 laboratories. The intercomparison was based on distributing 35 mL radon-in-air samples that are employed as part of a new transfer calibration standard for radon. The new system is based on measurements of the photon emission rate of radon daughters contained in small sample bulbs with a NaI(Tl) well counter that is calibrated against the NIST pulse-ionization-chamber-based primary radon measurement system. (2) The development and evaluation of the prototype polyethylene-encapsulated radium solution standards has satisfactorily progressed to a stage that the first prototypes will be available as a new SRM within the next few months. The provisional certificates for these standards will be based on the first developed measurement application. (3) Collaborations with several laboratories, including those within the commercial radon industry, are also ongoing to evaluate the prototype capsules and to develop calibration protocols for other measurement applications. (4) The Radioactivity Group participated and served as the referee for an international measurements intercomparison of instruments used to measure trace atmospheric concentrations of radon at remote marine environment locations around the globe. Such radon measurements are used to obtain information on the temporal and spatial distributions which are in turn used to test and validate global models that simulate the transport and removal of trace atmospheric species. The intercomparison was conducted at the Bermuda Biological Research Station, and NIST was responsible for providing standardized additions of radon concentration to the sampling tower used by the four participating laboratories. This exercise was the first such intercomparison of instruments used in different world-wide locations, and will provide a common reference for the global data. (J.M.R. Hutchinson and R. Collé)

FUTURE OPPORTUNITIES

- Two-Dimensional ESR Imaging of Surfaces for Electronics Materials. Electron spin resonance like nuclear magnetic resonance has potential for use in imaging. NIST has the opportunity to work with instrument manufacturers in developing ESR imaging techniques and helping industry exploit these techniques to study microstructure in high tech materials. A particular interest is to use ESR imaging to develop contour maps of paramagnetic centers in irradiated electronic devices. These data will be correlated with theoretical calculations and measurements of interface dosimetry.

- Tools for Radiation Therapy Treatment Planning. The physical aspects of radiation treatment planning are based on an analysis of the radiation source, the source dosimetry and the physical characteristics of the tumor. Future treatment planning will be carried out with larger and faster computer systems, which will allow the input of massive patient-specific input data (computed tomographic (CT) and magnetic resonance imaging (MRI) scans of the tumor for example). NIST techniques for mapping source
fields with radiochromic films will be incorporated into treatment planning packages.

- **Medical Industrial Radiation Facility (MIRF).** The Ionizing Radiation Division is designing a new facility for medical radiation therapy and industrial radiation processing applications. The MIRF will be a push-button 50 MeV electron/photon accelerator set up with work stations for medical radiation dosimetry with electron and bremsstrahlung photon beams, and for high current DC 10 MeV electron beams for dosimetry of electron processing and sterilization.

- **Neutron Interferometry.** Advanced neutron optical techniques, i.e., "neutron interferometry," are highly appropriate for performing fundamental tests of quantum mechanics, gravity, and special relativity. To exploit the exquisite sensitivity of these techniques advanced methods of vibrational control must be developed which, incidentally, are of interest in a variety of Hi-Tech and Bio-Medical application.

- **Advanced Techniques in Materials Dosimetry.** Newer methods of establishing fast neutron exposure of heavy section steel and the attendant degradation of toughness must be developed and evaluated for accuracy and modes of application. The need is underlined by the recent and first shutdown of an operating nuclear power reactor solely for reasons of possibly unsafe embrittlement of the steel plate and weldments of the reactor pressure vessel. Major directions to meet this challenge are innovative neutron detector development and benchmark experiments in new reference neutron fields.

- **Radionuclides in Industrial Process Control.** The increasing application of radionuclides and radiations in industrial process control will be monitored. The ability to follow the interaction of relatively few atoms, with negligible residual activity for short-lived radionuclides, offers interesting possibilities for tomography, for example.

- **Nuclear Waste Radionuclide Standards.** Standards for very long-lived radionuclides in nuclear waste should be developed. Measuring techniques using selective atom-counting instead of radiation spectrometry may be appropriate if complex chemistry is to be avoided.
TIME AND FREQUENCY DIVISION

MISSION
The mission of the Time and Frequency Division encompasses three primary objectives:
- development and operation of standards of time and frequency and coordination of them with other world standards;
- provision of time and frequency services to the United States;
- fundamental and applied research in support of future standards, dissemination services, and measurement methods.
Since length is now derived from the second, the Division has a secondary responsibility for that unit.

ORGANIZATION
The Division is organized into eight technical Groups: Ion Storage, Atomic Beam Standards, Phase Noise Measurements, Time & Frequency Services, Time Scale & Coordination, Laser Spectroscopy, Geophysical Measurements, and Optical Frequency Measurements. With a full time staff of 40, the Groups are necessarily small, and the Group Leaders are thus able to function primarily as technical leaders within their areas. The unifying theme of time and frequency technology requires strong interactions (even dependencies) among the Groups. During the last year, the Division hosted 20 long-term guest researchers and 5 postdocs.

CURRENT DIRECTIONS
As a result of the large service component of the Division program, substantial resources are devoted to certain routine operations. These include the operation of the NIST time scale and the primary frequency standards, broadcast of time and frequency signals, and operation of calibration services. Division research and development efforts are undertaken to provide the basis for the future of these operations as described below.

- Improved Time Scales. The NIST Time Scale continues to be the working clock system which provides accurate signals for services and applications and which serves as a reference for research on new standards and measurement methods. The reliability and stability of this time scale is based on the use of an ensemble of commercial cesium-beam standards and hydrogen masers combined together under computer control using a highly developed algorithm. The Division is working to improve the performance of the time scale through acquisition of more stable clocks, development of improved algorithms, and improvement of the electronic systems which read the output of the clocks.

- New Frequency Standard. The accuracy of the time scale is derived from primary frequency standards which provide the practical realization of the definition of the second. To meet advancing needs the Division has built a new frequency standard which uses optical pumping methods. A preliminary evaluation of the accuracy of this standard has been completed, although considerably more effort will be required to complete evaluation of errors at the full design accuracy of $1 \times 10^{-14}$. Looking toward still higher accuracy, the Division is studying trapped, laser-cooled atomic ions as the basis for advanced frequency standards. These offer promise of accuracy improvements of many orders of magnitude. While the ion studies have involved demonstrations of prototype clocks, the work is treated as basic research providing the knowledge base for future development of more accurate standards.

- Improved Methods of Time Transfer. Since the world operates on a unified time system, Coordinated Universal Time, highly accurate time transfer (to coordinate time internationally) is a critical ingredient in standards operations. The Division has long been a world leader in this field. The Division is working to further improve the NIST-developed, GPS Common-View Time Transfer Method which is the standard for international time coordination. The Division is also continuing efforts to develop and implement...
the Two-Way Time Transfer Method which promises still higher transfer accuracy.

- **Time and Frequency Broadcast Services.** The Division provides time and frequency broadcasts from stations WWV and WWVB in Fort Collins, Colorado and from WWVH in Hawaii and a time code broadcast from the GOES weather satellites operated by NOAA. The Division also operates a telephone time service, the Automated Computer Time Service (ACTS), designed for setting clocks in digital systems. These broadcasts serve applications in a broad range of systems in business, communications, science, transportation, and computers. Calibration laboratories are served by the Division's Frequency Measurement Service, a system which provides for highly accurate frequency measurements. The Global Time Service uses GPS common-view time transfer to provide the highest accuracy time and frequency dissemination. Work has started on an advanced Satellite Time Service with a projected accuracy over 1000 times better than the current GOES service.

- **Improved Optical Frequency Standards.** The Division is also engaged in developing improved optical sources for use in accurate optical frequency measurements which are important to future ion frequency standards in the optical region, advanced optical communication, analytical instrumentation, and length measurement. The emphasis in this program is on diode lasers which promise very high spectral purity, simplicity, tunability, and low cost.

- **Development of New Phase-Noise Measurements.** The Division’s development of new phase-noise measurements supports accurate specifications for a range of aerospace systems. Further development work is being undertaken to broaden the spectral coverage and simplify comparison of measurement accuracy between standards laboratories. Further work is being done on documentation for a new phase-noise calibration service.

- **Applications of Time and Frequency Technology.** Finally, the Division is engaged in the application of time and frequency technology to important problems in high-resolution spectroscopy and geophysics.

**TECHNICAL HIGHLIGHTS**

- **Preliminary Evaluation of NIST-7.** A preliminary evaluation of the uncertainty of NIST-7 has been completed. Results of the evaluation will be presented to the world’s standards community at the Conference on Precision Electromagnetic Measurements to be held in Paris in June of 1992. NIST-7 is an optically pumped cesium standard, developed by Bob Drullinger, Dave Glaze, John Lowe, Andrea DeMarchi (guest researcher), and Jon Shirley (guest researcher). It will eventually replace NBS-6 which is now 17 years old. The design goals for NIST-7 have been (1) an accuracy of $1 \times 10^{-14}$, (2) a high short-term stability providing for more rapid evaluation, and (3) highly automated evaluation of systematic errors allowing near continuous operation of the standard. This preliminary evaluation was done at a level of $1 \times 10^{-13}$, the same as the accuracy of NBS-6.

With this initial phase of development and demonstration now completed, NIST-7 will be moved into the main primary standards laboratory where systematic uncertainties will be further evaluated and control systems will be further improved. Evaluation of the new standard at the full design accuracy will take as long as two additional years. This will require very detailed measurements of (1) the AC Stark shift, (2) cavity-related errors, (3) several line pulling effects, (4) second-order Zeeman splitting, and (5) the second-order Doppler shift. One long-term goal is to develop electronic control of these last two error terms. Furthermore, a careful re-analysis of the entire servo-electronic system will be needed to assure achievement of the required line-center accuracy. In the final analysis, the second-order Doppler shift is likely to be the major accuracy-limiting effect.

- **Linear Paul Trap.** The main advantage of using a single ion in a Paul quadrupole trap is that the kinetic energy of micromotion can be on the order of the random thermal motion. This allows us to minimize the second-order Doppler shift, for example, holding it to a few parts in $10^{18}$ for a single mercury ion cooled to the Doppler-cooling limit. The disadvantage of using a single ion is that the experimental signal-to-noise ratio is low making measurements difficult. The development and demonstration of a linear Paul trap (see Fig. 1) that can store 50 - 100 ions in a string promises substantially improved signals while retaining the advantage of small second-order Doppler shift.

The ions in these strings can be treated as independent atomic clocks where the clock transition can be detected with 100% efficiency (using an electron-shelving scheme). If 50 ions are used, on a resonance of frequency 40.5 GHz
(the ground state hyperfine transition for $^{199}\text{Hg}^+$), and the Ramsey method of interrogation is used where the free precession time is 100 s, the frequency stability of this clock "ensemble" should be $\epsilon_p = 5.5 \times 10^{-14} \tau^4$.

In preliminary studies of strings of $^{199}\text{Hg}^+$ ions, Mark Raizen and John Gilligan (postdoctoral fellows) along with Dave Wineland, Wayne Itano, and Jim Bergquist have observed the 40.5 GHz hyperfine resonance. This trap can also be used to do very-high-resolution spectroscopy on optical transitions. With one or more ions localized in the trap to less than $\lambda/2\pi$ ($\lambda$ is the laser wavelength), several interesting experiments investigating interference, superradiance and subradiance, and cavity-QED should be feasible.

![Figure 1. Linear trap configuration.](image)

**Be$^+$ Hyperfine Pressure Shift.** Fred Moore (postdoc), John Bollinger and Dave Wineland in the Ion Storage Group have identified a shift of the $^9\text{Be}^+$ clock transition frequency, with unexpectedly large value, as the background pressure was increased. Of the residual gases studied in these experiments (H$_2$, N$_2$, O$_2$, H$_2$O, CO, CH$_4$, and CO$_2$), only CH$_4$ gave a large shift, a few $\times 10^{-5}$ per Pascal (about $2 \times 10^{13}/10^{10}$ torr). The pressure shift might affect all precision measurements of hyperfine structures of all ions at similar levels requiring cryopumping to achieve higher vacuums (thus minimizing the effect).

The large difference between the data for CH$_4$ and other gases we measured, and the difference between our data for CH$_4$ and ion hyperfine pressure shifts induced by inert gases (measured by other groups) is not understood at this time. One possible explanation is suggested by studies of radiative association of C$^+$ with H$_2$ to form CH$_2^+$. In the models of this process, it is assumed that the H$_2$ can stick to the C$^+$ for a long enough time to allow the C$^+$-H$_2$ complex to radiatively stabilize. This sticking is possible because the collision energy can be taken up by the internal degrees of freedom of the H$_2$ molecule or the H$_2$-C$^+$ complex. The sticking time can be orders of magnitude longer than the interaction time during a simple elastic collision. If a similar sticking mechanism is active in CH$_4$ + Be$^+$ collisions, it may account for the apparent large pressure shift.

- **Observation of "Atomic Projection" Noise.** In spectroscopy, "technical noise," such as laser amplitude fluctuations caused by an unstable power supply, often dominates the noise. These sources of noise can be eliminated by careful engineering. Two examples of more fundamental noise sources are the detection shot noise in a laser absorption spectroscopy experiment and the fluctuations in signal caused by the fluctuations in the number of atoms in an atomic beam experiment. These sources of noise can also be eliminated or significantly reduced. For example, laser shot noise can, in principle, be reduced by use of squeezed light. In a stored-ion experiment, the number of ions can be held constant thereby reducing the atomic number fluctuations to zero. Also, when absorption is detected using electron shelving, the detection noise approaches zero since 100% detection efficiency is possible. Because of this immunity from some sources of noise, we have been able to observe, in a clear way, what might be called "quantum projection noise." Basically, this source of noise is caused by the statistical fluctuations in the number of atomic absorbers (ions in our case) which are observed to make the transition in an absorption spectroscopy experiment.

Wayne Itano along with the rest of the Ion Storage Group have completed experimental working describing this previously unrecognized noise source. They developed the basic theory for this noise showing that it is maximum, for Ramsey excitation, at the point of maximum slope of a resonance curve. Measurements of a "clock" resonance in $^9\text{Be}^+$ (see Fig. 2) show that the observed noise is larger on the sides of the Ramsey resonance than on the peaks and valleys of the curve (noise due to frequency fluctuations was negligible).
Figure 2. A Ramsey resonance taken on the "clock" resonance of $^9\text{Be}^+$ ions in a Penning trap. The number of ions (approximately 20) was held fixed. The error bars indicate the standard deviation of the measurements.

- **Penning Trap Density Limitations.** John Bollinger, Fred Moore (postdoc), Dave Wineland, and Wayne Itano have discovered and investigated a particular limitation to the number and density of charged particles that can be stored in a Penning trap. The energy and angular momentum of a cloud of $^9\text{Be}^+$ ions were controlled with radiation pressure from two different lasers. One of the laser beams was directed through the radial edge of the ion cloud and supplied a radiation-pressure torque which increased the $^9\text{Be}^+$ rotation frequency and density. We discovered that a slight misalignment of the trap symmetry axis with the magnetic field would heat the plasma when we attempted to increase the rotation frequency (or density) beyond a certain value. With about 2000 ions in the trap, we could use this heating to align the trap symmetry axis with the magnetic field to better than 0.01°. Larger ion clouds were even more sensitive to this misalignment. In fact, in this trap, all other known methods of alignment were less sensitive. We were able to associate this heating with the excitation of a collective mode of the plasma by the static field asymmetry.

These static modes have important implications for experiments where storage of large numbers of charged particles are important. For example, they may provide a limit to the number of antiprotons or positrons which can be stored in a trap. The plasma modes also play an important role in the asymmetry-induced trans-

- **Theory for Sisyphus cooling for a bound atom (ion).** Cooling that results from optical dipole forces has been considered for a bound atom (or trapped ion). Through optical pumping, the atom can be made to feel decelerating optical dipole forces more strongly than the accelerating optical dipole forces. This effect, which has previously been realized for free atoms, is called Sisyphus cooling. Dave Wineland in collaboration with Jean Dalibard and Claude Cohen-Tannoudji of the Ecole Normale in Paris examined a simple model for a bound atom in order to reveal the basic aspects of cooling and heating when the atom is confined in the Lamb-Dicke regime. Results of semiclassical and quantum treatments show that the minimum energy achieved is near the zero-point energy and can be much lower than the Doppler cooling limit. Sisyphus cooling of trapped $^9\text{Mg}^+$ and $^9\text{Hg}^+$ have been examined theoretically.

- **Search for anomalous spin-dependent forces using $^9\text{Be}^+$.** The existence of weakly interacting bosons (such as axions) has been suggested previously. Laboratory experiments might detect scalar or pseudoscalar couplings of such particles to matter in the form of new spin-dependent forces. Dave Wineland, John Bollinger, Wayne Itano, and Mark Raizen (postdoc) have used spectroscopy of $^9\text{Be}^+$ to search for anomalous potentials having a dipole-monopole or dipole-dipole character. An experimental limit was placed on the strengths of the interactions by examining the $^9\text{Be}^+$ hyperfine "clock" transition frequency $\nu_0$ under various conditions.

In these searches, one particle in the postulated interaction was taken to be either the $^9\text{Be}$ nucleus or the unpaired outer electron of $^9\text{Be}^+$. In the search for a dipole-monopole force, the other particles are taken to be nucleons in the earth. A search was made for a change in frequency between the cases where the trap magnetic field was parallel or antiparallel to the vertical direction in the lab. In the search for a dipole-dipole force, the other particles were taken to be the electron spins in the iron pole faces of an electromagnet. In this case frequencies were compared when the field was created by the electromagnet or by a superconducting solenoid. From these data, upper limits on these weak forces were determined for the electron and the neutron.
New System for Precise Phase Noise Measurements. In response to emerging aerospace systems with tight phase noise specifications, Fred Walls has developed the first measurement systems which yield high-precision phase noise measurements over a broad frequency range. These phase-noise-measurement systems operate at carrier frequencies from 5 MHz to 26 GHz and 33 GHz to 50 GHz with bandwidths up to 10% of the carrier frequency. The measurement precision ranges from about 1 to 2 dB depending on the operating conditions. Funding for this program was provided in part by the Department of Defense to which NIST has delivered four measurement systems.

Commercial equipment for phase noise measurements has been available for several years, but there has been no satisfactory method for assuring that such systems were indeed giving accurate readings. The commercial systems are substantially more limited in dynamic range and precision. The NIST measurement systems have uncovered a number of measurement errors, some ranging from 5 to 20 dB, errors that are often intolerable. Both equipment and operator-procedure errors have been identified.

Phase noise has been rising in importance in radars, telecommunications, and other systems where high spectral purity of signals is critical. Its presence in the components of signal channels degrades spectral purity of the signal and thus the performance of the system.

Secondary Standards for Phase Noise Measurements. Fred Walls has developed a simple phase-noise artifact which can be used as a secondary reference in round-robin tests of measurement systems. The portable device provides a fixed noise floor with added phase noise introduced at the flip of a switch. The noise floor and the fixed, higher phase-noise level, both of which are highly stable, are calibrated using the new NIST phase-noise-measurement system. The present devices operate at carrier frequencies of 5, 10, and 100 MHz with phase noise that is nearly flat to Fourier frequencies 10% from the carrier. This new device allows for full assessment of the precision of phase noise measurements encompassing the entire measurement process (hardware, software, and operator procedures).

Extended tests have shown the phase noise of this device to be stable to ± 0.3 dB over the course of a full year. The demonstrated precision is ± 0.23 dB. In its first application to round-robin measurements, a large error, attributed to the operator's procedures, was uncovered.

Because of the popularity of the concept, devices are now being planned for other carrier frequencies.

PC Technology for Time-Scale Systems. Judah Levine has completed conversion of the NIST Time Scale from a main-frame type computer to a PC (486). This involved massive rewriting or conversion of software, and implementation of a careful interrupt scheme used for reading the atomic clocks at exactly chosen instants in time. This new system is operating in parallel with the current front-end computer. This provides an operational redundancy that was previously difficult to justify because of the high cost. Data from the two parallel time scale systems are independently archived.

This transition marks the beginning of a general program to phase out the use of main frame computers for this function. Because the cost differential (between the main-frame and PC systems) is more than an order of magnitude, this will allow the Division to not only run with a higher level of redundancy, but also to acquire needed backup computer equipment. In the process of rewriting the software, number handling and round-off errors were implemented in a manner that resulted in a noticeable reduction in "computer-added" clock noise. In addition, comparison of the time-difference measurements between the two systems has allowed us to evaluate the performance of the hardware and has already resulted in an improved data acquisition algorithm for both systems.

New Algorithm for NIST Time Scale. Marc Weiss and Tom Weissert (guest researcher) have completed development of an improved algorithm for combining the outputs of the various atomic clocks in the NIST Time Scale. The new algorithm called TA2 is used for post-processing time scale data in such a way as to provide corrections for current operation of the time scale. One example of such a correction involves sensitive detection of frequency steps which are very difficult to differentiate from noise in real-time operation. The algorithm, which gains efficiency by running the data both backwards and forward in time, includes an automatic step detection routine. Processing two and a half years of time scale data shows a significant improvement in long-term stability, although much longer data records will have to be processed before the value of the new algorithm can be established with solid statistical confidence.

The value of an algorithm for forming a time scale from an ensemble of clocks is now clearly evident.
established. Properly done, the output of such an algorithm is a time that is more stable than that of the best clock in the ensemble. NIST has provided leadership in developing and arguing the value of time-scale algorithms. While the current algorithm (AT1) has performed well for a number of years, it has become clear that there were shortcomings to be repaired. The imminent use of an improved primary standard has provided the incentive for this development. At an accuracy level of $1 \times 10^{-14}$ the current time scale will not be able to carry the accuracy of an evaluation for more than about one month.

**Synchronization Interface Standard for Telecommunications Networks.** David Allan and Marc Weiss provided leadership in the development of a new synchronization interface standard for use by the U.S. telecommunications community. The standard supports synchronous communications in a new fiber-optic based technology known as SONET. Standards for this technology are being developed by the Committee Telecommunications 1 (T1) which is accredited by the American National Standards Institute.

The group with synchronous interfaces was having substantial difficulty defining the amount of phase noise which SONET will have to tolerate. At the request of the industry, NIST analyzed communications noise data collected from the telephone network, made recommendations of useful phase noise measures, and served as a focal point for clarification of new network phase noise specifications. There were two key contributions that were made in this process. First, they developed a variation on the two-sample variance (Allan variance) called the time variance (TVAR) that is particularly suited to characterization of the performance of synchronization links. This measure received instant acceptance by the telecommunications industry and has now been accepted as an international standard. Second, in collaboration with Jim Jespersen of the Division, a simple picture was developed for this and other variances which shows how these variances can be viewed as simple filters in the frequency domain. This was a particularly useful contribution, since telecommunications engineers typically view the performance of their systems in this manner. The impact of this effort can be judged from the expected sales of the SONET equipment which should be measured at a level of hundreds of millions of dollars. Network providers are also interested in the huge operational cost savings that SONET equipment deployment could generate.

**New Software for Statistical Analysis of Time and Frequency Data.** Marc Weiss, Fred Walls, and Dave Allan have developed new statistical software packages that will be made available to users in industry, government, and science. These provide not only for the calculation of the standard time and frequency measures of performance, but also for certain complex data conversions. The software packages should prove to be useful in the characterization of a variety of systems including clocks, oscillators, communications networks, and general time measurement systems.

There are three agreed upon time-domain statistical measures used by the time and frequency community. These are the Allan variance, the modified Allan variance, and a relatively new variance called the time variance. In contrast to the first two variances which are used for characterizing frequency stability, the latter variance provides a means for measuring time or phase deviations. These three measures, often denoted as AVAR, MVAR and TVAR, are all calculated by these software packages. Because of the high interest in TVAR by the telecommunications industry, some very efficient algorithms for its calculation were developed. These allow for the processing of about a million points in an advanced PC in only a few minutes. In addition, one of these software packages will take a large variety of modelled spectral elements, pass-band filters, etc. and convert them from their normal frequency-domain representations into any of the three time-domain measures listed above.

**Ionospheric Receiver Technology Transferred to Industry.** Dick Davis and Marc Weiss have successfully transferred the technology for a codeless GPS ionospheric receiver to a local Colorado company that deals in atmospheric measurement technology. The general idea of a codeless GPS receiver had been conceived by several organizations including the Jet Propulsion Laboratory, but no implementation to date has been as simple and versatile as the NIST receiver.

The Division developed the receiver in order to provide for continuous measurement of the delay produced by the ionosphere in the Common-View Time Transfer Method (also developed by NIST). The receiver picks up signals from two different frequencies broadcast by the GPS satellites and, from the phase difference of the
signals, determines the ionospheric delay and thus the free electron content along the path to the satellite. The receiver stores a catalogue of all the GPS satellites and identifies each from its Doppler signature. It can track approximately ten satellites simultaneously providing ionospheric measurements for each.

While the market for the time-delay measurements for time comparisons is significant, the system can potentially provide useful corrections for geophysical GPS surveying, and for studies of the ionosphere. This latter application is significant, because the current measurement method is performed using the electron-content of the ionosphere involves a cumbersome use of reflected radar signals which then only provides a measure of the vertical ionospheric component.

- **New Modem for Satellite Time Transfer and Satellite Time Service.** Dick Davis, Marc Weiss, and Dave Howe have completed design and started construction of a second version of a spread-spectrum modem required for accurate time transfer and for range determinations for a proposed satellite time service. After completion of the first version, important design improvements were identified forcing a substantial revision of part of the circuitry. This complex telecommunications modem will be used with commercial, KU-band communication satellites for both time transfer and ranging. The modem supports sub-nanosecond timing resolution and a coding system that provides flexibility in addressing specific earth stations. It also incorporates variable communication rates. The system is run by a personal computer (386) allowing software control of all operational parameters.

The satellite time service is one of the two key applications of this modem. In this service, two-way exchanges of signals through a geostationary communication satellite between three geographically dispersed earth stations provides accurate coordinates for the satellite. These coordinates, along with a time message, are then broadcast from the satellite. The broadcast can then be picked up (receive only mode) by user receivers and processed to account for the delay in propagation from the satellite to the receiver. An accuracy of better than 100 nanoseconds should be readily achievable and the concept provides for extension of accuracy if it is required. Of course, the other application for this modem is in two-way time transfer supporting international coordination of time scales.

- **New Time-Code Generators and New Voice Systems for Radio Broadcasts.** The Division has recently acquired and installed specially designed time-code generators and digital-voice-recording equipment for control of broadcast operations at radio stations WWV (Fort Collins, Colorado) and WWVH (Kauai, Hawaii). The equipment replaces leased systems which were becoming difficult to maintain and which limited flexibility in modifying the digital time codes broadcast on subcarriers of the main shortwave frequencies. In addition, the use of directly recorded voice messages for certain other agency announcements has been problematic through the years because of the variability in voice clarity and enunciation associated with the different individuals recording messages and the unreliability of conventional tape-recording equipment. The other agency announcements include marine storm warnings, geophysical alerts relating to solar/ionospheric disruption of communications, OMEGA navigation status reports, and GPS status announcements.

In recent years, the Division has received a number of requests to modify the broadcast time codes in a manner which would provide information on the current year and allow for improved long-term anticipation of insertion of leap seconds and changes to and from daylight savings time. These changes allow for more complete automation of timekeeping at the users end. The hard-wired nature of the older time-code generators made it difficult to implement these changes. The new time-code systems are now in routine operation providing the improved time codes. User and manufacturer response has been excellent.

The new digital-voice-recording systems are providing higher quality and increased reliability for the recorded announcements. The routine time announcements (every minute) and the station identification announcements also use a digitally stored voice. The only problem identified to date is a dissatisfaction (by a few listeners) with the new voices which have replaced the familiar voices used for many years.

- **Advanced Systems for the Frequency Measurement Service.** George Kamasa and Mike Lombardi have implemented an improved version of the equipment used with the Division's Frequency Measurement Service. This reimbursable service provides measurement assurance for calibration labs with an accuracy as high as $1 \times 10^{-12}$. NIST equipment at the user's lab receives LF signals which are compared with the local standard,
and the performance of the user's equipment is monitored through a modem by NIST. The user pays an up-front fee for installation of the equipment and training on the equipment. A regular monthly fee then provides continuous assurance of the performance of the local standard.

Substantial hardware and software improvements were made in converting the system operation over to a PC (286) environment. User friendly screens provide ready access to data on the performance of the standard and the user system prints out a daily report. The older versions of this equipment are still supported, but users can opt to replace the older system with the new one (for somewhat higher fees). This measurement service provides for direct traceability of frequency measurements in more than 60 of the Nation's high level industrial and government laboratories.

**NIST Leadership of U.S. Delegation to CCIR.** For the last five years Roger Beecher has served as chairman of the U.S. delegation to Working Party 7A (dealing with time and frequency matters) of the Consultative Committee on International Radio (CCIR). Dave Allan of the Division has served as one delegate to the Working Party for the last 3 years. They have recently coordinated major U.S. inputs which have been accepted by WP 7A and are now in the form of formal recommendations of the CCIR.

The CCIR is a technical advisory group that, within the International Telecommunications Union (ITU), provides formal recommendations, technical advice, and technical information related to the allocation and use of the radio spectrum. When adopted, such recommendations of the CCIR have the force of international law, at least for the more than 150 member nations of the ITU. The best known recommendation of this type is CCIR Recommendation 460, which established the UTC (Coordinated Universal Time) system in 1972. WP 7A has historically taken a rather broad view of its scope considering questions such as methods for improving terrestrial frequency and time dissemination, stability of standard-frequency and time-signal emissions as received, time codes, techniques for time transfer, performance and reliability of frequency standards and their use in time scales, and standard frequency and time signals from satellites.

In its recent work WP 7A has produced several recommendations. One is a rather comprehensive recommendation on "Frequency and Time (Phase) Instability Measures." Other recommendations involve the use of satellite methods for time transfer. NIST participation in this process has assured that U.S. industry and government interests are well represented in the setting of international standards. In the most recent meetings in Geneva, the U.S. delegation gained acceptance of 13 of the 14 proposals put forward by the delegation, a very high level of success.

**Special Time and Frequency Issue of IEEE Proceedings.** Wayne Hanson and Jim Jespersen of the Division served as guest editors for a special issue of the IEEE Proceedings devoted to time and frequency technology. The special issue covers time and frequency standards, statistical characterization of frequency standards, techniques for time coordination and dissemination, emerging needs for accurate time and frequency, and requirements for accurate time in science. Of the twenty invited papers in this issue, four involved NIST authors. These NIST papers deal with ion frequency standards, cooled neutral-atom standards, characterization of frequency stability, and an overview of time generation and distribution.

**Diode Laser System for a Calcium Length Standard.** Leo Hollberg in collaboration with Reinhold Ellingsen (Norway), Vladimir Velichansky (Moscow), and Guglielmo Tino (Italy) has developed a diode laser system at 657 nm for detection of a calcium transition that has potential as an optical standard of length/frequency. This transition is substantially narrower (natural linewidth of 400 Hz) than that of the iodine transition used to stabilize He-Ne lasers used as length references. Furthermore, the calcium line is a singlet eliminating complications and systematic shifts encountered with using more complex lines. While a number of laboratories have looked at ways to improve upon the iodine-stabilized He-Ne laser, it seems clear that a movement towards calcium makes more sense. Furthermore, with the recent demonstration of laser cooling of calcium in Italy, Germany, and Japan, there is potential for still higher accuracy.

In this work, extended-cavity diode lasers have been used to observe Doppler-free saturated absorption signals in calcium (see Fig. 3). The best diode-laser measurements are now limited to a linewidth of 200 kHz, but with further improvement in the lasers this should be dramatically reduced.

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PHYSICS LABORATORY

TIME AND FREQUENCY DIVISION
Figure 3. Calcium spectrum. The measurement was done using Doppler-free saturated-absorption spectroscopy with a diode laser. The linewidth is limited by the linewidth of the diode laser. Much narrower resonances will be obtained as the laser linewidth is reduced. The natural linewidth is 400 Hz.

A major program at the PTB in Germany is nearing measurement of the absolute frequency of the calcium line through direct frequency multiplication from the cesium standard. With this measurement (after duplication by other laboratories), the calcium line can take on the role of an accepted secondary standard of length/frequency. Thus, the NIST work on development of a simple laser for exciting that transition is of significant practical importance.

- Major Tutorial Lectures on Applications of Diode Lasers. Leo Hollberg recently presented two major tutorials on applications of diode lasers. A special half-day tutorial at a meeting of the Division of Atomic, Molecular, and Optical Physics (DAMOP) of the American Physical Society in Washington, D.C. was attended by more than 100 scientists who paid an additional fee for the session. This tutorial, the first tutorial ever offered in conjunction with a meeting of DAMOP, was considered to be a resounding success. Hollberg also presented the introductory lecture at a one-day symposium on "Optical Spectroscopy Using Diode Lasers" held in conjunction with the Eighteenth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies in Anaheim, California. The invitations for these tutorials are no doubt related to the wide interest expressed in a paper, "Using Diode Lasers for Atomic Physics," published by Hollberg and Carl Weiman of JILA. More than 400 requests were received for this paper.

- Diode Laser Control and Characterization. In a collaborative effort, Professor Hugh Robinson (Duke University), Rich Fox (guest researcher) and Leo Hollberg have been studying the optical noise characteristics of semiconductor diode lasers. This work has focussed on both the amplitude and frequency noise of the devices. New hybrid optical and electronic methods have been developed to reduce the amplitude noise to near the quantum-limited shot noise. Optical stabilization methods have been developed to further narrow the spectrum of grating-tuned diode lasers. Progress has also been made in generating blue light from diode lasers by second harmonic generation in potassium niobate.

Reduction of the amplitude noise in diode lasers will enhance their application to ultra-sensitive detection of atoms and molecules as well as to other scientific areas. The line narrowing is important in a number of applications including frequency synthesis, high-resolution spectroscopy, and optical pumping of atomic frequency standards. The frequency doubling to produce blue light is of obvious importance to optical frequency synthesis, but might also provide sufficient blue light directly from the diode laser) to laser cool calcium.

- Laser Magnetic Resonance Spectroscopy for Ozone Chemistry Studies. Laser magnetic resonance (LMR), invented at NIST by Ken Evenson, is one of the world's most sensitive spectroscopic techniques. Its sensitivity has recently been further enhanced by an order of magnitude by increasing the modulation and using higher speed detectors. The technique has been selected by NASA for use in a balloon-borne experiment to measure the absolute concentration of atomic oxygen, the hydroxyl radical (OH), and the hydroperoxyl radical (HO$_2$) in the lower stratosphere (at an altitude of about 15,000 meters. The flying LMR spectrometer for this experiment is being developed in a joint project by Ken Evenson of the Division and staff of NOAA's Aeronomy Laboratory in Boulder.

The OH and HO$_2$ radicals are particularly important intermediates in numerous atmospheric reactions and are extremely reactive. The successful development of a sensitive measuring instrument for these radicals in the atmosphere is therefore crucial to the understanding of which reactions are dominant at a given latitude and altitude. An example of a topic of much current concern in which the role of OH/HO$_2$ is uncertain is that of polar ozone depletion. One proposed mechanism of ozone
depletion involves both the OH and HO$_2$ radicals. The LMR technique appears to be the only viable means for acquiring data of sufficient accuracy on these species.

- **Frequency and Wavelength Standard for the Far Infrared.** Visiting scientist Thomas Varberg and Kenneth Evenson have recently completed a high resolution study of the far infrared spectrum of gaseous carbon monoxide (CO). The frequencies of pure rotational transitions in the ground state of the molecule were measured using their laser-synthesized, tunable far infrared spectrometer. A complete set of frequencies were calculated from these data with an accuracy of about 5 parts in $10^9$. This is ten times more accurate than the previous best measurements.

  Accurate measurements of the spectrum of carbon monoxide are important for two reasons. First, CO is an abundant interstellar molecule, and many astrophysical measurements and tests of theory depend on the accuracy of CO rotational frequencies. Second, CO is often used as a reference standard to calibrate spectrometers (especially Fourier transform spectrometers) in the far infrared. With the completion of this work, the CO transitions are now the most accurate far infrared frequencies available in the frequency range from 100 to 4300 GHz (wavelengths of 3000 to 70 $\mu$m).

**FUTURE OPPORTUNITIES**

In the course of conducting current programs, the Division has developed capabilities putting it in a unique position to pursue certain programs. While the list of opportunities is far greater than the resources available to pursue them, it is nonetheless worthwhile to examine them here. These special capabilities include: (1) systems for trapping and cooling ions; (2) highly stable lasers and microwave sources for high resolution studies of atoms and molecules; (3) well-characterized atomic beams; (4) high-resolution systems for imaging atomic particles; (5) low-phase-noise components and systems; and (6) satellite-timing receivers and transmitters. The Division also has a strong tradition of accurate frequency measurement across the electromagnetic spectrum and leading-edge talent in statistical analysis of time series of data. Considering these assets, we list the following examples of research opportunities.

- **Atomic Physics.** In atomic physics, Division programs are centered on strengths in ion trapping, cesium beams, low-noise frequency synthesis, and accurate frequency measurements. Example measurements include:
  - Tests of Relativity Theory: Such tests include accurate measurement of the gravitational red shift and searches for spatial anisotropy (Hughes-Drever type experiments).
  - Measurement of Light Shifts: Both the influence of black-body radiation and electric fields (ac-Stark shifts) can be studied. The latter might provide the basis for an ultraviolet power standard.
  - Study of Radiation Statistics of Atomic Systems: Here, we observe transitions in systems involving one or a few atoms where cooperative effects and nonclassical statistics such as antibunching and sub-Poissonian statistics can be studied.
  - Study of Influence of Radiation Fields on Atoms: Here we compare predictions of quantum and semi-classical theory and study radiation damping and frequency pulling in cavities.
  - Precise Measurements of Mass Ratios: Laser fluorescence mass spectroscopy developed by the Division could yield measurement of such ratios as $m_e/m_\gamma$, $m_e/m_p$ and $m_p/m_\gamma$, as well as g-factors.
  - Laser Cooling of Neutral Atoms: Cooling of neutral atoms can provide higher resolution in study of atoms in neutral beams. This is important for frequency and length standards.

- **Molecular Physics.** Spectroscopy is being performed with coherent radiation using tunable far-infrared (TuFIR) and laser magnetic resonance (LMR) systems. Both of these provide for highly accurate and very sensitive measurements of atomic and molecular spectral line frequencies as well as line shapes. Such measurements are important not only as secondary frequency and wavelength standards, but also in atmospheric physics and astrophysical research. The Division capability can be used to observe and characterize spectra of unusual and rare molecules, molecular ions and free radicals which heretofore have not been observable in the laboratory. The dependence of line shape (and width) on temperature and pressure, which can also be precisely determined in the laboratory, can facilitate remote sensing of important upper atmospheric molecules. Further develop-
ment of diode lasers will certainly support all of this work, and will result in unique opportunity for ultrasensitive spectroscopic detection of atoms and molecules providing for practical monitoring of important species.

- **Optical Physics.** Studies in optical physics revolve around the need to develop very narrow-line sources of radiation at a variety of frequencies (from the microwave to the visible) and to accurately measure optical frequencies. Laser studies involve gaseous lasers, dye lasers, solid-state lasers and diode lasers. The standard approach to measuring optical frequencies involves frequency multiplication which requires the development of an understanding of mixers such as Schottky diodes, metal-insulator-metal (MIM) diodes, nonlinear crystals, vacuum-tunneling diodes and, perhaps, superconducting (Josephson or quasiparticle) junctions composed of the new high-Tc superconductors. The study of the fundamental noise processes in lasers will also be important in this effort. Another approach to the problem of frequency synthesis involving synchrotron division offers the opportunity to study laser excitations of a single relativistic electron in a Penning trap. Still another approach to frequency division involves diode lasers and nonlinear optics.

Laser cooling and Doppler-free spectroscopy are traditionally categorized under optical physics and should be included, since they constitute major components of the Division program.

- **Plasma Physics.** Stored ion clouds of beryllium and magnesium (which are being studied as frequency standards) constitute very interesting nonneutral plasmas. These plasmas have distribution functions which are closely related to those for neutral plasmas. Under proper laser-cooling conditions, such plasmas become strongly coupled and can be liquid or solid. Important experiments to consider involve study of Bragg scattering, ion diffusion, phase transitions, Coulomb clusters, the classical limit of Wigner crystallization, and multispecies ion plasmas. Such studies are also relevant to the development of frequency standards since a full understanding of the dynamics of ions in these systems provides the basis for estimating systematic errors (primarily Doppler shifts) arising from ion motion.

- **Satellite Timing.** One of the primary limitations to accuracy of satellite time transfer is the uncertainty in signal propagation time which arises from variations in the index of refraction of the troposphere and in the electron density of the ionosphere. Knowing the stability of the reference clocks, one can gain understanding of these delays through the additional uncertainties which they add. Alternately, they can be studied by using several carrier frequencies. The multifrequency method is particularly interesting as it applies to precise geophysical (length) measurements both between ground stations and satellites and between separated ground stations. Another important area for study involves the magnitude and the stability of delays which can be attributed to system hardware or to interfering signals.

- **Time Series Analysis.** Over the last two decades, the Division has led the development of the statistical analysis of time-series data using the two-sample (Allan) variance. In a preliminary way, these techniques have been applied in other disciplines, e.g., standard volt cells and mechanical gage blocks. It appears that significant insight into the long-term stability of these systems can be gained through these methods. The more common use of the standard deviation is not always justified, particularly where the behavior of systems is observed over long periods (as is done with standards) where assumptions about stationarity are usually incorrect. To take advantage of time-series methods requires further development of the treatment of unequally spaced data. Furthermore, the ideas must be simplified if they are to be widely used. Additional work on the modified Allan variance could lead to a more accurate assessment of noise performance, since the conventional approach tends to yield distorted results in the presence of high frequency noise.

- **Optimal Use of Ensembles of Clocks.** The NIST time scales are based on an algorithm which intelligently combines the outputs of many clocks to arrive at a smooth time scale which is more stable and reliable than any of the constituent clocks. It is clear that further study and development of such algorithms can improve the robustness of the clock ensemble and yield even better ensemble performance. Research in this area is needed to support comparisons between earth-bound atomic clocks and the regular pulsations of millisecond pulsars. Such comparisons could ultimately result in the detection of gravitational waves.
MISSION

Through the Quantum Physics Division, NIST participates in the Joint Institute for Laboratory Astrophysics (JILA), a cooperative enterprise between NIST and the University of Colorado (CU). The Division conducts long-term, high-risk research in quantum physics and related areas in support of the Nation’s science and technology. The Division’s objectives include:

- developing the laser as a refined measurement tool and applying it to tests of fundamental physical postulates and to measurements of physical constants and properties;
- devising and applying measurement techniques to advance understanding of critical rates and pathways for important chemical species and processes;
- researching new techniques for measuring and interpreting interactions involving electrons, atoms and molecules in ionized and excited gases;
- improving the theory and instrumentation required for measurements in both the astrophysical and geophysical domains.

The Division accomplishes its mission by interacting with University faculty and visiting scientists to maintain expertise at the forefront of research in physics; by transferring the results of its research and the technology developed to the Nation’s industries and other government agencies; and by exchanging ideas and skills with other scientists in NIST and in industry through scholarly publications, visits, seminars, and exchanges of personnel.

ORGANIZATION

The 26 permanent senior scientists (“Fellows”) of JILA form a governing body that sets policy, subject to review by the Director of NIST and the President of CU. A biennially-elected Chairman, assisted by an executive committee, is responsible for operating the Institute within the policies set out by the Fellows. Of the 25 active Fellows, 15 are full-time faculty members in the Departments of Physics, Chemistry, or Astrophysical, Planetary and Atmospheric Sciences (APAS); ten are NIST employees (nine in the Quantum Physics Division and one in the Time and Frequency Division). Although these scientists work side by side, sharing facilities and responsibility for the success of the Institute, each remains officially responsible to his respective employer, NIST and its Director in one case, CU and the pertinent academic department in the other.

Through their adjoint faculty appointments, NIST scientists at JILA have both the opportunity and responsibility to participate in faculty activities and to supervise graduate students and postdoctorals. Seven of the NIST scientists are Lecturers or Adjoint Professors in Physics, two are Adjoint Professors in Chemistry, and one is an Adjoint Professor in APAS. JILA is currently home to 84 graduate students and 50 postdoctorals. The Institute has 49 administrative and technical support staff, 16 senior scientific staff, and ten Visiting Fellows. At the present time, 66 graduate students and postdoctorals are being supervised by NIST scientists. The JILA Visiting Fellows Program is probably the next most important factor in maintaining an atmosphere of change and scientific excitement in JILA. Each year it provides partial funding for some ten internationally distinguished scientists to spend up to twelve months at JILA collaborating with resident scientists. Applicants are chosen according to scholarly achievement, demonstrated interest in the scientific and technical objectives of JILA, and the recommendations of their peers. Since its inception 27 years ago, the Program has become internationally renowned and more than 260 senior scientists from the United States and 29 foreign countries have participated.

CURRENT DIRECTIONS

A direct outgrowth of the national space program in the early 1960s, JILA was formed in response to perceived serious gaps in our basic understanding of the physics of gaseous atmospheres (terrestrial, planetary, solar and stellar).
JILA has since responded to changing national needs and to the requirements of its parent organizations, and become a world leader not only in atomic and molecular science and astrophysics but also in precision measurement (including gravity and geophysics), laser and optical physics, and chemical physics. Recent new scientific thrusts include:

- **New Frequency Standards.** We are contributing to the development of new optical and microwave frequency standards based on an atomic "fountain", developing a compact and manageable phase-locked system linking the optical and microwave frequency domains, and devising more accurate and transportable optical frequency standards.

- **New measurement techniques.** We are developing laser-based and other advanced measurement techniques such as extremely sensitive interferometric and seismic isolation devices to measure key physical constants such as atomic mass and to support both ground- and space-based observations of gravitational waves from astrophysical sources.

- **Scanning Tunneling Microscopy.** We are exploiting the scanning tunneling microscope (STM) as a tool for studying, at the level of individual atomic sites, the changes in reactivity and morphology of surfaces bombarded by electrons and reactant particles, and investigating measurement techniques fundamental to the development of STM-based nano-fabrication.

- **New Techniques for Semiconductor Fabrication.** We are applying advanced laser techniques to the controlled vaporization of cryogenic films and refractory materials for the development of new semiconductor dry etching and deposition techniques, and developing new measurement tools for characterizing etching and deposition processes and products.

- **Excitation of Ions by Electrons.** We are developing new techniques for making absolute measurements of electron-ion excitation cross sections for multiply-ionized atoms, and for theoretical investigations of relativistic effects in the interaction of electrons with heavy atomic systems such as occur in fusion plasmas, planetary atmospheres, and high-power switches.

**HIGHLIGHTS**

- **Using White-Light to Produce a Monovelocity, Cooled Atomic Beam.** A high flux beam of cooled atoms would be very useful in a variety of experiments and applications, including high-resolution spectroscopy, collision measurements, and atomic interferometry. Hall's group has demonstrated the feasibility of a new technique for generating such a beam using "white light." A primary challenge in cooling an atomic beam by radiation pressure from a narrow band laser results from the fact that the inhomogeneous broadening (due to the thermal velocity distribution) is usually much larger than the natural linewidth of the atomic transition used for the cooling process. Thus there cannot be much cooling unless the atoms can be kept in resonance with the laser field throughout the cooling process. Two methods have been devised to compensate for this changing Doppler shift: frequency chirping and the use of a spatially varying magnetic field, but each has its own limitations. One suggested alternative that circumvents these limitations is to use light with a broad spectrum so that there is always some portion of the light spectrum resonant with the atoms. However, the use of only a broadband light beam, counterpropagating to the atomic beam, causes all the atoms to experience a velocity-dependent radiation force, leading to deceleration with no velocity compression. Hall's group has now overcome this obstacle by using sharply-filtered radio frequency electronic "noise" to modulate an optical beam to produce a window of optical frequency "white light." All of the vastly increased number of beam atoms (sodium was used) within this spectral window can now be captured into the cold atomic beam, a ten-fold improvement.

- **Laser Gravitational-Wave Observatory in Space.** Bender, Faller and collaborators have made substantial improvements in the last two years in the conceptual design for a laser gravitational-wave observatory in space (LAGOS). Laser heterodyne measurements will be used to determine changes in the arm-length difference for a Michelson interferometer with 10⁷ km arm lengths. Test masses freely floating inside four separate spacecraft in orbit around the L-5 point of the Earth-Sun system will support the end mirrors for the two arms of the interferometer. The gravitational wave frequencies of interest are from 10⁻⁵ to 1 Hz. Studies of expected gravitational wave signals due to binary star systems concluded that the power spectral density of signals due to different types of binary star systems will likely exceed the instrumental sensitivity for frequencies from roughly 10⁻⁵ to
$10^2$ Hz. Recent work on the conceptual design for the LAGOS antenna has concentrated on methods for meeting the present detailed error budgets for the spurious accelerations of the test masses and for the measurement of the separations between the test masses. The total error allowances are $1 \times 10^{15}$ m/sec$^2$/Hz for the sum of the accelerations of the test masses in the frequency range $2 \times 10^5$ to $1 \times 10^5$ Hz, and $4 \times 10^{11}$ m/VHz for the sum of the measurement errors for the difference in arm lengths at frequencies of $10^{-3}$ to 1 Hz. Bender and Faller substantially changed the design and layout of major components in each of the four spacecraft so as to minimize changes in the gravitational field component along the interferometer arm and in temperature gradients inside the spacecraft due to fluctuations in the power dissipated in the electronics and in the solar energy absorption by the solar cells.

- **Isolation Systems for Gravitational Wave Antennas.** The performance of ground-based gravitational wave antennas could be extended through improved seismic isolation. For example, the ground noise spectral amplitude, which increases toward lower frequency, is an important limitation on the low frequency performance in present interferometer designs. Extending the operating band down to 1 Hz through better vibration isolation would afford access to a band that may contain signals indicative of massive black hole formation or collisions near the time of galaxy formation. Bender and Faller are working to demonstrate that a two- or three-stage isolation system can be designed that will provide the necessary isolation without introducing too much thermal noise. During the past year they have developed a design for a preliminary six-degree-of-freedom isolation stage with an isolation factor of 100 from 1 to 100 Hz. A multistage system with an overall isolation factor of roughly $10^4$ at 1 Hz and $3 \times 10^7$ at 10 Hz appears to be needed in order to bring the vibrational noise at the support points of the test mass pendulums down to the desired level in low-frequency interferometric detectors similar to the 4 km arm length detectors in the Laser Interferometric Gravitational-Wave Observatory (LIGO) proposed jointly by Cal Tech and MIT. The required noise level is not well known, but is in the range of $10^{-15}$ to $10^{-14}$ m/VHz at 1 Hz for the common mode motion of the support points for the final isolation pendulums in a low-frequency gravitational wave detector. Each isolation stage needs to attenuate oscillations in all six degrees of freedom in order to avoid cross-coupling between the different types of motion. The preliminary stage is now under construction. It is large enough to support a vacuum system which can contain the two planned main isolation stages. The preliminary stage also can be used later as a shake table to test the performance of the two main stages.

- **Alignment Effects in Energy Transfer.** Energy transfer processes are important in a wide variety of environments, including lasers and discharge media, interstellar space, and the upper atmosphere. Several new results in this area have come out of the study of alignment effects on electronic energy transfer of Ca. In new experiments, Leone's group has measured the first alignment effects before and after the collision. One laser is used to populate an initially aligned p-orbital, and a second laser probes the alignment of the final p-orbital in the state-changing collision. The system studied is

$$\text{Ca}(4s5p \, ^1P_1) + \text{He} \rightarrow \text{Ca}(4s5p \, ^3P_2) + \text{He}.$$  

In this three-vector correlation experiment, it is possible to obtain both real population cross sections as well as "coherence" terms. The three vectors are the two laser polarizations and the relative velocity. The coherence terms provide new information about how the phase of an initially prepared superposition state is transferred to a final superposition state. The experiments have obtained all of the population cross sections and several of the coherence terms. Another single-collision experiment has led to the detection of a high degree of alignment in the energy transfer from translationally fast H atoms and H$_2$O. The H$_2$O molecules which are excited in their antisymmetric stretch mode by the 2.2 eV H atoms are also excited preferentially with rotational motion in the plane of the molecule. The dynamics are detected by measuring the $K_r$ and $K_q$ rotational substructure (in-plane vs. out-of-plane, respectively).

- **Energetic Barriers to Silicon Etching by High Kinetic Energy Chlorine Molecules.** Plasma etching of silicon is a complex process involving charged species, neutral molecules and radicals, and surface reactions. It is difficult to determine which reactions are central to the materials removal process and which are subsidiary. Recently, well-defined beams of translationally fast chlorine molecules were demonstrated by Leone's group using a laser vaporization technique. This method allows the chemistry of the etching process to be explored in much more
precise detail, and the results will provide an important new microscopic basis for understanding etching. Chlorine molecules are deposited onto a cold transparent substrate, and an intense pulsed laser is used to vaporize the film. The resulting superheated film evolves chlorine molecules with kinetic energies of 1-10 eV, energies which are sufficient to break the chemical bonds of atoms at the surface. The chlorine molecules impinge on a substrate of silicon in an ultrahigh vacuum region and silicon chloride products are detected with a mass spectrometer. With thermal chlorine emanating from an effusive beam, no detectable etching is observed, but at the increased kinetic energies of 2-6 eV, sustained etching is detected. In addition, when the kinetic energy is increased, the rate of etching also increases dramatically – by a factor of more than 30 over a thermal beam. By selecting out one velocity with a high speed slotted chopper, it will be possible to define precise energetic barriers for the etching process.

The figure shows a schematic of the apparatus; the laser pulses come in from the left and the beam and etching products are measured by the mass spectrometer. Similar work is also being carried out with a well-defined source of chlorine atoms. It was immediately observed that the etching behavior of chlorine atoms and molecules are fundamentally different.

- New Results from Infrared Laser Absorption Spectroscopy. The Nesbitt group has developed slit supersonic expansion technology to a point where direct laser absorption sensitivities of $10^4$ W/Hz in a 50 cm path length at a few degrees Kelvin and with sub-Doppler (30 MHz) resolution are now quite routine. This has permitted a detailed high resolution IR study of van der Waals complexes (Ar, Ne, He with hydrogen halides, water, methane, ammonia), and the physics of internally tunneling species such as in H$_2$ and H$_2$O containing complexes. From a theoretical perspective, the group is investigating the multidimensional quantum mechanical "tools" necessary to interpret such large amplitude motion, as well as developing new inversion methods for extracting multidimensional potential energy surfaces from spectroscopic data. This method has recently been pushed to obtain the first near-IR spectra of multiple complexes such as Ar$_3$HF (n = 2,3 and 4), which begin to probe systematically the transition to "solvated" chromophores. The figure shows typical results. The group is also studying the dynamics of hydrogen bonding such as in Lewis acid-base complexes (e.g., N$_2$, N$_2$O, CO, HX/DX, with HX/DX). Recently, they have been able to demonstrate that the hydrogen bond between OCO and HF is extremely "floppy", as expressed by a bending potential which changes by less than 5 cm$^{-1}$ over angular excursions of up to 75 degrees! By way of contrast, the hydrogen bonds in N$_2$HX/DX complexes appear to be up to 10 times "stiffer" in the bending potential. Such efforts require theoretical efforts into the quantum mechanics of "semi-rigid benders" and double internal rotors, which the group has been pursuing in parallel.

- First Results from New Technique for Electron-Ion Excitation Measurements. The combination of a merged-beams and an electron-energy-loss technique has permitted ground-breaking absolute measurements of a cross section for electron-impact excitation of a multiply-charged atomic ion. Dunn's group has demonstrated the power of this new technique involving the third ionic stage of silicon, but an entirely new spectrum of measurements has now been proven feasible. Highly charged atomic ions are pervasive and critical elements in high-temperature plasmas (fusion, astrophysical, laser, and others). Excitation of ions remains the most elusive of the electron-ion scattering processes as far as getting adequate number of experimental tests. People using theoretical approaches are calculating literally millions of such cross sections, and it remains a challenge to get experimental
verification of even select cases -- almost all past measurements involved singly-charged ions and a very restricted set of transitions for which fluorescence from excited states could be used as the detector. This new collisions technology, combined with the availability of abundant ions from advanced ion sources, permits greatly enhanced signals (merged rather than crossed beams) and detection efficiencies (all electrons involved rather than just some photons) compared with that attainable with traditional ion sources and crossed-beams collision geometries. A key element in the new technique is a real-time charged-particle beam probe that can be used both as a beam diagnostic and to quantitatively determine the beam density distribution in all three dimensions. The figure shows a schematic of the new device, including the beam probe near the interaction region where the electron and ion beams are merged.

- Atoms Trapped for High Accuracy Atomic Mass Measurements. A Penning ion trap has been constructed by Dunn’s group that employs a highly uniform and stable magnetic field and accurate electric fields so that one should in principle be able to make atomic mass measurements to parts in \(10^{10}\), and perhaps eventually to parts in \(10^{12}\). Masses with such accuracies play a role in possible determination of the neutrino mass, more accurate determination of Avogadro’s constant, physics and chemistry of isomers, and the possible adoption of a non-artifact mass standard. They have just recently succeeded in observing three ions with excellent signal to noise. The method involves cyclotron resonance of single ions in a cold (4K) ion trap. The basic method has recently been demonstrated at University of Washington and at MIT, though some differences exist with Dunn’s system. The latter Z motion side-band detection system utilizes a high Q (7500) resonant circuit with a low noise FET amplifier at 860 Khz. They have demonstrated trap ion Q’s of several million and have characterized various properties of the trap such as the anharmonicity, etc. They will next attempt to obtain preliminary mass comparisons at high resolution and then attack the problems that are showing up. Progress has been made toward changing the system so that arbitrary ions can be injected. One of the first ions that will be looked at when this is operational will be silicon, with an eye to the atomic mass standard. As things progress, they may look to moving the apparatus to Gaithersburg and injecting fully stripped ions from EBIT. There is an alternate possibility (remote, but finite) that the existing ECR ion source at Oak Ridge may be moved to JILA, in which case multiply charged ions could be injected without moving to Gaithersburg.

- Kinetics and Plasma Chemistry of Silane-Germane Glow Discharges Probed. Gallagher and his group have uncovered a wealth of new information that could lead to major improvements in deposition rate, large-area reliability, stability, and efficiency of inexpensive photovoltaic devices. Hydrogenated amorphous silicon (a-Si:H) is a leading contender for solar power generating systems as well as large-area photoconductors. Thin film transistors of a-Si:H are also being developed in many companies for display and reading devices. Thin films of hydrogenated amorphous silicon-germanium (a-SiGe:H) alloy have exciting potential for tandem-photovoltaics (those that combine the best features of silicon and germanium). The attraction arises from the continuous optical band-gap (between 1.2 and 1.8 eV) that can be provided, in principle, by simply changing the ratio of silicon to germanium in the composition. Radio frequency or dc discharge decomposition of silane-germane and disilane-germane mixtures are the currently preferred techniques for the deposition of these alloy films. Unfortunately, for reasons as yet unknown, the films formed seem to have electronic properties that are much inferior to those of the pure a-Si:H films. The explanation may lie in the complex plasma chemistry and kinetics involved in the deposition process, about which practical-
ly nothing is now known. In a mass spectrometric study of stable gas production and depletion in silane-germane and disilane-germane glow discharges, it was found that germane depletes about four times faster than silane, nearly independently of their relative initial fractions, and that germane is much more reactive than silane. Complimentary studies of the spatial distribution of reactive atoms and molecules using spatially resolved measurements of optical emission, and of deposition using measurements of film deposits on fiber probes, revealed that the discharge operates in a "hybrid" regime, and that ion effects are important near the electrodes.

- **Measurements of Deuterium in the Local Interstellar Medium.** How did the Universe begin? There are only a very few observable quantities with which to test the broad range of theoretical models concerning the origin of the Universe. For example, theories of how atomic nuclei were synthesized in the early universe are sensitive to the assumed primordial abundances of the simplest elements. One important test, therefore, is the ratio of deuterium, also called "heavy hydrogen," to ordinary hydrogen in primordial matter that has not been altered by nuclear processes occurring in the centers of stars. Linsky and collaborators have been carrying out observations with NASA’s Hubble Space Telescope (HST) to attempt to answer this question. They observed the nearby star Capella (the brightest star in the constellation Auriga) with the High Resolution Spectrometer on HST. The observation is of the brightest line of atomic hydrogen, called the Lyman alpha line, of the far ultraviolet spectrum near 121.6 nanometers. The figure shows the bright emission line emitted by the star and the absorption features produced by atomic hydrogen (the broad dark feature) and atomic deuterium (the narrow feature). These features are absorptions of stellar light due to interstellar gas in the line of sight to the star. These data are being analyzed to infer the abundance of deuterium relative to hydrogen in interstellar gas.
FUTURE DIRECTIONS
The following is a brief summary of some of the new problems and areas of research currently planned or underway in each of the Division’s four groups. The largest new effort in the next few years will be in furtherance of a Competence Proposal funded in 1991, championed by Dr. John Hall. The Division has advertised a position for an experimentalist to take a leadership role in this program.

- **Fundamental and Precision Measurements.** The goal of the Competence Program is, by exploiting laser, nonlinear optical, and rf electronic techniques, to achieve advances in the sensitivity of optical measurements well beyond that attainable within previously accepted "quantum" limits. Potential applications include enhanced detection sensitivity for trace materials, practical absolute optical power standards based entirely on quantum physics concepts, more secure communications, ultrasensitive wideband laser spectroscopy, precise manipulation of atoms and molecules, advanced optical and microwave frequency standards, spectacular advances in atomic clocks, and novel tests of fundamental physical principles.

- **Chemical Physics.** A new series of experiments will use IR laser direct absorption methods to probe the collisional alignment of molecular angular moments in supersonic jets. The approach is to use polarization modulation of a diode laser beam to sample the differential distribution of M projections in the laboratory frame via modulation of the absorption signal. In essence, these studies will measure the collisionally induced birefringence of molecules and probe the orientation dependence of state-to-state energy transfer cross sections. One long-term interest is in developing an intense source of oriented molecules for studying the steric influence on energy transfer and reactive collisions under molecular beam conditions.

- **Atomic and Molecular Collisions.** Detailed measurements have been made of resonant-excitation-double-autoionization (REDA) for electron impact on He-like ions C\textsuperscript{4+}, N\textsuperscript{5+}, and O\textsuperscript{6+} in the metastable triplet state. Such indirect processes can be very large for some ions, and it is important to understand them for simple systems such as these. The apparatus has been reconfigured for further ionization measurements on simple ions of fusion interest, and preliminary measurements have been made of the cross section for ionization of Cl\textsuperscript{+}. Edge plasmas of Tokamaks have ionization stages ranging from neutral to +9, and Cl is one of the elements found in the edge plasma. Work is currently under way for ionization of Si\textsuperscript{+} for which there is great interest.

- **Astrophysical Measurements.** The Division will continue to be a very active contributor to the development of new space experiments. Linsky is working with other astronomers on NASA Science Working Groups to design and oversee the development of three new astronomical instruments to fly on space satellites: the Space Telescope Imaging Spectrograph (STIS), an echelle spectrograph to cover the spectral region from the ultraviolet to the near infrared planned as a replacement instrument to be placed in the Hubble Space Telescope in 1997; the Advanced X-Ray Astronomical Facility (AXAF), intended to obtain high resolution x-ray images and spectra of astronomical sources; and the Far Ultraviolet Spectrograph Explorer (FUSE), scheduled for launch in 1999 to obtain high resolution spectra in the extreme and far ultraviolet spectral regions.
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reaction: O' + HF goes to F' + OH(v=0,1)," J. Chem. Phys. (in press).


Nelson, P.G. "An active vibration isolation system for inertial reference and precision


NOTE: Names in parentheses are authors who are not connected with JILA, NIST or CU. List does not include JILA publications by JILA CU Fellows and their associates.

*Entries with stars are those resulting from the work of JILA Visiting Fellows.
APPENDIX B

INVITED TALKS
LABORATORY OFFICE


ELECTRON AND OPTICAL PHYSICS DIVISION (841)


Pierce, D.T., "Introduction: The Importance of Magnetic Materials and Measurements to Cur-


ATOMIC PHYSICS DIVISION (842)


Gillaspy, J.D., "Tests of the Pauli exclusion principle and QED with high resolution laser spectroscopy," Purdue University, February 1991.


Kim, Y.-K., "Relativistic effects in atoms and molecules," Pohang Institute of Technology, Pohang, Korea, April 1991.


Mohr, P.J., "Recent progress in bound-state QED," Institute for Theoretical Atomic and Molecular Physics, Harvard University, June 1991.


Phillips, W., "Optical molasses, laser cooling and the coldest atoms ever," at the Notre Dame University, Notre Dame, IN.


Phillips, "Laser cooling of atomic beams," at the University of Sao Paulo, Sao Carlos, Brazil, August 1991.

Phillips, W., "Optical molasses," at the University of Sao Paulo, Sao Carlos, Brazil, August 1991.

Phillips, W., "New mechanisms for laser cooling," at the University of Sao Paulo, Sao Carlos, Brazil, August 1991.


Rolston, S., "Laser cooling and optical clocks," Towson State University, Towson, MD, April 1991.


Wiese, W.L., "Regularities in the widths and shifts of plasma-broadened lines," Jagellonian University, Krakow, and Pedagogical University, Opole, Poland, May 1991.


MOLECULAR PHYSICS DIVISION (843)


Fraser, G.T., "Inversion and Internal Rotation in Ar-NH₃", Symposium on Clusters and Cluster Ions," East Coast Regional Meeting of the American Chemical Society, January 1991.


Hellwell, E.J., "Vibrational Energy Transfer in Metal Carbonyl Systems, Department of Chemistry Seminar Series, University of California at Davis, November 1991.


King, D.S., "Fragment Energy and Vector Correlations in the Overtone Dissociation of HN_3," NATO Advanced Research Workshop on Dynamics of Stereochemistry, Santa Cruz, CA, November 1990.


King, D.S., "Surface State Mediated Photochemistry: Laser-Induced Desorption of NO from Si(111)," FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands, July 1991.

King, D.S., "Dissociation Dynamics of Vibrationally Excited van der Waals Dimers," Southeastern Regional Meeting of the American Chemical Society, Richmond, VA, November 1991.


Suenram, R.D., "Using van der Waals Complexes to Investigate Reaction Mechanisms," Department of Chemistry, Wesleyan University, Middletown, CT, October 1991.
RADIOMETRIC PHYSICS DIVISION (844)
Asmail, C.C., "BRDF," 1991 MODIL 9th Industrial Briefing, NIST, Gaithersburg, MD, April 30-May 1, 1991.


QUANTUM METROLOGY DIVISION (845)

Danos, M., "Quantum Field Theory" Colloquium at the University of Chicago, Feb. 4, 1991.

Danos, M., "Consistent Quantum Field Theory," at the University of Texas, Math Department Colloquium, May 17, 1991.


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IONIZING RADIATION DIVISION (846)


Hutchinson, J.M.R., "NIST Large Area Alpha-Particle Calibration Systems," Radiac Working Group Conference, Naval Electronics Systems


McLaughlin, W.L., "Chemical Dosimetry" Short Course on Radiation Dosimetry, University of Maryland, College Park, MD, October 1991.


TIME AND FREQUENCY DIVISION (847)


Hollberg, L.W., "Diode Lasers and Precision Measurements," Lebedev University, Moscow, USSR, November 1991.


Itano, W.M., "Quantum Zeno Effect," Workshop in honor of ECG Sudarshans Contributions to Theoretical Physics, University of Texas, Austin, TX, September 1991.


Wineland, D.J., "Experiments on Laser Cooled Ions," University of Sao Carlos, Sao Carlos, Brazil, August 1991.


QUANTUM PHYSICS DIVISION (848)


Dunn, G.H., "Compound state effects in ion-neutral and ion-electron collisions," Colloquium Physics Department, University of Colorado, Boulder, September 1991.

Dunn, G.H., "Research briefing on selected opportunities in atomic, molecular and optical sciences," delivered at Directorate of Mathematical and Physical Sciences, National Science Foundation, June 1991.

Dunn, G.H., "Research briefing on selected opportunities in atomic, molecular and optical sciences," delivered at Office of Naval Research, June 1991.


Faller, J.E., "Fifth force physics and the gravity of spinning tops," George Mason University, April 1991.

Faller, J.E., "Fifth force physics and the gravity of spinning tops," University of Santa Barbara, La Jolla, CA, April 1991.


Faller, J.E., "Fifth force and little 'g'," Ohio State University, Columbus, OH, February 1991.


Linsky, J.L., "Scientific rationale and present implementation strategy for the Far Ultraviolet Spectrograph Explorer (FUSE)," International Workshop on Space Projects to probe the internal structure and magnetic activity of the Sun and Sun-like stars, Catania, Italy, November 1991.


Linsky, J.L., "Why do magnetic B- and A-type stars have radio emission properties similar to stars with convective envelopes?" National Radio Astronomy Observatory, Socorro, NM, January 1991.


Nesbitt, D.J., "IR Laser studies of mode selective energy transfer dynamics i fragile molecules," Department of Chemistry, Tel-Aviv University, Tel Aviv, Israel, May 1991.


Nesbitt, D.J., "Investigating the forces between molecules" High resolution spectroscopy and dynamics of weakly bound and hydrogen bond-


APPENDIX C

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP
TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

LABORATORY OFFICE

Wayne A. Cassatt
Chairman, Subcommittee on “Nuclear Data Needs of the 1990’s”, national Nuclear Science Advisory Committee to DoE and NSF.

Chris E. Kuyatt
Member, Advisory Panel to International Organization for Standardization (ISO) TC 12: Quantities, Units, Symbols, Conversion Factors.
Member, Council for Optical Radiation Measurements (CORM).
Chairman, NIST Washington Editorial Review Board.
Chairman, NIST Radiation Safety Committee.
Member, Board of Editors, NIST Journal of Research.
Member, NIST Calibrations Advisory Group.

William R. Ott
Member, Panel on Optics Technology Applications for the SDIO Technology Applications Office.
DoD Liaison, SDI-Related Metrology at NIST.
NIST Liaison, Society of Photo-Optical Instrumentation Engineers (SPIE).
Member, Program Committee for SPIE Conference, Ultraviolet Technology IV, July 1992.

Member, DoC Interagency Committee on Classification Reform.
Member, total quality management (TQM) team reviewing operations of the Planning and Engineering Office of the NIST Plant Division.
Member, interagency committee advising the DoC Director of Personnel on personnel classification reform.
Consultant to staff at the Office of Personnel Management on issues concerning classification reform and personnel management.

Barry N. Taylor
Consultative Committee on Electricity and Consultative Committee on Units of the International Committee for Weights and Measures (CIPM).
Chair, American Physical Society Topical Group on Fundamental Constants and Precise Tests of Physical Laws.
CODATA Task Group on Fundamental Constants.
NIST Representative, Comptroller, and member of the Executive Committee of the Conference on Precision Electromagnetic Measurements (CPEM).
Board of Editors, Metrologia.
Technical Advisor to the U.S. National Committee of the International Electrotechnical Commission (IEC) on Technical Committee (TC) 25 Matters (TC 25: Quantities and Units and Their Letter Symbols), and member of TC 25, Working Group (WG) 1, Advisory and Preparatory.
U.S. Technical Advisory Group (TAG) for International Organization for Standardization (ISO)/ TC 12, Quantities, Units, Symbols, Conversion Factors, and International Advisory Panel to TC 12.

NIST/CODATA liaison to the National Academy of Sciences/National Research Council Advisory Committee on Fundamental Constants and Standards.

Advisory Committee to the Particle Data Group, Lawrence Berkeley Laboratory.

Institute of Electrical and Electronics Engineers (IEEE) Standards Coordinating Committee 14, Quantities, Units and Letter Symbols.

Subcommittee on Standards and Metric Practice of the Metrification Operating Committee of the Interagency Committee on Metric Policy.

American Society for Testing and Materials Committee E-43 on SI Practice.
ELECTRON AND OPTICAL PHYSICS DIVISION (841)

Charles W. Clark
Member, Executive Committee, Division of Atomic, Molecular, and Optical Physics, American Physical Society.
Member, Collaborative Computational Project 2: Continuum States of Atoms and Molecules, Science and Engineering Research Council (UK).
Chairman, National Academy of Sciences/National Research Council Committee on Line Spectra of the Elements - Atomic Spectroscopy.

Robert J. Celotta
Member, American Physical Society - Davisson-Germer Prize Committee.

David L. Ederer
Member, Executive User Committee of the Advanced Light Source, Berkeley, CA.
Member, User Proposal Review Committee, National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY.

Lanny R. Hughey
Member, Design Review Board for Title II Vacuum Design of the 6 GeV Electron Storage Ring (APS), Argonne National Laboratory, Argonne, IL.
Member, Planning Committee for the Second Topical Conference on Vacuum Design of Synchrotron Light Source, Argonne National Laboratory, Argonne, IL.
Member, Stage Three Vacuum Design Review Board for the APS Storage Ring and Associated Accelerators at Argonne National Laboratory.

Michael H. Kelley
Cooperating U.S. Scientist for Joint NIST-Yugoslovakian Project (JFP-598) entitled "Electron Impact Cross-Sections for Atomic Particles."

Paul Lett
Member, NASA Preliminary Design Review Committee for Project "Sunlite", NASA Langley Research Center, Langley, VA.

Robert P. Madden
Member, Optical Society of America Nominating Committee.
Member, Advisory Program Committee for the 75th Annual Meeting of the Optical Society of America.
Member, Council of U.S. Synchrotron Radiation Laboratory Directors.
Member, International Committee of the International Conference on X-Ray and VUV Synchrotron Radiation Instrumentation.
Member, DARPA Advisory Committee for Oversight of the Development of a Synchrotron Source for Lithography.
Member, NSLS Program Advisory Committee, Brookhaven National Laboratories.
Member, Advisory Committee for the U.S. National Synchrotron Radiation Instrumentation Conference.

Jabez J. McClelland
Member of the International Organizing Committee of the Polarization and Correlation Conference, Adelaide, Australia, July 18, 1991.

Daniel T. Pierce
Program Committee, 34th Conference on Magnetics and Magnetic Materials.
Mark D. Stiles
President, Greater Washington Solid State Physics Colloquium Steering Committee.

Richard N. Watts
ATOMIC PHYSICS DIVISION (842)

Daniel E. Kelleher
Member, International Program Committee, International Conference on Spectral Line Shapes.

Yong-Ki Kim
Member, Report Committee on Secondary Electron Production by Electron-Impact, "International Commission on Radiation Units."

William C. Martin
Member, IAEA Network of Atomic Data Centers for Fusion.

Peter J. Mohr
Member, International Program Committee, Nobel Symposium on "Heavy-Ion Spectroscopy and QED Effects in Atomic Systems," to be held in 1992.

William D. Phillips
Member, Steering Committee, Laser Science Topical Group of the American Physical Society.
Vice Chair, 1991 Gordon Conference on Atomic Physics and is the 1993 Chair.
Chair, Optical Physics Group of the Optical Society of America.

James R. Roberts
Member, National Research Council, National Academy of Science, Panel on Plasma Processing of Materials.

Arlene Robey

Jack Sugar
Chairman of the Organizing Committee, 4th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas.

Wolfgang L. Wiese
Member of Organizing Committee, International Astronomical Union, Commission on Atomic and Molecular Data.
President, Commission on Atomic and Molecular Data, International Astronomical Union.
Member, Network of Atomic Data Centers for Fusion, coordinated by the International Atomic Energy Agency (IAEA).
Member, Organizing Committee, 4th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas. □
MOLECULAR PHYSICS DIVISION (843)

Edwin J. Heilweil
Discussion Leader, KAST International Workshop, Kinagawa Academy of Science and Technology, Kawasaki, Japan, June 10-12, 1991.

Jon T. Hougen

Marilyn E. Jacox
Member, AFOSR High Energy Density Materials Panel.
Chairman, Award Recognition Committee, NIST Chapter of Sigma Xi.

Paul S. Julienne
Member, International Committee of the International Conference on the Physics of Electron and Atomic Collisions.

Frank J. Lovas
Member, Working Group 5 (Molecular Spectra), Commission 14: Fundamental Spectroscopic Data, International Astronomical Union.

Alfons Weber
Member, 1991 Lippincott Award Committee (Optical Society of America, Coblentz Society, and Society for Applied Spectroscopy).
Member, Council of the American Physical Society.
Chairman, Audit Committee, American Physical Society.
Member, Membership Committee, American Physical Society.

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RADIOMETRIC PHYSICS DIVISION (844)

Clara Asmail
Member, ASTM E-12.09, Scattering.

Yvonne Barnes
Member, ASTM E-12 Committee, Appearance of Materials, Subcommittees E-12.01 on Editorial and Terminology, E12.02 on Spectrophotometry and Colorimetry, E-12.03 on Geometric Properties.

Kenneth L. Eckerle
Member, ASTM E-13 Committee on Molecular Spectroscopy, Subcommittees E-13.01 on Ultraviolet and Visible Spectroscopy, E-13.03 on Infrared Spectroscopy, E-13.06 on Molecular Luminescence.

Laurance E. Fink
NIST Representative, ANSI IT2 on Image Evaluation and IT2.28 on Densitometry Standards.

Charles E. Gibson
Member, ASTM E-19 Committee, Temperature Measurements, Subcommittee E-20.2 on Radiation Thermometry.

Jonathan E. Hardis
Member, U.S. National Committee of the CIE.

Jack J. Hsia
Associate Director, CIE Division 2, Physical Measurement of Light and Radiation.

Secretary, U.S. National Committee of the CIE.

Member, ASTM E-12 Committee, Appearance of Materials, Subcommittees E-12.01 on Editorial and Terminology, E-12.02 on Spectrophotometry and Colorimetry, E-12.03 Geometric Properties, E-12.09 on Scattering.

Member, ASTM E-13 Committee, Molecular Spectroscopy; Subcommittees E-13.01, Ultraviolet and Visible Spectroscopy; E-13.03, Infrared Spectroscopy, and E-13.06, Molecular Luminescence.

Delegate, Inter Society Color Council.

NIST Alternate Representative, ANSI IT2 on Image Evaluation and IT2.28 on Densitometry Standards.

John K. Jackson
Member, CORM Radiometry Subcommittee CR-1.

Klaus D. Mielenz
President, U.S. National Committee of the CIE.

Director, CIE Division 2, Physical Measurement of Light and Radiation.

Member, ASTM E-13 Committee, Molecular Spectroscopy; Subcommittee E-13.06, Molecular Luminescence.

Member, IES Subcommittee CO12, Nomenclature.

Ex officio member, CORM Board of Directors.

Member, OSA International Affairs Committee.

Member, Advisory Board, Munsell Color Science Laboratory, Rochester Institute of Technology.

Albert Parr
CORM Radiometry Subcommittee CR2 on Radiometric Lamp Availability.

CIE Division 2 Reporter, "Application of Cryogenic Radiometry."

NIST representative to CCPR and Subcommittees on UV Standards and Radiometric Lamp Availability.

Ex Officio Member CORM Board of Directors.

Robert D. Saunders, Jr.
Member, ANSI Z311, Photobiological Safety of Lamps and Lighting Systems.

Member, CIE TC2-05, Definition and Measurement of Distribution Temperature.
Alternate, ASTM E-20, Temperature Measurements.
Alternate, ASTM E-44, Solar Energy Conversion.
Member, USNC/CIE.
Member, USDA Steering Committee for UV-B Measurements.

E. Ambler Thompson
Member, IES Photobiology Committee.
Member, ASTM E13.06 on Molecular Luminescence.

James H. Walker
Member, CORM Radiometry Subcommittee CR-1.
QUANTUM METROLOGY DIVISION (845)

Paul L. Cowan
General User Oversight Committee, National Synchrotron Light Source.

Richard D. Deslattes
Member, Executive Committee of the PRT/IDT Council for the National Synchrotron Light Source.

Completed tenure as Chairman, University of Chicago Review Committee for Physics Division, Argonne National Laboratory.

Member, organizing committee, International Nuclear Physics Conference, Wiesbaden, Germany, July 26 - August 1, 1992.


Member evaluation panel, Texas Higher Education Board for proposals in Physics, Astronomy and (portions of) Engineering.

Member, selection committee for SBIR proposals, NSF Physics Division.

Chairman, Nominating Committee, APS Topical Group on Fundamental Constants and Precision Tests of Physical Theory.
IONIZING RADIATION DIVISION (846)

Jacqueline M. Calhoun

Member, Subcommittee U. S. Council for Energy Awareness (USCEA)/NIST Measurement Assurance Program for the Nuclear Power Industry.

Member, Subcommittee USCEA/NIST Measurement Assurance Program for the Nuclear Medical Industry.

Co-Chair, Publicity Committee of the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE).

Member, National Institute of Standards and Technology, Day Care Scholarship Committee.

Member, National Institute of Standards and Technology Handicap Committee.

Allan D. Carlson

Chairman, Standards Subcommittee, Cross Section Evaluation Working Group (CSEWG), National Data Center.

Member, Evaluation Committee of CSEWG.

Chairman, Nuclear Energy Agency Nuclear Data Committee (NEANDC)

Working Group on the $^{10}\text{B}(n,\alpha)$ Cross Section Standard.

Randall S. Caswell

Chairman, Science Panel, Committee on Interagency Radiation Research and Policy Coordination (CIRRPC), Office of Science and Technology Policy.

Alternate Member, Main Committee, CIRRPC.

Honorary Member, National Council on Radiation Protection and Measurements (NCRP).

Member and Secretary, ICRU.

Sponsor, ICRU Report Committee on Stopping Power for Protons and Alpha Particles.

Sponsor, ICRU Report Committee on Stopping Power for Heavy Ions.

Sponsor, ICRU Report Committee on Absorbed Dose Standards for Photon Irradiation and Their Dissemination.

Sponsor, ICRU Report Committee on In-Situ Gamma-Ray Spectrometry in the Environment.

Sponsor, ICRU Report Committee on Beta-Ray Dosimetry for Radiation Protection.

Member, Department of Energy Site Visit team to Environmental Measurements Laboratory, New York, NY (May 1991).

Ronald Collé

Member, Radon Working Group, Interagency Committee on Indoor Air Quality.

Louis Costrell

Chairman, National Instrumentation Methods Committee.

Chairman, American National Standards Institute (ANSI) Committee N42, Radiation Instrumentation.

Member, ANSI Nuclear Standards Board.

Member, ANSI Nuclear Standards Board Planning Committee.

Secretary, Institute of Electrical and Electronic Engineers (IEEE) Nuclear Instrumentation and Detectors Committee.

Ex-Officio Member, IEEE Nuclear and Plasma Sciences Society Administrative Committee.

Chairman, IEEE Nuclear and Plasma Sciences Annual Meetings Committee.

Member, Organizing Committee, 1991 IEEE Particle Accelerator Conference.

Member, U.S. National Committee of the International Electrotechnical Commission (IEC).

Chief U.S. Delegate, IEC Committee TC45, Nuclear Instrumentation.

Chairman, IEC Committee TC45 Working Group 9, Detectors.
APPENDIX C: COMMITTEE PARTICIPATION & LEADERSHIP

Bert M. Coursey
Chairman, International Committee for Radionuclide Metrology (ICRM) Applications in Radionuclide Metrology Working Group.
Member, ANSI Committee N42.02 on Nuclear Instruments, Procedural Standards for Calibration of Detectors for Radioactive Measurements.
Alternate Member, Science Panel, CIRRPC.
Member, Task Group 3, Accredited Dosimetry Calibration Laboratories, American Association of Physicists in Medicine (AAPM).
Delegate to Section I, Consultative Committee for Ionizing Radiations (CCEMRI), Conférence Générale des Poids et Mesures, Paris, France.

Marc F. Desrosiers
Member, IAEA Coordinated Research Program on Alanine Dosimetry at the Radiation Therapy Level.
Program Chairman, Washington Electron Paramagnetic Resonance (EPR) Discussion Group.

Charles E. Dick
Member, Technical Organizing Committee, Industrial Applications, International Conference on the Applications in Research and Industry.
Member, Editorial Review Board of Industrial Metrology.

Charles M. Eisenhauer
Member, CIRRPC Science Panel; Chairman, Subpanel on Predisaster Planning for Human Health Effects Research.
Member, Working Group 2, Reference Radiations Subcommittee 2, Technical Committee 5, International Standards Organization.

David M. Gilliam
Delegate, CCEMRI Section on Neutron Measurements (Section III), Conférence Générale des Poids et Mesures, Paris, France.

NIST Representative, National Council on Radiation Protection and Measurements (ICRM).

Geoffrey L. Greene
Member, National Steering Committee for the Advanced Neutron Source (1986-present).
Program Committee for the Moriond Workshop on Tests of Fundamental Laws in Physics.

James A. Grundl
Member, NCRP Task Group SC-63 on Public Knowledge About Radiation Emergencies.
Member, CIRRPC Science Panel, Subpanel on Public Education.

Dale D. Hoppes
Member, International Committee for Radionuclide Metrology (ICRM).
Member, ICRM Beta- and Gamma-Ray Spectrometry Working Group.
Member, USCEA-NIST Standards Program Committee.
Chairman, International Committee of Weights and Measures (BIPM), Consultative Committee on Standards for Measuring Ionizing Radiations, Subcommittee Section II: Radionuclide Measurements.
Member, ANSI Subcommittee N42.2 on Procedural Standards for Calibration of Detectors for Radioactive Materials.

Jimmy C. Humphreys
Co-Chairman, American Society for Testing and Materials (ASTM) E10.01 Subcommittee (Radiation Processing Dosimetry) task group developing a standard on "Statement of Uncertainties in Radiation Dosimetry."

J. M. Robin Hutchinson
Chairman, Ad hoc ICRM Committee to draft "Guidelines for International Acceptances of Radioactivity Calibration Sources."
Secretary, ANSI N42.2, Radioactivity Measurements.
Kenneth G. W. Inn
Member, ANSI N42.02, Quality Assurance for Radiochemistry Laboratories.
Member, ASTM Committee C26.05.01, Methods for Test, Environmental Methods.
Member, ASTM Committee D19, Water, Radioactivity Test Methods.

Emmert D. McGarry
Member, ASTM Committee E10; Subcommittee E10.05, Nuclear Metrology.
Chairman, Awards Committee of ASTM Subcommittee E10.05.
Member, Planning Committee for the 9th ASTM-EURATOM Symposium on Reactor Dosimetry.

William L. McLaughlin
Technical Advisor, Council of Europe Parliamentary Assembly, Work Group on Aerospace Physiology, Medicine, and Radiation Measurement.
Technical Advisor, Council of Europe Parliamentary Assembly, Work Group on Space Biophysics.
Member, R & D Associates Committee on Irradiated Food Products.
Member, IAEA Advisory Group on High Dose Measurement and Standardization for Radiation Processing.
Member, AAMI Subcommittee on Radiation Sterilization Dosimetry (Working Groups on Gamma Ray Sterilization and Electron Beam Sterilization).
Technical Advisor, NCRP Scientific Committee 63, Radiation Exposure Control in a Nuclear Emergency.
Chairman, IAEA Advisory Panel on Electron Beam Dosimetry for Industrial Radiation Processing.
Member, IAEA Advisory Panel on Guidelines on Dosimetry for Industrial Radiation Processing.
Member of Organizing Committee and Chairman for Invited Speakers for 2nd International Workshop on Dosimetry for Radiation Processing.

Francis J. Schima
Research Associate Member, IAEA, Coordinated Research Program on Gamma-ray Standards for Detector Efficiency Calibration.
Member, ICRM Working Group on Gamma and Beta-ray Spectrometry.

Roald A. Schrack
Department of Commerce Representative to Environmental Protection Agency Interagency Working Group on Residual Radioactivity of Federal Installations.

Robert B. Schwartz
Member, ICRU Report Committee on Practical Determination of Dose Equivalent.
Member, Health Physics Society Standards Committee, The Selection and Use of Neutron Radiation Instruments for Dose Equivalent Determination.

Stephen M. Seltzer
Member, ICRU Report Committee on Stopping Power.
Consultant, ICRU Report Committee on Material Equivalent and Tissue Substitutes.
Participant, IAEA Coordinated Research Program on Atomic and Molecular Data for Radiotherapy.
Consultant, Lawrence Livermore National Laboratory, to provide electron and positron interaction data for the LLNL Evaluated Nuclear Data Library (ENDL).

Christopher G. Soares

Member, Health Physics Scientific Subcommittee Work Group for the revision of ANSI N545, "Performance, testing, and procedural specifications for thermoluminescence dosimetry (environmental applications)" and the writing of ANSI N13.29, "Criteria for testing environmental dosimetry performance."

U.S. Technical expert appointed by ANSI to the ISO sub-group (TC 85/2/2/0) for the revision of ISO 6980, "Reference beta radiations for calibrating dosimeters and doseratemeters and for determining their response as a function of beta radiation energy."

Julian H. Sparrow

Marlon L. Walker
Chairman, President's Committee on New Directions and Plans for NOBCChE.
Member, NOBCChE.
Member, National Society of Black Physicists.

Michael P. Unterweger
Member, ASTM Committee D022 on Sampling and Analysis of Atmospheres.

Oren A. Wasson
Member, DoE Nuclear Data Committee.
TIME AND FREQUENCY DIVISION (847)

David W. Allan
Member of U.S. Study Group 7A, Consultative Committee on International Radio
Member of Commission A on Time and Frequency, URSI.
Member of Consultative Committee on the Definition of the Second.

Roger E. Beehler
Chairman of U.S. Study Group 7A, Consultative Committee on International Radio

James L. Jespersen
Chairman of Timing Committee, InterRange Instrumentation Group (IRIG).
Member of Telecommunication Subcommittee on Time and Synchronization (T1X1.3).

George Kamas
Measurement Assurance Subcommittee, National Conference of Standards Laboratories.

Judah Levine
Member of NIST Research Advisory Committee.

Donald B. Sullivan
Member of Commission A on Time and Frequency, URSI.
Executive Committee for the Conference on Precision Electromagnetic Measurements.
Executive Committee for the Annual Symposium on Frequency Control.

David J. Wineland
NIST Precision Measurement Grants Committee, 1978 - present.


QUANTUM PHYSICS DIVISION (848)

P. L. Bender
Member, NASA Management and Operations Working Group for UV and Optical Astronomy and Relativity.

Member, Interferometry Panel, Astronomy and Astrophysics Survey, National Research Council.

Member, Control Structure Interaction Program Advisory Committee, NASA.

Member, Lunar Laser Ranging Management and Operations Working Group.

Member, Crustal Dynamics Working Group, NASA.

G. H. Dunn
Member, Executive Committee of DAMOP.

Chairperson, Committee on Atomic, Molecular and Optical Sciences (CAMOS) of the National Research Council.

Chairperson, Prize Selection Committee for Davisson-Germer Prize of the American Physical Society.

Chairperson, DOE Subpanel for Low Energy Scattering of Committee to Assess Future Opportunities in Atomic, Molecular and Optical Physics.

Member, Advisory Committee for Physics Subcommittee on National Needs in Atomic, Molecular and Optical Physics of National Science Board.

Chairperson, Program Review Panel for Atomic Physics at Lawrence Berkeley Laboratory.

Member, Fellowship Committee of DAMOP.

Co-chairperson, panel on Future Opportunities in Atomic Molecular and Optical Sciences of the National Research Council.

J. E. Faller

Member, Working Group II of the International Gravity Commission.


Member, Directing Board of IGC (International Gravity Commission).

J. L. Hall
Delegate, Consultative Committee for the Definition of the Meter (BIPM), Sèvres, France.

Chairman, International Steering Committee for Conferences on Laser Spectroscopy.

Member, NIST Committee for Precision Measurement Grants.

Member, Program subcommittee, QELS 91 and 92 Conferences, American Physical Society and Optical Society of America.

Member, AMO Subcommittee of Physics Division, Academy of Science.

D. G. Hummer
Co-Director, International Stellar Opacity Project.

Director, IRON Project for Large Scale Computation of Electron Excitation Cross Sections of Atoms and Ions.

S. R. Leone
Program Committee, Division of Atomic, Molecular and Optical Physics, American Physics Society.

Nominating Committee, Division of Atomic, Molecular and Optical Physics, American Physical Society.

Steering Committee, Laser Science Topical Group, American Physical Society.

J. L. Linsky
Member, User’s Committee, International Ultraviolet Explorer Satellite.

Member, Lyman Far Ultraviolet Spectrograph Explorer Phase B Science Team.

Member, NASA Peer Review Panel for the Phase C/D Proposals for scientific instruments
on the Advanced X-ray Astrophysics Facility (AXAF).

Member, Science Advisory Council, Mount Wilson Institute.

Member, Astrophysics Council, NASA.

Member, IUE Long Range Planning Committee.

Chairman, Steering Committee, Synoptic High Resolution Spectroscopic Observing Group.

Chairman, Management Operations Working Group, Science Operations Branch, NASA.

Chairman, US Scientific and Technical Working Group for the Large Earth-Based Solar Telescope (LEST), High Altitude Observatory, NCAR.

Chairman, Final Archives Definition Committee for the IUE Satellite Data, NASA.

Member, Review Panel for the Solar Physics Program at the NASA Goddard Space Flight Center.

Member, Policy Panel of the Astronomy and Astrophysics Survey Committee.

Member, UV/Optical From Space Panel of the Astronomy and Astrophysics Survey Committee.

Member, Status of the Professional Panel of the Astronomy and Astrophysics Survey Committee.

Member, Computing and Data Processing Panel of the Astronomy and Astrophysics Survey Committee.

Member, Scientific Organizing Committee for the International Astronomical Union Joint Commission Meeting on "Solar and Stellar Coronae," Buenos Aires, Argentina.

Member, Observatories Visiting Committee, Association of Universities for Research in Astronomy (AURA).

Member, Scientific Organizing Committee for the Seventh Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun, Tucson, AZ.

Member, COSPAR Commission E that plans astrophysics workshops at COSPAR meetings.

D. J. Nesbitt

Member, Organizing Subcommittee, International Quantum Electronics Conference (IQEC) '88, "Fundamental Laser Spectroscopy and Physics."

Member, Organizing Committee, International Laser Spectroscopy (ILS) Conference.

D. W. Norcross

Secretary, TAMOC, an informal group representing scientists in the theoretical atomic and optical physics community.
APPENDIX D

SPONSORED WORKSHOPS, CONFERENCES, AND SYMPOSIA
LABORATORY OFFICE

W. R. Ott organized and chaired a two-day DoD/SDI program review of NIST advanced metrology projects, November 1991.

W. R. Ott was a co-host at NIST of a two-day SDIO workshop, the 9th Optics MODIL (Manufacturing Operations Development and Integration Laboratory) Industrial Briefing, April 1991.

ELECTRON AND OPTICAL PHYSICS DIVISION (841)


ATOMIC PHYSICS DIVISION (842)

W. D. Phillips was Co-director of an Enrico Fermi Summer School/NATO Advanced Study Institute on "Laser manipulation of atoms and ions." The summer school was held in Varenna, Italy July 9-19, 1991, and was attended by over 100 students from Europe, North and South America, Asia and Africa. Lectures and seminars were given by leading researchers in the field, including two Nobel laureates. The published notes of these lectures should constitute a landmark text on the subject.

MOLECULAR PHYSICS DIVISION (843)

E.J. Hellwell organized the "Vibrational Relaxation Processes in Molecules and Liquids Symposium," December 8, 1991, at the Annual Optical Society Meeting in San Jose, CA. The symposium was attended by about 40 persons interested in ultrafast laser and nonlinear spectroscopy of molecules, liquid crystals, and related systems.

D.S. King was Vice-Chairman of the XII International Conference on Molecular Energy Transfer, held in Nijmegen, The Netherlands under the sponsorship of the European Science Foundation. Attended by about 100 scientists from industry, government, and academic labs from five continents, this conference dealt with issues of molecular physics that will influence major experimental and theoretical research efforts over the next two years.

IONIZING RADIATION DIVISION (846)

B.M. Coursey organized a workshop cosponsored by the US Nuclear Regulatory Commission, "Workshop on the Standardization of 192 Ir High-Dose-Rate Brachytherapy Sources," to examine the calibration issues for the high-dose-rate (HDR) iridium-192 radioactive sources used in cancer therapy. The 30 invited participants represented three national standards laboratories, three federal agencies and a number of industrial and university research facilities.

J.M.R. Hutchinson co-organized the "ICRM Symposium on Low-level Measuring Techniques and Alpha-Particle Spectrometry," June 4-7, 1991 in Monaco. The Symposium was attended by 85 participants representing laboratories world-wide. It included sessions on radon, quality control and standards, sampling, software, techniques for long-lived radionuclides, alpha-particles, spectrometry, and applications.

W.L. McLaughlin served on the Organizing Committee, "4th Annual Sterilization Technology and Regulatory Symposium," held in Snow Mass, Colorado, March 5-8, 1991. Twelve executive representatives from major medical device manufacturers attended and were briefed on the use of radiation measurement and materials engineering necessary for meeting regulation requirements by the Bureau of Devices of the Food and Drug Administration (FDA). The main goal of the symposium was to help industry achieve more effective measurement quality assurance through measurement services and by traceability to NIST standards.
W.L. McLaughlin served on the Organizing Committee for the "Stabilization of Polymers and Organic Materials in Radiation Fields Symposium," University of Maryland, College Park, Maryland, July 15-19, 1991. There were 36 participants from 14 countries, who discussed the science and technology of radiation resistance of polymers, elastomers, composites, aircraft and reactor components, and methods for enhancing these properties. The result of the meeting was an IAEA Technical Report for member states, which will be used to advance this technology of space, medical, biomedical, industrial, and agricultural applications of organic materials that are used in radiation measurements.

W.L. McLaughlin and J.C. Humphreys served as instructors for the "Short Course on Radiation Dosimetry," University of Maryland, October 4-5, 1991. Approximately 50 students from health care and materials processing industries attended as paying students. This was an intensive course for practitioners in radiation measurements for diverse industrial applications, and it included two afternoon laboratory exercise sessions. The students were primarily technologists responsible for quality control in radiation processing industries. Such industries sterilize medical devices, process foods for shelf-life extension and pest control, manufacture specialty polymers, elastomers, composite films and insulation materials.

W.L. McLaughlin served as Chairman and member of the Organizing Committee for invited speakers and Workshop Coordinator for the 2nd International Workshop on "Dosimetry for Radiation Processing," held at the University of Maryland, October 6-11, 1991. The Symposium was attended by more than 120 participants, mainly from the radiation sterilization and health care industries. Topics ranged from dosimetry calibration; gamma-ray and electron beam processing; process control; process audits, statistics and practical applications. Mr. McLaughlin led a panel discussion of experts in radiation processing dosimetry, who discussed matters vital to public health and safety that is of concern in the multi-billion-dollar a year business of sterilizing medical products, prosthetic devices, and pharmaceuticals by ionizing radiation.

W.L. McLaughlin (Chairman) and M.F. Desrosiers (secretary) organized the "Third International Symposium on ESR Dosimetry and Applications," October 14-18, 1991, at NIST, Gaithersburg, MD. The Symposium was attended by 135 persons from 24 different countries who presented their new developments in ESR applications for radiation dosimetry, archeological dating, accident dosimetry, medicine, and irradiated food detection.

**TIME AND FREQUENCY DIVISION (847)**

D.A. Howe and P.J. Tomingas organized "Time and Frequency Seminar." June 25-27, at NIST, Boulder, CO. This 3-day tutorial seminar, which was attended by 45 people (maximum feasible attendance) from industry and government, included lectures by NIST and other invited experts covering the theory and application of time and frequency measurement and dissemination systems. This annual seminar provides the key U.S. means for training scientists and engineers in this field.
TECHNICAL ACTIVITIES

JOURNAL EDITORSHIPS

LABORATORY OFFICE
Taylor, B.N., Chief Editor of the Journal of Research of the National Institute of Standards and Technology

ELECTRON AND OPTICAL PHYSICS DIVISION (841)
R.J. Celotta, Co-Editor, Methods of Experimental Physics (Academic Press).
C.W. Clark, Topical Editor for Atomic Spectroscopy, Journal of the Optical Society of America B.
D.L. Ederer, Member, Editorial Board, Review of Scientific Instruments.
T.B. Lucatorto, Co-Editor, Methods of Experimental Physics (Academic Press).

ATOMIC PHYSICS DIVISION (842)
Reader, J. Editor, Line Spectra of the Elements, Handbook of Chemistry and Physics. CRC Press.
Fuhr, J.R., Editor, Atomic Transition Probabilities, Handbook of Chemistry and Physics.
Wiese, W.L., Associate Editor, Journal of Quantitative Spectroscopy and Radiative Transfer.
Wiese, W.L., Member, Editorial Advisory Board, Spectrochimica Acta B (Atomic Spectroscopy), Pergamon Press.
Wiese, W.L., Editor, Atomic Transition Probabilities, Handbook of Chemistry and Physics.
Wiese, W.L., Member, Editorial Board, Supplement Series to the Journal, Nuclear Fusion.

MOLECULAR PHYSICS DIVISION (843)
Hougen, J.T., Member, Editorial Advisory Board, Journal of Molecular Spectroscopy.
Jacox, M.E., Member, Editorial Board, Journal of Chemical Physics.

IONIZING RADIATION DIVISION (846)
Coursey, B.M., Editorial Board, Radioactivity and Radiochemistry.
Dick, C.E., Member, Editorial Board, Industrial Metrology.
McLaughlin, W.L., Editorial Board, Radiation Physics and Chemistry.
McLaughlin, W.L., Editor, Radioactivity Measurements, Principles and Practice.
McLaughlin, W.L., Consulting Editor, Special Issue of Applied Radiation and Isotopes 43, "Low Level Radioactivity Measurements."

TIME AND FREQUENCY DIVISION (847)
Jespersen, James and D.W. Hanson, Editors for Special Issue of the Proceedings of the IEEE on Time and Frequency, July 1991.
QUANTUM PHYSICS DIVISION (848)
Hummer, D.G., Member, Editorial Board, Computer Physics Communications.

Leone, S.R., Associate Editor, Annual Review of Physical Chemistry.
Linsky, J.L., Associate Editor, Newsletter of the American Astronomical Society.
Linsky, J.L., Member, Editorial Board, Solar Physics.
APPENDIX F

INDUSTRIAL INTERACTIONS
INDUSTRIAL INTERACTIONS

ELECTRON AND OPTICAL PHYSICS DIVISION (841)

- Methods for Isotopically-Selective Ionization. The Photon Physics Group works with Eastern Analytical, Inc., College Park, MD, under the auspices of a CRDA. Joint research is performed on multiphoton ionization of Ca, the goal being the optimization of methods for isotopically-selective ionization. Such methods would be used to enrich stable, low-abundance isotopes of Ca, which are in demand for a variety of biomedical applications, principally studies of human nutrition. Eastern Analytical's portion of the work has been funded by venture capital and NIH and DoE contracts. An Eastern Analytical employee works full time in the Photon Physics Group's laboratories.

- Optics for X-Ray Lithography. The Photon Physics Group works with Hampshire Instruments, Inc., Rochester, NY, under the auspices of a CRDA. Joint research is performed on the development of collimating optics for x-ray lithography. The Photon Physics Group has collaborated in a design study of alternative approaches, and will characterize special-purpose multilayer optics. Hampshire Instruments portion of the work is funded by DARPA.

MOLECULAR PHYSICS DIVISION (843)

- Narrowband Broadly Tunable Solid State Laser Source. D.S. King collaborated with Light Age, Inc., the major manufacturer of solid state, Alexandrite-based laser systems for research, environmental, and health care applications, on research that was funded by the National Science Foundation through the SBIR program. Phase I work was completed during FY 91. Application is pending for Phase II funding, to proceed with this research. This work is significantly advancing tunable laser technology, especially in the realms of narrow band and vacuum ultraviolet capabilities.

IONIZING RADIATION DIVISION (846)

- Tomosynthetic dental x-ray system. C.E. Dick and J.H. Sparrow cooperate with the Bowman Grey School of Medicine, Wake Forest University, in a program to develop a dental tomographic system. Such a system will mark a major improvement in the diagnosis and treatment of periodontal disease, the major cause of tooth loss in adults.

- Industrial x-ray radiography systems. C.E. Dick and M.R. McClelland have a CRDA with Rayex, Inc. for the research and development of one-sided computerized tomography (CT) systems for medical and industrial radiography, and for design and testing of a new generation of high-power x-ray tubes.

- Radiographic film development. W.L. McLaughlin is in a long-term collaboration with the International Specialty Products Division of GAF Corporation to develop a series of novel radiographic films. These films are beginning to be used for treatment planning dosimetry, for clinical radiography, brachytherapy, teletherapy, and stereotactic neurosurgery.

- Diamond detector development. W.L. McLaughlin has begun a three-way collaboration between NIST, Energy Sciences, Inc., and Trygon Corp. to develop N-doped diamond detectors for radiation monitoring on radiation-processing assembly lines. These detectors show promise of providing the needed continuous record of dose fluctuations for feedback control of beam parameters.

- Development of industrial ESR instruments. M.F. Desrosiers is assisting Bruker Instruments and Micro-Now Instruments in developing ESR readers for alanine dosimeters developed at NIST. The collaboration has established an interactive feedback between dosimeter design and reader sensitivity requirements. Such low-cost readers will be used in on-line free-radical measurements in product and process quality assurance for irradiated materials.

- Monte Carlo electron transport code development. S.M. Seltzer provided close consultation to members of the Simulation Technology Division, Sandia National Laboratory, on the incorporation of recently-developed electron-photon cross sections and sampling algorithms into their Monte Carlo codes.
Search for evidence of 17-keV neutrino. S.M. Seltzer consulted with the Physics Department at the College of William and Mary on theoretical calculations of the response of Si detectors used in high-statistics measurements of beta spectra in the search for evidence of the 17-keV neutrino.

Electron irradiation of silicon solar cells. C.E. Dick consulted with COMSAT Laboratories on the radiation damage effects on solar cells for space applications. The NIST 4-MeV electron Van de Graaff accelerator was used to irradiate cells in order to simulate the ageing effects of radiation on devices in orbiting spacecraft.

Dosimetry of radionuclide sources for interstitial therapy. C.G. Soares, J.T. Weaver and others collaborated with the 3M Company on measuring the dose rate, spectrum, and radial dose distributions from radionuclide sources of $^{125}$I, which are widely used in interstitial radiation therapy.

Yttrium-90 measurements for radionuclide therapy. J.M. Calhoun and B.M. Coursey consulted with Nordion International and Biotechnology Research Laboratories on radionuclide calibrator measurements of $^{90}$Y on glass microspheres (used in the treatment of liver cancer), and on monoclonal antibodies (for potential use in treatment of colon cancer).

Radionuclide measurement traceability testing. Continuing program with the trade association USCEA test activity measurements made by major radiopharmaceutical manufacturers such as Dupont-NEN, Malinkrodt, Bristol-Meyers-Squibb, and Medi-Physics against national standards established for important radionuclides by the Radioactivity Group. A similar program demonstrates the traceability of measurements made in the radiochemistry departments of 18 utilities using nuclear power generation and also includes eight suppliers of certified calibration sources or measuring services. Six members of the Group and two research associations are involved.

Glow-discharge resonance ionization spectroscopy investigations. J.M.R. Hutchinson and collaborators in the Analytical Mass Spectrometry Group, Franklin & Marshall College, and Eastern Analytical Company have installed a glow-discharge source in one of the NIST RIMS machines. The ultimate purpose is to assay environmental radioactivity either in the original matrix or with minimum chemical steps being performed before being measured.

Solid state track recorder (SSTR) R&D. Ultralight mass determinations in the nanogram and picogram range for SSTR dosimeters is a cooperative research effort with the Westinghouse Industrial Technology Center directed by E.D. McGarry. The endpoint is a new neutron dosimeter concept that makes use of a fissile layer placed adjacent to a polymer material which becomes conducting as a result of implantation of energetic heavy ions from nuclear fission. The trend in the nuclear power industry is for increased use of SSTR dosimetry as well as a recognized need for new types of neutron dosimeters that provide a wider dynamic range, permanently recoverable response, and ease of application.

LiF chip gamma dosimeters. This novel high-dose, passive gamma dosimeter developed by D. Gilliam works on the principle of optical absorbency at specific wave lengths. In situ performance trials are underway at the Davis-Besse nuclear power reactor in cooperation with Toledo Edison Co. Gamma-ray heating and coupling with thermal neutron intensities are important for understanding radiation damage to critical reactor structures.

Power reactor industry benchmark irradiation. Radiometric dosimeters including NIST developed PUD detectors, SSTR’s and other dosimeter techniques have been irradiated simultaneously in an operating power reactor. Backed by NIST neutron fluence standards, this interlaboratory effort is needed to validate the diverse methods of dosimetry methods proposed for industry use. This collaboration with the Babcock & Wilcox Lynchburg Research Center is under the direction of E.D. McGarry.

Calibration of D-T neutron source. A special setup directed by David Gilliam at the NIST $^{252}$Cf Neutron Irradiation Facility was used to determine the absolute neutron output of a 14-MeV minitron used by Schlumberger-Doll Research for oil well logging.

TIME AND FREQUENCY DIVISION (847)

Ionospheric Measurement Receiver. Dick Davis and Marc Weiss collaborated with Atmospheric Instrumentation Research in transferring technology for a NIST developed ionospheric measurement GPS receiver. The receiver has applications in time transfer, geophysical measurements and research on the properties of the ionosphere.
Synchronization Interface Standard. Dave Allan and Marc Weiss consulted with a consortium of telecommunications companies in the development of a Synchronization Interface Standard for Telecommunications Networks. This eliminated a key problem with full specification of equipment performance. Sales of equipment for the system, known as SONET, is expected to be at a level of hundreds of millions of dollars per year.

Absolute Gravity Instruments. J. E. Faller is collaborating and consulting with AXIS Instruments Company of Boulder, CO, on the engineering design and construction of instruments for the absolute measurement of gravity. This is a technology transfer exercise, in which these instruments are being engineered from designs based on the original research instruments developed at JILA. The first two commercially produced instruments will be manufactured by AXIS and delivered to NIST for testing, evaluation and ultimate delivery to the National Geodetic Survey of NOAA. They will be used in NOAA’s Global Change Program.
APPENDIX G

OTHER AGENCY RESEARCH AND CONSULTING
OTHER AGENCY
RESEARCH AND CONSULTING

ELECTRON AND OPTICAL PHYSICS DIVISION (841)
T. B. Lucatorto, E.B. Saloman, research for DOE: Isotopically selective multiphoton ionization.
R.P. Madden, L.R. Canfield, research for NASA: Improved radiometric methods and standards for the VUV spectral region in support of NASA solar physics experiments.
R.P. Madden, intercomparisons for NASA: Coordination of a radiometric inter-comparison of NASA solar irradiance experiments.
J.A. Stroscio, R.A. Dragoset, D.T. Pierce, R.J. Celotta, research for ONR: Scanning tunneling microscopy studies of low dimensional systems including 1-D and 2-D alkali phases on III-V semiconductors. Investigate the microscopic aspects of ultrathin epitaxially grown magnetic films on metals.
J. Unguris, D.T. Pierce, M.H. Kelley, R.J. Celotta, research for ONR: Study interlayer exchange coupling in magnetic structures using scanning electron microscopy with polarization analyzers. Correlate the variation in period of the coupling with the structure of the metal layers.

ATOMIC PHYSICS DIVISION (842)
J. Bridges, research for NASA: Ultraviolet and vacuum ultraviolet radiometry for space qualified portable sources.
W.C. Martin, research for NASA: Critical compilations of atomic spectroscopic data needed for space astrophysics.
W.C. Martin, research for NASA: Building of an atomic spectroscopic database needed for space astronomy.
W.D. Phillips, research for NRL: Laser cooling and trapping of neutral atoms.
J. Reader, research for DOE: Spectroscopy of highly ionized atoms to obtain data needed for diagnostics of magnetic-fusion plasmas.
J. Reader, research for DOE: Spectroscopy of laser-produced plasmas at National Laser Users’ Facility (Rochester) to obtain data for research on soft x-ray lasing ions.
J. Roberts, research for SEMATECH: Ultraviolet irradiance measurement technology for SVGL Microscan photolithography systems.
J. Roberts, research for SEMATECH: Ultraviolet irradiance measurement technology for GCA excimer and I-line photolithography systems.
J. Sugar, research for DOE: Critical compilation of atomic spectroscopic data of magnetic-fusion interest.
C.I. Westbrook, research for NRL: Laser cooling and trapping of neutral atoms.
W.L. Wiese, (Principal Investigator), research for the Fusion Energy Office, DOE: Determination of atomic data for the fusion energy program. This is a 5-component program, covering experimental and theoretical work on spectroscopy and collision physics in the Atomic Physics Division and at JILA.
W.L. Wiese, (P.I.) research for NASA: Critical evaluation and compilation of transition proba-
bility data pertinent to the space astronomy program.

W.L. Wiese, (P.I.) research for NASA: A comprehensive spectroscopic database for astronomy.

W.L. Wiese, (P.I.), research for NASA: Far ultraviolet radiometric calibrations of solar physics experiments.

MOLECULAR PHYSICS DIVISION (843)
M.P. Casassa, D.S. King, and J.C. Stephenson, research for AFOSR, High Energy Density Materials Program: Ultraviolet laser photolysis studies of cluster molecules like O$_3$ · H$_2$O.

M.E. Jacox, research for ARO: Spectroscopy of reaction intermediates in nitramine decomposition and combustion.

P.S. Julienne, research for ONR: Theory of collisions of laser-cooled atoms, in conjunction with the experimental NIST program in this area.


W.J. Lafferty and A. Weber, research for NASA: Collision induced IR absorptions in O$_3$ and N$_2$ and high resolution IR spectra of chlorine containing species.


RADIOMETRIC PHYSICS DIVISION (844)
Division Staff, research for the Calibration Coordination Group (CCG), made up of representatives from the primary DOD calibration and metrology laboratories:
- Improve spectrophotometric standards including hemispherical total reflectance;
- Develop photodetector transfer standards calibrated against the HACR;
- Design and build a laboratory for characterization of infrared detectors in the 2 to 25 micrometer wavelength region;
- Develop bidirectional scattering distribution function measuring laboratory and initiate appropriate calibration assurance efforts;
- Design and build a facility and develop procedures to test infrared imaging systems.

Division Staff, research for U.S. Army Strategic Defense Command:
- Develop a low background infrared (LBIR) facility for low background infrared research;
- Develop and test infrared sources and characterize infrared detectors;
- Develop high sensitivity detectors and study the properties of materials at low temperatures;
- Utilize laser heterodyne techniques to study optical density over many orders of magnitude.

Division Staff, research for NASA: provide radiometric calibration services and develop new services for use in preflight calibration of various spacecraft radiometric systems.

Division Staff, research for EPA and Department of Agriculture: develop ultraviolet radiometers which can be used for monitoring the solar UV radiation.

Division Staff and staff from the Atomic Physics Division, research for SEMATECH: improve the ultraviolet and optical radiation measurement technology used in the semiconductor industry for lithography by developing methodologies for calibrating and testing process monitoring systems.

IONIZING RADIATION DIVISION (846)
R.S. Caswell and L.R. Karam, research for the Department of Energy: Calculations of the alpha-particle spectra and energy deposition spectra at the cells at risk in the bronchial epithelium from radon daughters deposited in the bronchial airways.

R.S. Caswell and S.M. Seltzer, research for the Department of Energy: Calculations of the energy deposition from neutrons in nanometer- and micrometer-size volumes aimed at understanding the biological effects of high-linear energy transfer particles such as neutrons.

L. Costrell, study for the Department of Energy: Needs and development of instrumentation and bus systems for data acquisition and control for nuclear particle and radiation physics.

M.F. Desrosiers and coworkers, with support from the Department of Defense: Developing electron spin resonance (ESR) techniques for post-irradiation measurements of free-radical centers in bone samples. The studies are focus-
ing on hardware and software developments to lower the sensitivity and develop an analytical method.

M.F. Desrosiers, collaborations with the Department of Energy: ESR measurements of tooth enamel from victims of the Chernobyl accident. ESR tooth dosimetry has been used for the Hiroshima victims, and it is expected that with newer, more sensitive techniques to play an important role in the long-term monitoring of those exposed to radiation at the Chernobyl accident.

M.F. Desrosiers, collaborations with U.S. Army Aberdeen Proving Grounds, with support from the Environmental Protection Agency: Measurements of shell samples from estuaries around nuclear facilities. The electron spin resonance technique will be applied to measure the radiation-induced signal in shell samples.

C. Eisenhauer et al., consulting and measurement assurance for DOD/AFRRI: Microdosimetry measurements and determination of neutron kerma parameters for biological experiments carried out at a Triga reactor irradiation facility.

D. Gilliam, research for DOE: Study of neutron transport in water spheres with a fission neutron source to establish a benchmark for criticality safety calculations.

J.M.R. Hutchinson, study for the U.S. Navy: Responses of all commercially available alpha-particle monitors were compared to guide the U.S. Navy in their procurement efforts for next generation of such monitors. A 45 page report was issued.

E.D. McGarry and J.A. Grundl, research and consulting for the Nuclear Regulatory Commission: Selectively evaluate neutron dosimetry results from metallurgical test irradiations, power rector environments and benchmark experiments in support of surveillance dosimetry for Light Water Reactor structures and components.

S.M. Seltzer, electron-transport calculations for Department of Energy: The ETRAN code is used in calculating microdosimetric quantities of interest for radiation effects studies in medical sciences and health physics.

S.M. Seltzer, electron-transport calculations for NASA with support from their radiation health program: A Monte Carlo program is being developed to allow prediction of dose to space personnel for a given incident electron spectrum.

J.H. Sparrow, assists Navy and contractor personnel in a continuing review of the measurement aspects of the Navy quality assurance for radiographic inspections of large missile motors using linear accelerators. This includes on-site equipment calibration, verification, and monitoring of radiographic image quality.

J.H. Sparrow and C.E. Dick, collaborations with National Institute for Dental Research and the Bowman Grey School of Medicine: Development of a real-time computed tomographic (CT) system in which eight digital images are acquired of the same tooth from different incident x-ray angles, and a CT image is constructed.

M.D. Walker, collaborations with the Center for Devices and Radiological Health (CDRH) of the FDA: Spectral measurements for diagnostic x rays. The CDRH and the states must ensure the compliance of all diagnostic x-ray machines with specifications for exposure and spectrum quality.

J.T. Weaver and P.J. Lamperti, collaborations with Naval Surface Warfare Center: Measurement quality assurance studies and new instrument characterization for Navy radia instruments and TLD dosimeters.

**TIME AND FREQUENCY DIVISION (847)**

D.W. Allan, research and consulting for Space Division, Air Force: Analysis of GPS data and systems and consultation on operations.

D.W. Allan, consulting to Jet Propulsion Laboratory, NASA: Time transfer to NASA sites, and analysis of time transfer data.

R.E. Bechler, consulting to National Weather Service, NOAA: Broadcast of marine weather alerts on WWV and WWVH.

R.E. Bechler, consulting to Coast Guard, DoT: Broadcast of status of GPS satellites on WWV and WWVH.

R.E. Drullinger, research for Space Division, Air Force: Basic research on the physics of atomic standards.

K.M. Evenson, research for Astrophysics Laboratory, NASA: Far infrared spectroscopy for atmospheric and space studies.
D.W. Hanson, consulting to Naval Observatory: Calibration and testing of USNO earth station in Washington, D.C.

L. Hollberg, research for Office of Space Science, NASA: Molecular frequency calibration standards and tunable laser spectroscopy.

F.L. Walls, research for Metrology and Calibration Division, Army: Development of measurement methods for phase noise.

F.L. Walls, research for Fort Monmouth, Army: Development of phase noise artifacts as transfer standards.

F.L. Walls, research for Guidance and Metrology Center, Air Force: Development of phase noise measurement system for Air Force.

D.J. Wineland, research for Office of Naval Research: Frequency standards and basic studies with cooled, trapped ions.

D.J. Wineland, research for Office of Naval Research: Strongly-coupled, one-component plasmas stored in electromagnetic traps.

D.J. Wineland, research for Air Force Office of Scientific Research: Precision frequency metrology using laser cooled ions.

QUANTUM PHYSICS DIVISION (848)

P.L. Bender, research for NASA: Determination of worldwide tectonic plate motions and large-scale intra-plate distortions.

P.L. Bender, research for NASA: Regional translocation analysis: comparison of LAGEOS II and LAGEOS I results.

P.L. Bender, research for NSF: Low frequency isolation systems for gravitational wave interferometers.

P.L. Bender, research for LAGEOS: Preliminary mission studies for a laser gravitational wave observatory in space.

J. Linsky, research for NASA: Coronal stars in the Rosat WFC survey.

J. Linsky, research for SUNY: The naked T Tauri stars and the pre-main sequence evolution of low mass stars.

G. Dunn, research for DOE: Determine atomic, molecular, and nuclear data pertinent to the magnetic fusion energy program.

G. Dunn, research for NSF (GG)*: Research in atomic and molecular physics.

J. Faller, research for DMA: Absolute gravity meter development.

J. Faller, research for DMA-N: Absolute "g" co-op program.

J. Faller, research for NGS: Absolute gravity meter development and repair/maintenance.

A. Gallagher, research for DOE: Spectroscopic diagnostics of electron-atom collisions.

A. Gallagher, research for NOAA: CVD processes.

A. Gallagher, research for NSF (GG)*: Research in atomic and molecular physics.

A. Gallagher, research for SERI: Growth mechanisms and characterization of hydrogenated amorphous silicon alloy films.

J.L. Hall, consulting to an Advisory Committee to the Global Oscillation Network Group, National Solar Laboratory.

J.L. Hall, consultant on a Panel on laser interferometric gravity wave detection of the National Science Foundation.

J. Hall, research for AFOSR: Optical frequency standards; Hertz-level working standards and their absolute frequency measurements.

J. Hall, research for NSF (GG)*: Research in atomic and molecular physics.

J. Hall, research for ONR: Precision atomic-beam spectroscopy with stabilized lasers.

S. Leone, research for AF: Diode laser probing of energy transfer in XeF.

S. Leone, research for AFOSR: Theoretical/experimental investigations of the structure and dynamics of highly energetic dicaton species.

S. Leone, research for AFOSR: Laser probing of the kinetics and dynamics of III-V semiconductor growth.

S. Leone, research for ARF: Semiconductor deposition and etching interactions of laser-generated translationally hot atoms and radicals.

S. Leone, research for DOE: Time-resolved FTIR emission studies of laser photofragmentation and chain reactions.
S. Leone, research for NASA: Laboratory studies of low temperature rate coefficients.

S. Leone, research for NSF: State-resolved molecular dynamics.

S. Leone, research for NSF (GG)*: Research in atomic and molecular physics.

S. Leone, research for AFOSR: State-resolved dynamics of ion-molecule collisions in a flowing afterglow.

J.L. Linsky, consulting to the National Optical Astronomy Observatory (NOAO) and to the Association of Universities for Research in Astronomy (AURA) concerning operation of the National Solar Observatory and Sacramento Peak Observatory.

J. Linsky, research for NASA: An all-sky X-ray survey of IRS and CVn and related objects.

J. Linsky, research for NASA: International ultraviolet studies of astronomical sources.

J. Linsky, research for NASA: Understanding the circumstellar shell of the star TX PSC.

J. Linsky, research for NASA: The formation process of the He I Lambda 10830 line in cool giants.

J. Linsky, research for NASA: Advanced X-ray astrophysics facility (AXAF).

J. Linsky, research for NASA: Space telescope imaging spectrograph instrument.

J. Linsky, research for NASA: High resolution spectrograph observing program.

J. Linsky, research for NASA: Ultraviolet observations of selected astronomical sources.

J. Linsky, research for NASA: Can shock waves heat cool giant chromospheres?

J. Linsky, research for NASA: X-ray observations of late-type stars using the ROSAT all-sky survey.

J. Linsky, research for NASA: Diagnostics of the hydrogen Lyman and Balmer lines during the impulsive phases of solar flares.

J. Linsky, research for NSF: U.S.-Finland cooperative research on the magnetic structure of stellar atmospheres.

J. Linsky, research for NASA: Analysis of stellar emission from submillimeter to centimeter wavelengths.

D. Nesbitt, research for AFOSR: Direct absorption laser studies of spectroscopy, kinetics and state-to-state collisional dynamics of atmospheric IR emitters.

D. Nesbitt, research for NATO: Van der Waals dynamics.

D. Nesbitt, research for NSF: Direct IR laser and double resonance absorption spectroscopy in slit supersonic jets: vibrational Dynamics of novel molecular clusters.

D. Nesbitt, research for NSF (GG)*: Research in atomic and molecular physics.

D. Norcross, research for DOE: Electron Impact excitation of atomic ions.

D. Norcross, research for NSF (NSF Group Grant, Atomic and Molecular Physics and Related Areas at the Joint Institute for Laboratory Astrophysics.): Research in atomic and molecular physics.

D. Norcross, research for NSF: Theoretical atomic, molecular and optical physics.
APPENDIX H

CALIBRATION SERVICES AND STANDARD REFERENCE MATERIALS
CALIBRATION SERVICES
AND STANDARD REFERENCE MATERIALS

ELECTRON AND OPTICAL PHYSICS DIVISION (841)

<table>
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Total: 31
Recalibrations: 11
SURF-II calibrations: 10
# ATOMIC PHYSICS DIVISION (842)

## CALIBRATION SERVICES PERFORMED

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RADIOMETRIC PHYSICS DIVISION (844)

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*Number of lamps, detectors, optical filters or reflecters tested.
RADIOMETRIC PHYSICS DIVISION (844)

STANDARD REFERENCE MATERIALS

1. SRM 1001, X-Ray Film Step Tablet
   For calibration of optical densitometers and similar equipment used in the photographic, graphic arts, and x-ray fields. Certified for transmission densities from 0 to 4.

2. SRM 1008, Photographic Step Tablets
   For calibration of optical densitometers and similar equipment used in the photographic, graphic arts, and x-ray fields. Certified for transmission densities from 0 to 4.

3. SRM 1010a, Microscopy Resolution Tests Charts
   For determining the resolving power of microscopy systems.

4. SRM 2015 and 2016, White Opal Glass for directional-Hemispherical Reflectance from 400 to 750 nm.
   For use in calibrating the reflectance scale of an integrating sphere reflectometers.

5. SRM 2003, First Surface Aluminum Mirror for Specular Reflectance from 250 to 2500 nm.
   SRM 2011, First Surface Gold Mirror for Specular Reflectance from 600 to 2500 nm.
   SRM 2023, 2024, and 2025 Second Surface Aluminum Mirror for Specular Reflectance from 250 to 2500 nm.
   For use in calibrating the photometric scale of specular reflectometers.

6. SRM 2009, Didymium-Oxide Glass, Wavelength Standards between 400 and 760 nm.

7. SRM 2034, Holmium oxide in Perchloric Acid Solution as Wavelength Standards between 241 and 640 nm.


9. SRM 1931, Fluorescence Emission Standards for the Visible Region.
# IONIZING RADIATION DIVISION (846)

Neutron Interactions and Dosimetry Group

## CALIBRATION SERVICES PERFORMED

### NEUTRON DOSIMETRY

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|                           | Atlan-Tech. Corp.             | 44010C | 2            |
|                           | Naval Research Laboratory     | 44010C | 1            |
|                           | **Sub Total**                 | **N/A**| **6**        |

| In-house (NIST) Sources   | N/A                           | 4            |
| Total                     | **N/A**                       | **10**       |
IONIZING RADIATION DIVISION (846)

Radiation Interactions and Dosimetry Group

HIGH-DOSE CALIBRATION SERVICES PERFORMED FY 1991

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IONIZING RADIATION DIVISION (846)

Radiation Interactions and Dosimetry Group

DOSIMETRY INSTRUMENT AND SOURCE CALIBRATIONS, FY 1991

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SERVICE CODE    TYPE OF SERVICE                                                                 SP250 NUMBER
A               X-Ray and Gamma-Ray Measuring Instruments
B               Dosimeter Irradiations
C               Special Tests-Precision Electrometers
D               Dosimetry of High Energy Electron Beams (Fricke Dosimetry)
E               Gamma-Ray and Beta Particle Sources

46010C & 46011C
46020C & 46021C 46030S
48010M & 48011M
47010C, 47011C & 47030C
**IONIZING RADIATION DIVISION (846)**

Radioactivity Group

**RADIOACTIVITY CALIBRATIONS**

August 1, 1990 to August 1, 1991

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<th>CATEGORY</th>
<th>Scheduled Calibrations</th>
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<th>Non-Scheduled Tests</th>
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*SP-250 numbers refer to scheduled calibrations*
## Standard Reference Materials

Radioactivity Standards Issued - FY 1991

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<th>SRM</th>
<th>Radionuclide</th>
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<td>4417L-K</td>
<td>Indium-111</td>
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<td>4919G</td>
<td>Strontium-90</td>
<td>Monitoring of fission products in the nuclear fuel cycle</td>
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Total Radioactivity SRMs distributed: 855
TIME AND FREQUENCY DIVISION (847)

CALIBRATION SERVICES PERFORMED

Note that a large percentage of calibration and traceability to NIST is accomplished through direct user reception of NIST broadcasts from WWV, WWVB, WWVH, GOES, and ACTS. In general, for time and frequency metrology, it is only in special situations where in-house calibrations can achieve results not easily obtainable by signal transfer to the user.

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<th>FREQUENCY MEASUREMENT SERVICE</th>
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<td>This reimbursable service provides measurement assurance for calibration labs. NIST equipment at the users lab receives LF signals as reference. Performance of users equipment is monitored through a modem by NIST. An initial setup fee and a monthly fee are charged to the user. The total service income for FY 1991 was $234,000.</td>
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<td>Government Users: 21</td>
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This report summarizes research projects, measurement method development, calibration and testing, and data evaluation activities that were carried out during calendar year 1991 in the NIST Physics Laboratory. These activities fall in the areas of electron and optical physics, atomic physics, molecular physics, radiometric physics, quantum metrology, ionizing radiation, time and frequency, quantum physics, and fundamental constants.