NISTIR 89-4184

Center for Atomic, Molecular, and Optical Physics

U.S. DEPARTMENT OF COMMERCE
National Institute of Standards
and Technology

1989
Technical Activities

Image of a cloud of laser cooled Be^+ ions confined in a Penning trap. The spherically symmetric cloud (partially illuminated by three laser beams) is arranged in a liquid-crystalline phase of eleven concentric shells. This cloud contains approximately 15,000 ions and is 550 microns in diameter. Transitions from disordered to ordered states are being studied in cooled ion clouds in the Time and Frequency Division of the Center for Atomic, Molecular and Optical Physics.

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1989 Technical Activities

December 6-7, 1989

Katharine B. Gebbie, Acting Director
Center for Atomic, Molecular, and Optical Physics
National Measurement Laboratory

U.S. DEPARTMENT OF COMMERCE, Robert A. Mosbacher, Secretary
National Institute of Standards and Technology, Raymond G. Kammer, Acting Director

ABSTRACT

This report summarizes the research and technical activities of the Center for Atomic, Molecular and Optical Physics (CAMOP) during the Fiscal Year 1989. These activities include work in the areas of fundamental constants, radiation physics, surface science, molecular spectroscopy, electron and optical physics, atomic and plasma spectroscopy, time and frequency, quantum metrology, and quantum physics.

Keywords: Astrophysics; atomic physics; calibrations; chemical physics; fundamental constants; gravity; laser physics; molecular physics; optical physics; plasmas; radiation; solid state physics; spectroscopy; standards; surface science; time and frequency; wavelength standards.

INTRODUCTION

This report is a summary of the technical activities of the National Institute of Standards and Technology (NIST) Center for Atomic, Molecular, and Optical Physics (CAMOP) for the period October 1, 1988 to September 30, 1989. The Center is one of the four technical operating units in the National Measurement Laboratory.

The summary of activities is organized into eight sections, one for the technical activities of the Center office staff, and one each for the seven divisions of the Center. Each division tells its own story in its own way. In general, there is an overview followed by a series of short reports on current projects. Then the publications, invited talks, committee participation, and some of the technical interactions during the year are listed.

To obtain more information about particular work, the reader should address the individual scientists or their division, c/o Center for Atomic, Molecular and Optical Physics, B160 Physics Building, National Institute of Standards and Technology, Gaithersburg, Maryland 20899.

TABLE OF CONTENTS

FUNDAMENTAL CONSTANTS DATA CENTER

B. N. Taylor

OBJECTIVES: (1) To provide an international information center on the fundamental physical constants and closely related precision measurements (FCPM); (2) to analyze the consistency of measured values of the constants in order to test fundamental physical theory and to obtain sets (or subsets) of "best" or recommended values of the constants for international use; (3) to organize conferences or sessions at conferences on FCPM; and (4) to contribute to the work of various international and national committees and organizations active in the FCPM (or a closely related) field. Two other major objectives are (5) to serve as Chief Editor of the *Journal of Research of the National Institute of Standards and Technology* (*J. R. NIST*); and (6) to administer the NIST Precision Measurement Grant (PMG) program.

MOTIVATION: The fundamental constants have long been of importance to NIST because of their close relationship to precision measurements, basic measurement units such as the ampere, volt, and ohm, fundamental physics, state-of-the-art measurement technology, theoretical calculations, and the compilation and analysis of critical reference data. One of the aims of the Data Center is to provide assistance and guidance in the FCPM area to both NIST and university scientists, for example, to advise them on the potential impact of the experiments they are considering carrying out and to keep them informed of related work underway in various laboratories throughout the world.

NIST PMG's are awarded to scientists in U.S. academic institutions in order (1) to promote research in the FCPM field and train future measurement-oriented scientists; and (2) to foster contacts between NIST scientists and those researchers in the academic community who are actively engaged in such work. While NIST has much FCPM research underway, there is considerable expertise and relevant work in U.S. colleges and universities. The PMG program taps this reservoir and fosters the training of students who might eventually become NIST staff by awarding grants to outstanding academic researchers.

ACTIVITIES: These include (1) keeping apprised of and maintaining a complete reprint collection of the latest accomplishments throughout the world in FCPM; (2) carrying out least-squares adjustments of the fundamental constants to obtain sets or subsets of recommended values; (3) participating in the work of national and international groups, for example, the Committee on Data for Science and Technology (CODATA) Task Group on Fundamental Constants, the NAS/NRC Advisory Committee on Fundamental Constants and Standards, the Consultative Committee on Electricity (CCE), and the American Physical Society Topical Group on Fundamental Constants and Precise Tests of Physical Laws; (4) organizing FCPM conferences or FCPM sessions at conferences; (5) answering inquiries from both within and without NIST relating to the FCPM field; (6) soliciting papers for *J. R. NIST* and overseeing its publication; and (7) awarding two new $30K/year PMG's each year and renewing four existing $30K/year PMG's.

ACCOMPLISHMENTS: The work emphasis in FY 89 has been on selecting values of the Josephson and von Klitzing constants (K_J and R_K) to serve as the basis for new international representations of the volt and ohm to come into effect starting January 1, 1990; to document fully the selection process; and to help NIST inform science, commerce, and industry, but most especially the users of its electrical calibration services, about the new representations and how to bring standards and instruments into conformity with them. (Note that it is assumed $K_J = 2e/h$ and $R_K = h/e^2$, where e is the elementary charge and h is the Planck constant.) This was done by serving as a principal member of the CCE's Working Group on the Josephson Effect, Coordinator of the CCE's Working Group on the Quantum Hall Effect, NIST representative to the CCE, preparing articles, and delivering talks (see lists which follow). The calibration reports for NIST voltage standard calibrations, including the information sheet, were rewritten.

A detailed plan for carrying out the next least-squares adjustment of the fundamental constants was worked out in collaboration with T. J. Quinn, Chairman of the CODATA Task Group on Fundamental Constants, and E. R. Cohen, a principal member of the Task Group. It is to be completed in early 1993 and published simultaneously in *Rev. Mod. Phys.* and *J. Phys. Chem. Ref. Data* as agreed by the editors of both journals.

The FCDC assisted S. E. Chappell, Chief of the NIST Office of Standards Management, in revitalizing ISO (International Standardization Organization) Working Group 3, "Expression of Uncertainties" and assumed responsibility for representing NIST and the U.S. on the Working Group.

During FY 89, a three pronged approach to revitalizing the *J. R. NIST* was initiated: (1) papers were solicited via memoranda to the NIST staff, Center Directors, and Division Chiefs, plus numerous personal contacts and wide distribution of revised instructions for manuscript preparation; (2) the appearance of *J. R. NIST* was improved via a new, modern cover color and typography; and (3) an effort was made to increase subscriptions via a strong advertisement campaign. Additionally, the Board of Editors was reconstituted and its charter modified and updated.

Steven Chu, Stanford University, and Edward E. Eyler, University of Delaware, were the two new recipients of PMG's in FY 89. Chu's project, "Precision Optical Spectroscopy of Positronium," will determine the $1\ {}^3S - 2\ {}^3S$ interval in positronium via two photon laser spectroscopy with a relative uncertainty approaching 1 part in 10^{10}, thereby providing one of the best tests of the two-body problem in quantum electrodynamics. Agreement between theory and experiment at this level can be used to set an upper limit (at the same level) on the particle-antiparticle mass difference of the electron and positron, thus critically testing the CPT theorem.

Eyler's project, "Far Ultraviolet Spectroscopy with Single-Frequency Lasers," will develop and characterize intense tunable single frequency laser sources in selected regions of the far ultraviolet (50-200 nm) suitable for precision two-photon spectroscopy. The lasers will be used to measure the $1\ ^1S$ - $2\ ^1S$ interval in atomic helium with an accuracy approaching 0.001 cm^{-1} (6 parts in 10^9), thereby providing a precise experimental test of recent calculations of Lamb shift and relativistic corrections in the groundstate of helium and establishing a much improved set of calibration lines for vacuum ultraviolet spectroscopy in this region.

The following PMG's were renewed: E. A. Hinds and M. G. Boshier, Yale University, "Two-Photon Spectroscopy of H and He^+"; R. G. Hulet, Rice University, "Measurement of the Recombination Rate of Spin-Polarized Ultra-Cold Atoms"; W. P. Kirk, Texas A&M University, "Quantized Hall Resistance and Fine-Structure Constant Investigations: A Study of Uncertainty Contributions"; J. D. Morgan III, University of Delaware, "High Precision Calculation of Helium Atom Energy Levels."

FUTURE PLANS: In FY 90 the FCDC will focus on the preparation of a status report on the fundamental constants for presentation at the 1990 Conference on Precision Electromagnetic Measurements (CPEM 90) to be held in Ottawa, Canada, in June 1990. This report will be prepared in collaboration with E. R. Cohen of Rockwell International and will be a very concise update of the 1986 CODATA least-squares adjustment of the constants. However, it will not give new recommended values. The report was requested by the CODATA Task Group on Fundamental Constants and will be discussed at the Task Group meeting to be held at the time of CPEM 90. It will serve as the starting point for the 1993 CODATA least-squares adjustment of the fundamental constants to be completed by the end of 1992 or very early in 1993.

Efforts will continue to increase the number of papers submitted for publication in *J. R. NIST* by the NIST technical staff.

With regard to the PMG program, FY 90 plans naturally focus on renewing the four eligible current grants and awarding two new grants. Current and past recipients will be invited to visit NIST and to present talks as appropriate, and visits to current and past recipients will be made in conjunction with other travel. A session at the APS Spring Meeting in Washington, DC, in honor of the 20th anniversary of the PMG program is being planned.

PUBLICATIONS - FY 89

1. <u>In Print</u>

"Report to the Comité Consultatif d'Électricité from the Working Group on the Josephson Effect," R. Kaarls, B. P. Kibble, B. N. Taylor, and T. J. Witt, Bur. Int. Poids et Mesures (BIPM) Rapport 88/7, August 1988, 31 pp. Revised version in BIPM Com. Cons. Électricité **18**, pp. 76-96 (September 1988).

"Report to the Comité Consultatif d'Électricité from the Working Group on the Quantum Hall Effect," F. Delahaye, T. Endo, O. C. Jones, V. Kose, B. N. Taylor, and B. M. Wood, BIPM Rapport 88/8, August 1988, 32 pp. Revised version in BIPM Com. Cons. Électricité **18**, pp. 97-118 (September 1988).

"Technical Guidelines for the Reliable Measurement of the Quantized Hall Resistance," F. Delahaye, T. Endo, O. C. Jones, V. Kose, B. N. Taylor, and B. M. Wood, BIPM Rapport 88/9, August 1988, 16 pp. Revised version in BIPM Com. Cons. Électricité **18**, p. 119-129 (September 1988).

"The 1986 CODATA Recommended Values of the Fundamental Physical Constants," E. R. Cohen and B. N. Taylor, *J. Phys. Chem. Ref. Data* **17**, No. 4, pp. 1795-1803 (1988).

"Atomic Constants," B. N. Taylor, in *1989 McGraw-Hill Year Book of Science and Technology*, Ed. by S. P. Parker (McGraw-Hill Book Co., New York, 1988), pp. 49-51.

"New International Electrical Reference Standards Based on the Josephson and Quantum Hall Effects," B. N. Taylor and T. J. Witt, *Metrologia* 26, No. 1, pp. 47-62 (1989).

"New Internationally Adopted Reference Standards of Voltage and Resistance," B. N. Taylor, *J. Res. Natl. Inst. Stand. Technol.* 94, No. 2, pp. 95-103 (March-April 1989).

"Basic Standards and Fundamental Constants," B. N. Taylor, *IEEE Trans. Instrum. Meas.* **IM-38**, No. 2, pp. 164-166 (April 1989).

"NBS Determination of the Fine-Structure Constant, and the Quantized Hall Resistance and Josephson Frequency-to-Voltage Quotient in SI Units," M. E. Cage, R. F. Dziuba, R. E. Elmquist, B. F. Field, G. R. Jones, Jr., P. T. Olsen, W. D. Phillips, J. Q. Shields, R. L. Steiner, B. N. Taylor, and E. R. Williams, *IEEE Trans. Instrum. Meas.* **IM-38**, No. 2, pp. 284-289 (April 1989).

"Guidelines for Implementing the New Representations of the Volt and Ohm Effective January 1, 1990," N. B. Belecki, R. F. Dziuba, B. F. Field, and B. N. Taylor, NIST Technical Note 1263 (U.S. Dept. of Comm., Natl. Inst. Stand. Technol., Gaithersburg, MD, June 1989), 72 pp.

"The New 1990 Volt and Ohm Standards," B. N. Taylor, *IEEE Spectrum* 26, No. 7, pp. 20-23 (July 1989).

"New Measurement Standards for 1990," B. N. Taylor, *Physics Today* 42, No. 8, Pt. 1, pp. 23-26 (August 1989).

2. <u>In Press, In Review, or Nearing Completion</u>

"The New International Volt and Ohm Standards," B. N. Taylor, in *Proceedings of the International Symposium on Electromagnetic Metrology*, ISEM89 (International Academic Publishers, Beijing, August 1989), pp. xxx-xxx.

"New International Representations of the Volt and Ohm Effective January 1, 1990," B. N. Taylor, *IEEE Trans. Instrum. Meas.* **IM-39**, No. 1, pp. xxx-xxx (February 1990).

"Constants, Fundamental," B. N. Taylor, in *Encyclopedia of Physics*, Ed. by R. G. Lerner and G. L. Trigg (VCH Publishers, Inc., New York, December 1990), pp. xxx-xxx.

INVITED TALKS - FY 89

Critical Comparison of Values of the Fine-Structure Constant, University of Washington, Seattle, WA, January 1989.

Quantum Phenomena, Fundamental Constants, and Electrical Units, Annual Meeting of the American Association for the Advancement of Science, San Francisco, CA, January 1989.

The New Internationally Adopted Volt and Ohm Standards Based on the Josephson and Quantum Hall Effects, Natl. Conf. Stands. Labs. Ad Hoc Committee 91.4, Changes in the Volt and Ohm, Anaheim, CA, January 1989.

Report on the 18th Meeting of the Consultative Committee on Electricity, 1989 Measurement Science Conference, Anaheim, CA, January 1989.

The New International Volt and Ohm Standards Effective January 1, 1990, National Physical Laboratory of Israel, Jerusalem, Israel, April 1989.

New Internationally Adopted Reference Standards of Voltage and Resistance Based on the Josephson and Quantum Hall Effects, IEEE Instrumentation and Measurement Technology Conference, Washington, DC, April 1989.

The Fundamental Physical Constants and New Electrical Standards Based on the Josephson and Quantum Hall Effects, American Physical Society Spring Meeting, Baltimore, MD, May 1989.

The Basis for the New International Representations of the Volt and Ohm Effective January 1, 1990, National Research Council of Canada, Ottawa, Canada, May 1989.

The Basis for the New International Representations of the Volt and Ohm Effective January 1, 1990, Swiss Federal Office of Metrology, Wabern-Bern, Switzerland, June 1989.

EDITORSHIPS, TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION

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

B. N. Taylor is NIST representative to the Consultative Committee on Electricity (CCE) of the International Committee of Weights and Measures (CIPM).

B. N. Taylor serves as Vice Chairman of the American Physical Society Topical Group on Fundamental Constants and Precise Tests of Physical Laws.

B. N. Taylor is a principal member of the CODATA (Committee on Data for Science and Technology) Task Group on Fundamental Constants.

B. N. Taylor serves as NIST representative to, Controller, and member of the Executive Committee of the Conference on Precision Electromagnetic Measurements (CPEM).

B. N. Taylor is a member of the Board of Editors of *Metrologia*.

B. N. Taylor is a member of the Editorial Board of the *Journal of Physical and Chemical Reference Data.*

B. N. Taylor serves as a Technical Advisor to the U.S. National Committee (USNC) of the International Electrotechnical Commission (IEC) on TC25 Matters (TC25: Quantities and Units, and Their Letter Symbols).

B. N. Taylor is the NIST representative to ISO TAG-4/WG-3 (International Standards Organization, Technical Activities Group 4, Working Group 3), Expression of Uncertainties.

B. N. Taylor is NIST liaison member of the NAS/NRC (National Academy of Sciences/National Research Council) Advisory Committee on Fundamental Constants and Standards, National Data Advisory Board (NDAB).

B. N. Taylor is a member of the Advisory Committee of the Particle Data Group, Lawrence Berkeley Laboratory.

B. N. Taylor is a member of the Institute of Electrical and Electronics Engineers (IEEE) Standards Coordinating Committee 14 (SCC14), Quantities, Units, and Letter Symbols.

B. N. Taylor is a member of NCSL (National Conference of Standards Laboratories) Ad Hoc Committee 91.4, Changes in the Volt and Ohm.

COLLABORATIONS, CONSULTING, MISCELLANEOUS ACTIVITIES

B. N. Taylor is collaborating with E. R. Cohen, Rockwell International, and the CODATA Task Group on Fundamental Constants, on various aspects of data analysis relevant to the fundamental physical constants.

B. N. Taylor is collaborating with S. E. Chappell, Chief of the NIST Office of Standards Management, on the U.S. contributions to the work of ISO TAG-4/WG-3.

LASER COOLING GROUP: LASER COOLING AND TRAPPING OF NEUTRAL ATOMS

W. D. Phillips, C. I. Westbrook, S. L. Rolston, R. N. Watts, C. E. Tanner
Visiting Scientists: H. J. Metcalf, P. L. Gould, J. Weiner, H. Thorsheim

Objectives: To study the basic physics of laser cooling and electromagnetic trapping of neutral atoms, and of the interaction of atoms and radiation; to develop applications of these studies to new classes of physical measurements. Areas of interest include high resolution spectroscopy, ultra-low-energy collisions, ultra-low-energy atom-surface interactions, Bose-Einstein condensation, and atomic beam manipulation. This work is complementary to work in the Time and Frequency Division on cooling and trapping of ions, and is being carried out, in part, in collaboration with scientists in the Molecular Physics and Electron and Optical Physics Divisions, as well as with scientists from The State University of New York at Stony Brook, the University of Connecticut, the University of Maryland, Harvard University, and the École Normale Supérieure (ENS) in Paris.

Current Activities: We have a laser-cooled atomic beam apparatus which produces a continuous beam of atoms having velocities below a few tens of meters per second. This can be used to load optical or magnetic atom traps and optical molasses. These in turn are used to study the quantum optics and atomic processes involved in laser cooling and trapping, and to study the physics and chemistry of atomic collisions.

Accomplishments: Last year we discovered an entirely new class of laser cooling mechanisms. Our experiments showed that the temperature achievable by laser cooling was far lower than the lower limit imposed by the generally accepted theory of laser cooling. Attempts by theoretical groups to explain our results led to the identification of a new kind of laser cooling, different both conceptually and practically from had been presumed to be the mechanism for laser cooling. Surprisingly, the Doppler effect, long thought to account for the velocity dependence of the radiation pressure essential for laser cooling, plays no role in the new mechanism. Our work this year has focused on gaining a better experimental and theoretical understanding of the new cooling mechanism.

<u>Measurements on optical molasses</u>. Optical molasses is a three-dimensional arrangement of counterpropagating laser beams which captures, cools, and viscously confines atoms. It has become a standard tool for loading atoms traps and as a source of very cold atoms. Our investigation of its properties led to the discovery of the new cooling force. Much of this year's work involved careful measurements of the dependence of atomic temperature and confinement time on various controlled parameters for detailed comparison with theory. For example, we have improved both our experimental arrangements and our measurement technique so as to achieve temperatures as low as 25 ± 10 μK, compared to 45 ± 20 μK last year. Data for such a determination, which is also supported by other techniques, is shown

in figure 1. Measurements of the temperature as a function of laser intensity have been particularly helpful in testing the predictions of the theory, which has been found to be in good agreement with experiment.

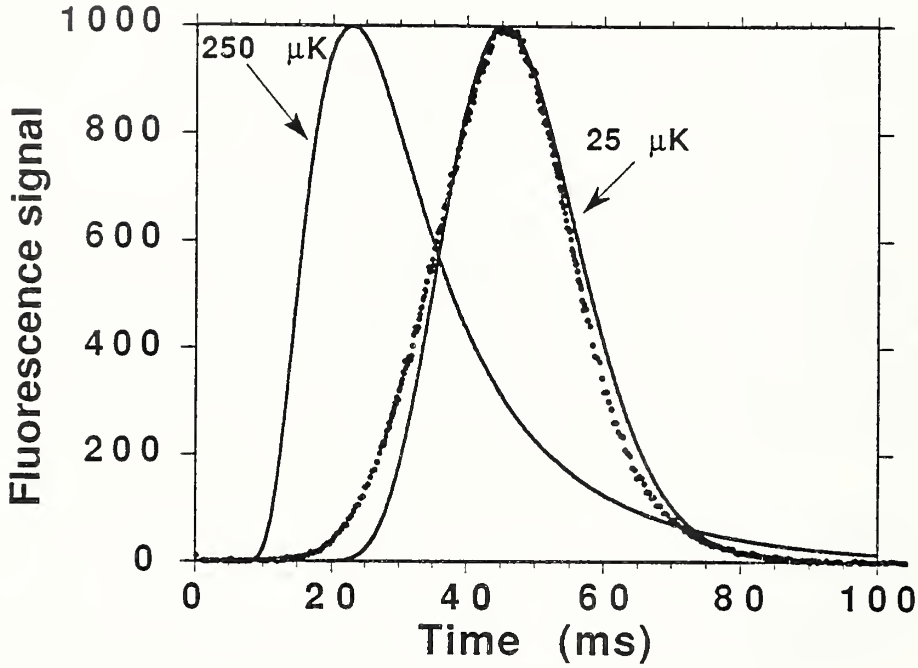

Figure 1. Time-of-flight measure of temperature. Atoms released from optical molasses are detected some distance away. The distribution of arrival times reflects the temperature. The data correspond best to a temperature of 25 μK. For comparison, we show the expected result if the temperature had been 250 μK, the lowest temperature allowed by the traditional theory.

The 25 μK temperature is the lowest reported temperature achieved by laser cooling, and is the lowest temperature ever recorded for gas phase atoms. Such low temperatures are difficult to measure and led us to consider a direct spectroscopic measurement of the Doppler width of the fluorescent spectrum emitted by the atoms. This led to a successful measurement by an optical heterodyne technique. The measurement was important from a scientific viewpoint because of the unexpected nature of the results (see figure 2). The broad part of the spectrum corresponds to the Doppler width, about 600 kHz, much narrower than the 10 MHz natural width. The narrow feature, however, is only 70 kHz wide and is apparently due to motional (Dicke) narrowing of the Doppler line by confinement of atoms in wavelength-size optical potential wells. This phenomenon, long speculated to be possible, had never before been directly observed. The development of this technique presents a new and qualitatively different method for studying optical forces.

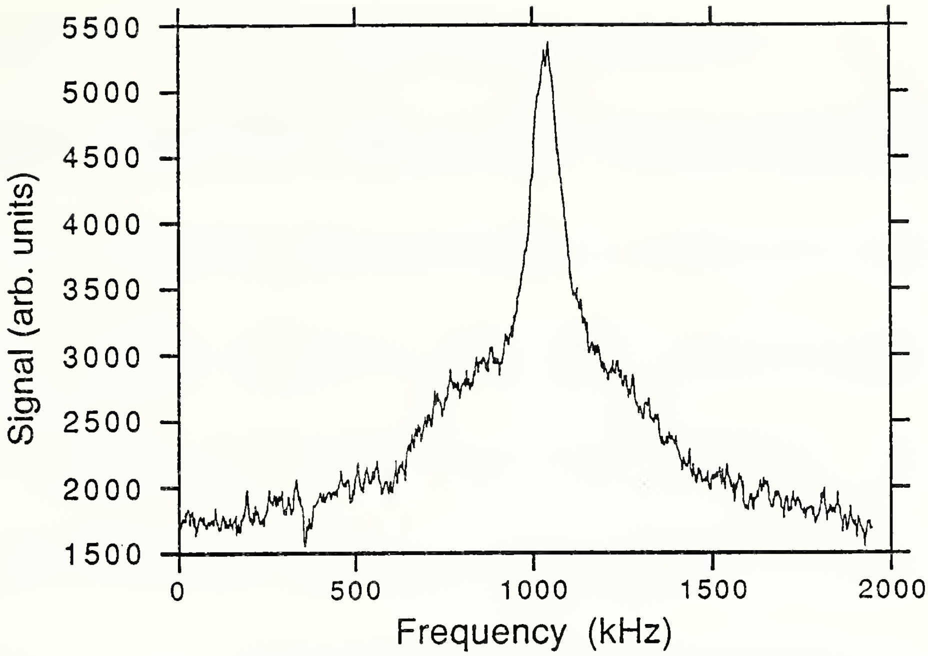

Figure 2. Fluorescence spectrum of Na atoms in optical molasses, obtained by an optical heterodyne technique. The broad and narrow features represent the Doppler-broadened and Dicke-narrowed spectra respectively. The much larger natural width is absent in this technique.

<u>Theory of cooling at the recoil limit</u>. The temperatures we measure are now so low that they approach the recoil limit, the energy gained by an atom at rest from the recoil of a single photon. In Na this is 2.4 μK. Since 1979, when the theory of laser cooling was first carefully considered, there has been no systematic treatment of recoil limited cooling, because it violates the usual semiclassical assumptions of an atom localized within a wavelength of light. We have performed a Monte Carlo analysis that gives qualitatively different results from previous work, and is in agreement with recent quantum mechanical results obtained at ENS in Paris. The result is that one cannot cool below the recoil limit with a single, narrow band laser frequency.

Future Plans: We are continuing our theoretical and experimental investigations of the new cooling force, particularly with respect to the new results from heterodyne spectroscopy. Specifically, we are attempting to provide a semi-quantitative theory of the motion of atoms in optical molasses which explains the details of the observations. In addition we are constructing and installing apparatus for laser cooling of both heavier and lighter atoms to study the influence of the recoil energy on the cooling process. We are developing the techniques for cooling atomic hydrogen with Lyman-α radiation for applications to fundamental spectroscopy and Bose-Einstein condensation of trapped hydrogen. We are pursuing the construction of an atomic fountain for high resolution spectroscopy, using a technique, conceived in our laboratory, for avoiding heating of the atoms as they are thrown up in the fountain. Since transverse temperature is one of the major figures of merit for an atomic fountain frequency standard, this should provide a significant improvement in expected performance.

INVITED TALKS - FY 89

W. D. Phillips, "New Physics with Cold Atoms," Physics Department Colloquium, University of Illinois, Urbana, Illinois, October 1988.

W. D. Phillips, "Laser Cooling and Trapping," Physics Department Colloquium, Williams College, Williamstown, Massachusetts, October 1988.

W. D. Phillips, "New Physics with Cold Atoms," Department of Physics and Chemistry, University of Maryland, Baltimore, Maryland, November 1988.

W. D. Phillips, "Laser Cooling Below the Doppler Limit," Atomic Physics Seminar, Columbia University, New York, New York, November 1988.

W. D. Phillips, "The Hottest News About the Coldest Atoms," Physics Department Colloquium, Purdue University, Lafayette, Indiana, December 1988.

W. D. Phillips, "Hot News About Cold Atoms: Laser Cooling at NIST," Physics Department Colloquium, Duke University, Durham, North Carolina, January 1989.

W. D. Phillips, "Laser Cooling, Optical Molasses, and the Coldest Gas in the University," Physics Department Colloquium, University of Texas, Austin, Texas, February 1989.

W. D. Phillips, "Collisions of Ultra-Cold Atoms," Atomic Physics Seminar, University of Texas, Austin, Texas, February 1989.

C. I. Westbrook, "New Mechanisms for Laser Cooling," Atomic Physics Colloquium, Harvard University, Cambridge, Massachusetts, February 1989.

C. E. Tanner, "Parity (and Time Reversal) Nonconservation in Atomic Cesium," Physics Department Colloquium, University of Notre Dame, South Bend, Indiana, February 1989.

C. E. Tanner, "Parity Violation in Cesium," Center for Atomic, Molecular, and Optical Physics Colloquium, NIST, Gaithersburg, Maryland, February 1989.

W. D. Phillips, "Laser Cooling, Optical Molasses, and the Coldest Gas in the Universe," Department of Physics Colloquium, Pennsylvania State University, State College, Pennsylvania, March 1989.

W. D. Phillips, "Laser Cooling of Atoms," Physics Department Colloquium, Juniata College, Huntington, Pennsylvania, March 1989.

R. N. Watts, "Hot Topics in Cold Atoms," Chemical Physics Seminar, NIST, Gaithersburg, MD, March 1989.

C. I. Westbrook, "The Coldest Gas in the Universe," Atomic Physics Seminar, State University of New York, Stony Brook, New York, March 1989.

S. Rolston, "Laser Cooled Sodium," Wesleyan University, Middletown, Connecticut, March 1989.

R. N. Watts, "Ultra Cold Atoms," Surface Science and Electron Physics Seminar, NIST, Gaithersburg, MD, April 1989.

R. N. Watts, "Laser Cooling Below the Doppler Limit," Quantum Electronics and Laser Science Conference, Baltimore, Maryland, April 1989.

S. Rolston, "Laser-Cooled Sodium," Physics Department Colloquium, University of Cincinnati, Cincinnati, Ohio, May 1989.

W. D. Phillips, "Cooling Below the Doppler Limits: New Surprises," 9th International Congress on Laser Spectroscopy, Bretton Woods, New Hampshire, June 1989.

W. D. Phillips, "New Mechanisms for Laser Cooling: Experimental Tests," Gordon Research Conference on Atomic Physics, Brewster Academy, New Hampshire, July 1989.

C. E. Tanner, "Laser Cooling," Purdue University, Lafayette, Indiana, August 1989.

C. E. Tanner, "Parity Non-Conservation in Atomic Cesium," Purdue University, Lafayette, Indiana, August 1989.

PUBLICATIONS - FY 89

"NBS Determination of the Fine-Structure Constant and of the Quantized Hall Resistance and Josephson Frequency-to-Voltage Quotient in SI Units," M. E. Cage, R. F. Dziuba, R. D. Elmquist, B. F. Field, G. R. Jones, Jr., P. T. Olsen, W. D. Phillips, J. Q. Shields, R. L. Steiner, B. N. Taylor, and E. R. Williams, IEEE Trans. Instrum. Meas. IM-38, No. 2, pp. 284-289 (April 1989).

"Optical Molasses," P. D. Lett, W. D. Phillips, S. L. Rolston, C. E. Tanner, R. N. Watts, and C. I. Westbrook, Journal of the Optical Society of America - B 6 (1989).

"Laser Cooling and the Recoil Limit," S. Rolston, P. Lett, and W. Phillips, Technical Digest of the Quantum Electronics and Laser Science Conference, April 24-28, 1989, Baltimore, MD.

"Laser Cooling Below the Doppler Limit," P. Lett, C. Westbrook, S. Rolston, C. Tanner, W. Phillips, P. Gould, and H. Metcalf, Technical Digest of the Quantum Electronics and Laser Science Conference, April 24-28, 1989, Baltimore, MD.

"Associative Ionization of Ultra-Cold Laser-Trapped Sodium Ions," P. D. Gould, P. D. Lett, R. N. Watts, C. I. Westbrook, P. S. Julienne, W. D. Phillips, H. R. Thorsheim, and J. Weiner, Atomic Physics 11, S. Haroche, J. C. Gay and G. Grynberg Eds. (World Scientific, Singapore, 1989) p. 215.

"Observation of Atoms Laser-Cooled Below the Doppler Limit," W. D. Phillips, C. I. Westbrook, P. D. Lett, R. N. Watts, P. L. Gould, and H. J. Metcalf, Atomic Physics 11, S. Haroche, J. C. Gay, and G. Grynberg Eds. (World Scientific, Singapore, 1989) p. 633.

"Atoms Laser Cooled Below the Doppler-Cooling Limit," P. D. Lett, C. I. Westbrook, R. N. Watts, S. L. Rolston, P. L. Gould, and W. D. Phillips, Frequency Standards and Metrology, A. DeMarchi Ed., (Springer, Berlin, 1989) p. 264.

"Prospects for Electromagnetic Manipulation of Antihydrogen," P. D. Lett, P. L. Gould, and W. D. Phillips, Hyperfine Interactions 44, 335 (1988).

ELECTRON AND OPTICAL PHYSICS DIVISION

FISCAL YEAR 1989 TECHNICAL ACTIVITIES

The Electron and Optical Physics Division focuses on measurement programs related to the use of electron, laser, ultraviolet, and soft x-ray radiation in the energy range from about 5 eV (250 nm) to 1 keV (1.3 nm).

In support of this mission, radiation standards and advanced measurement techniques are developed. Through our standards program, the Division provides the central national basis for the measurement of far ultraviolet and soft x-ray radiation. The NIST synchrotron radiation facility and a detector calibration facility based upon well-characterized photoionization chambers serve as national radiation standards. Measurement services are available for the calibration of the quantum efficiency of uv photodiodes and the spectral responsivity of vacuum ultraviolet spectrometer systems.

Through our electron measurements program, new types of electron sources and detectors are developed to investigate the properties of matter on an atomic scale. For example, specially designed spin-polarized electron sources and detectors are used to determine fundamental atomic scattering properties and to measure surface magnetism. A scanning tunneling microscope is being used to provide "images" of surfaces on an atomic scale and to study relationships between macroscopic material properties and surface microstructure.

With the goals of improving standards and understanding the fundamental physical phenomena upon which they are based, the Division also conducts theoretical and experimental research on the electronic structure of atomic and molecular systems, the interaction of the systems with photon and electrons, and radiation deposition and energy transfer processes. Theories are developed for the scattering and transport of electrons in materials of fundamental and technological interest. New techniques and instrumentation are developed to study radiative reactions with matter, including photoexcitation and photoionization processes and non-linear effects in intense laser fields. Studies are underway to relate the behavior of condensed matter systems to their fundamental atomic and molecular properties.

The Division has two major research facilities: a dedicated synchrotron ultraviolet radiation facility (SURF-II), and a microstructure measurement research facility.

SURF-II is a dedicated synchrotron radiation facility, consisting of a 300 MeV electron storage ring, a 10 MeV microtron injector, and associated synchrotron radiation beamlines. It produces radiation in a narrow, intense, highly polarized beam with a continuous and accurately known spectrum from the infrared, through the visible and the far ultraviolet, and into the soft x-ray region. SURF-II is unique among synchrotron light sources by virtue of its uniform and precisely known circular orbit. This allows accurate determination of all the spectral and geometrical properties of the radiation and hence its use as an absolute radiometric standard.

This facility serves staff from our own Division, users from other NIST Divisions, and outside users in radiometric standards and calibration work, optical physics research, surface science, biochemistry, spectroscopy, and other research areas utilizing far ultraviolet radiation. It helps to fill a growing demand for radiation in the ultraviolet and soft x-ray region of the electromagnetic spectrum. Of the 11 light ports at SURF, 6 are now instrumented for user applications and for calibration of optical instruments and transfer standard photodiodes. Some of these ports are shared by more than one experimental station. Three of the remaining ports are used for beam current monitoring, electron counting, and machine diagnostics. Most experiments and calibrations can run simultaneously, unless they require special beam parameters.

The microstructure measurement research facility is used to study the atomic and magnetic microstructure of advanced materials, in collaboration with industry. Magnetic microstructure is measured with a spatial resolution of about 500 Angstroms (0.05 microns) by a technique called Scanning Electron Microscopy with Polarization Analysis (SEMPA). An ultrahigh vacuum scanning tunneling microscope (STM) is used to investigate, on an atomic scale, the nucleation and growth of thin films on clean metallic and semiconductor surfaces.

In the same complex, two additional instruments are being developed: a "magnetic" tunneling microscope, to enable magnetic domain measurements with atomic scale resolution by combining SEMPA and STM technology; and a high current, high resolution SEMPA instrument, to improve SEMPA performance by a factor of 10 in collaboration with Honeywell, Inc., Control Data Corporation, and Perkin Elmer Corporation.

Division staff are also collaborating on two projects at the National Synchrotron Light (NSLS) facility at Brookhaven. The first involves radiation probing of exotic materials with soft x-rays. With colleagues from the U. of Tennessee and Oak Ridge National Labs, we are studying core-hole excitation and soft x-ray fluorescence in solid materials of fundamental and industrial significance such as GaAs, quasi-crystals, and high Tc superconductors. This is being done using an IR-100 award-winning, high sensitivity, soft x-ray emission spectrometer with an efficiency 1000 to 10,000 higher than conventional spectrometers in the energy range 20 eV to 1 keV.

In the second project, Division staff are part of a consortium of 10 principal investigators from 8 major laboratories representing industry, universities, and government. This "Materials Research Group", funded principally by NSF, is studying surface magnetism using spin polarized photoemission techniques on materials prepared with molecular beam epitaxy methods. This work is being done on an undulator beamline at NSLS.

As can be seen in the following sections, the Division staff have been active in publishing research papers, providing calibration services, presenting invited talks, sponsoring conferences, providing consultation services, and participating in technical and professional committees. We have also been active in technical collaborations within NIST and with universities, industry, and other government agencies. Some highlights of the past year include:

1. A workshop on SEMPA was organized at the IEEE International Magnetics Conference. About 200 scientists and engineers attended the 1 1/2 hour tutorial. Potential applications were discussed by a panel of scientists from Carnegie Mellon University, M.I.T., Honeywell, Inc, and Control Data Corporation.

2. Our scanning tunneling microscope was used to measure the transition from atomic behavior to metallic behavior in atomic scale clusters of Fe atoms adsorbed on a GaAs substrate. If the 10-30 A clusters are considered to be the ultimate magnetic "bit", they would represent a million-fold improvement in information storage density.

3. SURF-II had a record, stored-beam current of 302 mA in March, 1989, and a record average of 215 mA during April-September, 1989, about 20% higher than last year's record. Increased current means increased flux. Experiments can be done faster, more sophisticated measurements can be made, and the quality of the work is higher.

4. Special narrow band XUV photometers (filtered detectors) were developed, in collaboration with industry, and calibrated at SURF-II for user applications. One of the photometers, about the size of your thumb, was flown on a solar sounding rocket.

5. An enhanced XUV optics program was initiated at SURF-II to provide measurement services to scientists and engineers developing and using high efficiency, multilayer, soft x-ray optical devices. New collaborations were established with AT&T Bell Labs, IBM, Lawrence Livermore, Lawrence Berkeley, Princeton University, Johns Hopkins University, U. Arizona, U. Colorado, and Ovonics Corporation.

6. A new "competence" project for "Advanced Studies in Laser Cooling and Trapping" was initiated as a collaboration between three Divisions with expertise in atomic, molecular, and optical physics. The Electron and Optical Physics Division, in collaboration with U. Maryland, is developing a vuv laser source to cool hydrogen atoms to within a few K.

7. A new data service was established to support the development of advanced methods of elemental and isotopic analysis. The service provides formatted data and application sheets to permit the routine use of laser resonance ionization techniques in analytical chemical measurements.

8. Thirty two major visiting scientist collaborations were active in FY89: 11 in the Far UV Physics Group; seven in the Electron Physics Group; and 14 in the Photon Physics Group.

FAR UV PHYSICS GROUP

Far UV Detector Calibrations (L. R. Canfield, N. Swanson, and J. Kerner)

An ongoing calibration service, now listed in NIST Special Publication 250, is the calibration of specially selected far ultraviolet detectors for quantum efficiency in the spectral region 5-254 nm. This is accomplished at two facilities: a dedicated beamline at the SURF-II synchrotron radiation facility for the region 5-50 nm; and a vacuum ultraviolet radiation facility for the longer wavelengths. Transfer standard detectors are made available to outside users involved in a wide variety of research disciplines in the far ultraviolet, such as plasma diagnostics, aeronomy, astronomy, solar physics, etc. This competence has served the radiometric detector needs of the space community for almost twenty years. Over this period, several hundred calibrations have been furnished; during FY89 an additional 26 services were provided.

At present, two types of photoemissive photodiodes cover the entire far uv region: a NIST-fabricated windowless photodiode for the 5-122 nm region; and a MgF2-windowed photodiode, made to NIST specifications, for the 116- 254 nm region. Working standards of both types derive their calibration from rare gas ionization chambers, which are an absolute detector in a portion of the region covered (5-92 nm). For the longer wavelengths, a special windowless thermopile is used to transfer an ionization chamber calibration to longer wavelengths. These standards are then used to calibrate, by intercomparison, outgoing transfer standards of the same type, or to recalibrate similar standards previously issued.

In a collaboration with industry, a new detector type is under study to assess its suitability as a transfer standard in the far uv. This is a new kind of silicon photodiode developed to meet radiometric quality criteria in the far uv. It has been determined thus far that the efficiency of these devices can be far greater than the present standards, reaching an improvement of almost 300 times at the shortest wavelengths. Less sensitivity to surface contamination, a common potential problem with vacuum system environments, is also a benefit as compared with the windowless photoemissive photodiodes. The nature of semiconductor fabrication is such that it lends itself to the relatively economical creation of high-efficiency array detectors for the far uv.

SURF-II Operations (L. Hughey, A. Hamilton, R. Madden and W. Wooden)

The performance of SURF-II continues to improve. The average beam current for this year is 203 mA (last year it was 170 mA) while the average for the last six months is 215 mA. A new record beam of 302 mA was achieved on March 16, 1989, by SURF operator William Wooden. Beam lifetime at full energy continues to improve as well. The beam current-lifetime product now exceeds 700 mA-Hr. SURF-II availability remains high. Throughout the year, beam was provided to users approximately 95% of the scheduled beam time (9 hours/day, 4 days/week) with a high of 98% during the period from August 1988 to January 1989.

The improvements in beam current and in beam lifetime have come about both from changes to existing parts of the system and refinement of others. In the former category, the microtron injector performance has been enhanced by reducing the complexity of the interconnections among the various timing circuits. This in turn reduced the time jitter in the system and thus allowed the operator to make more subtle adjustments during the tuning process. In the latter category, a nearly continual refinement takes place in the programs which control the correction coil currents and RF energy while the ring is ramping from injection to full energy. In addition, a periodic evaluation is made of the phase of the RF cavity signal to adjust for maximum lifetime under varying ring conditions.

During FY89, a new cryopump was installed on the microtron. This has reduced the cycle time for repairs or adjustments to the microtron RF cavity or the microtron filament from more than a day to a few hours.

SURF-II Users Programs (R. Madden)

SURF-II was used by a variety of NIST and outside users in FY89 for spectrometer and detector calibrations and for research in surface science, molecular physics, and uv and soft x-ray optical physics. Heavy use was made of the surface science beamlines. This group expanded operations this year by establishing a completely refurbished station on BL-1, and moving the earlier experimental chamber to a toroidal grating monochromator on BL-8. The detector calibration beamline, BL-9, was also used extensively for photodiode calibrations and other measurements on optical devices. The high resolution spectrometer on BL-3 was operational this year, doing research on rare gases and molecular nitrogen. The reflectometer on BL-8 was also used heavily in the latter part of the year for the study of multilayer systems, in a cooperative program involving many outside researchers. The high flux normal-incidence monochromator on BL-5, unused earlier this year, is now being used for the experimental development of timing circuitry in preparation for two photon pump-probe experiments, and two outside user groups are preparing to use it during the next year for both gas and solid state experiments.

A. Surface Science Beamline, BL-1 and BL-8 (R. Kurtz and S. Robey, Surface Science Division, CAMOP, R. Stockbauer, Louisiana State Univ.; T. Madey, Rutgers Univ.)

The NIST research efforts in surface science are supported at SURF-II with two beamlines and associated ultra-high vacuum chambers that are used for a wide range of studies of solid surfaces. The principal experimental technique applied in these efforts is ultraviolet photoelectron spectroscopy (UPS), where variable-wavelength photons are used to probe the valence electronic structure of bulk solids and the molecular orbitals of adsorbed species. In addition, photon stimulated desorption (PSD) of ions from surfaces is studied to elucidate the mechanisms involved in radiation damage of materials. These studies have shown that the atomic-scale structure of defects and steps may be revealed by stimulated desorption techniques.

Photoemission has been used to study the initial stages of chemisorption of simple molecules on oxide surfaces. This work, a collaboration with the Instituto Ciencia de Materiales of Madrid, looked at the interaction of H_2O and NH_3 with TiO_2 surfaces and discovered that new models are required for dissociation of these species on oxide surfaces. These models profoundly impact thinking for the mechanism involved in the catalytic activity of these model systems.

As part of the surface standards program, improvements on a technique for measuring electron attenuation lengths have been made. New substrate materials have been used in these overlayer measurements, different measurement geometries have been studied, and a new technique for dosing the surface has been explored. These improvements have resulted in data of improved quality.

The exciting work being pursued on high-temperature superconductors has continued with single-crystal superconductors being investigated. Photoemission measurements that can be compared directly with band structure measurements have been made. In addition, studies of the chemistry of these oxides has been extended to include a wider range of materials and have shown that materials improvements can have a substantial positive impact on the chemical stability of these materials upon exposure to atmosphere.

Since the first application of high-T_c superconductors will come in the area of thin-film devices, the photoemission measurements at SURF-II are being extended to include thin-film superconducting materials produced in situ. A research-scale molecular-beam epitaxy chamber is presently under construction to produce the thin films by co-evaporation. Detailed investigations of the factors affecting the epitaxial growth of high-T_c superconductors on different substrates can be pursued as well as such things as the effect of substrate interactions and buffer layers.

The Surface Science Division has played a strong role in developing techniques and instrumentation for studies of both electron-and photon-stimulated desorption processes. A large effort has been devoted to the development of an ellipsoidal-mirror analyzer and this instrument has been installed on Beamline 1. Initial testing indicates that the analyzer is operating within design expectation. Photoemission and ion desorption spectra have been obtained and the next phase in making the instrument fully operational will involve the refinement of the angle-resolving capabilities. This will allow us to simultaneously measure charged-particle kinetic energies, mass, and angular distribution as a function of the incident photon wavelength that stimulates the emission process. These measurements will result in a more complete description of the systems of interest than had been possible previously.

B. Radiometric Instrumentation Calibration, BL-2 (M. Furst and R. Graves)

The synchrotron radiation from the SURF-II storage ring is used as an irradiance standard for characterizing instrument response over a wide range of wavelengths from 4-400 nm. There were 16 instruments calibrated by 8 user groups over a period of 35 weeks during FY89. Facility users included NASA/Goddard Space Flight Center, North Carolina State University, Laboratory for Atmospheric and Space Physics/University of Colorado, Space Sciences Laboratory/University of California at Berkeley, Lawrence Livermore National Laboratory, and Space Sciences Center/University of Southern California.

Several improvements were made to the facility. A cryopump was added to the beamline at the 11 m station to decrease the amount of time necessary for evacuating user instrumentation and for baking out beamline components for both user stations. The vacuum chamber gimbals drive system was redesigned and the angular range of motion was increased. Data transmission rates for the 17 m station were increased by a factor of four over previous rates.

C. High Resolution Spectrometer, BL-3 (M. Ginter and D. Ginter, Univ. of Maryland; R. Morrison, Talladega College; D. Cleary, Naval Postgraduate School, Monterey, CA; H. Morgan and J. Fortna, Univ. of District of Columbia)

In the first set of experiments since being installed at SURF-II, the 6.65m high resolution spectrometer was used to perform a high resolution photoabsorption study of N_2. The work was motivated by the need of the atmospheric physics community to resolve an inconsistency between plasma density measurements of the F2 region of the ionosphere by various remote sensing techniques. The problem required detailed knowledge of the N_2 absorption cross section near O^+ emission lines. Preliminary measurements made here this year are consistent with lower cross section values proposed by D. Cleary, and it is intended to continue the study in the near future.

New users this year are a group from Univ. of District of Columbia, led by H. Morgan and J. Fortna. They plan to join in improving the N_2 photoabsorption measurements, and to extend studies to other atmospheric gases.

D. Optical Properties of Materials, BL-8 (E. Saloman and J. Kerner; J. Roberts, Atomic and Plasma Radiation Division, CAMOP; R. Keski-Kuha, Goddard; D. Husk, Univ. of Virginia)

The 2.2 m grazing incidence spectrometer and reflectometer chamber on BL-8 were used to measure reflectivity of various multilayer samples, as well as deposited metal mirrors. The measurements of these samples have been made for the wavelength region between 80 and 500 Å. Samples from different laboratories, including the University of Arizona, the University of Colorado, Johns Hopkins University, NASA, Lawrence Livermore, Lawrence Berkeley, IBM, AT&T Bell Labs, Princeton University, and Ovonics

Corporation have been measured. Collaborations with some of these and other institutions, including Bell Labs, have been set up for future experiments in lithography and biological microscopy.

The measurement and vacuum systems have been improved and new sample holders for flat as well as curved samples have been incorporated. In order to properly address the new emerging technology of soft x-ray optics characterization, further improvements of the existing apparatus are planned. Plans for a new computer controlled monochromator and reflectometer chamber are underway. Plans also include a capability of in-situ thin film deposition and load-lock sample introduction.

E. Detector Calibration, BL-9 (L. R. Canfield and J. Kerner)

Beamline-9 is a dedicated detector calibration facility that is routinely used to calibrate standard detectors for the spectral region 5-50 nm. Detectors are calibrated by intercomparison with a working standard, which has been previously calibrated in this same facility using a rare gas ionization chamber as the absolute reference. The continuum radiation from SURF-II is dispersed by a toroidal grating, giving monochromatic light of approximately 1 nm bandpass for calibration purposes. The ionization chamber is pressurized with a rare gas, usually neon, while the ultra-high vacuum of the storage ring is protected by a transmitting thin film filter sealed to the ionization chamber.

During FY89, several research activities were also carried out with this facility.

(1) Special thin film filters were characterized for two different groups involved in rocket studies of solar flux, and for one of these groups, a narrow bandpass solid state detector, i.e., an XUV photometer, was calibrated for a similar application.

(2) The photoemission and transmission of diamond thin films was measured, as were several metals interesting as far uv filter materials.

(3) A proportional counter system was assembled and attached to BL-9 to evaluate the purity of the dispersed radiation in the 45-60Å region. It is extremely difficult to measure the degree of impurity contamination present in the dispersed radiation with the detectors normally calibrated in this system, but the proportional counter, which can be used as an absolute detector, can be quite discriminating against impurities from longer wavelengths. Thus such a counter gives an independent method of absolute detection, and can also be used for the evaluation of scattered light.

(4) A study of special silicon semiconductor photodiodes, optimized for use in the far uv, continues on this beamline in collaboration with United Detector Technology, Inc. These photodiodes have considerably more efficiency that the windowless standards presently used--as much as a factor of 300 at 70 nm--and are a likely candidate as an alternate standard for the future. Recent studies on BL-9 have shown immunity to radiation damage in the 5-50 nm region, and the spatial uniformity has been shown to be quite acceptable. In the region 50-160 nm some radiation damage

manifests itself with extensive exposure, and this is currently under study. The long-term stability continues to be monitored.

ELECTRON PHYSICS GROUP

The Electron Physics Group has ongoing research efforts in electron collision physics including electron-atom collisions, electron-surface interactions, surface magnetism, electron interaction theory, electron polarization phenomena, tunneling and scanning electron microscopy, and electron optics and instrumentation. The wide applicability of electron-based measurement technologies allows us to contribute to the solution of many diverse scientific and technological problems.

In the past year, we have seen significant achievements in all of our areas of research. The STM has been used to characterize metal induced band gap states and the SEMPA project has coupled theory and experiment to greatly improve our understanding of domain wall structure. The electron atom scattering experiment has obtained its first elastic scattering data and a greatly improved spin detector has been developed for the NSLS polarized photoemission project. Our theory efforts include an important paper on polarized metastable de-excitation and a good start on high Tc superconductivity. Our interactions with industry continue to be strong, as do our other collaborative efforts.

We continue our focus on interfacial phenomena with special emphasis on the use of microscopy to study microstructures, clusters, defects, growth, and dynamics on the atomic scale. Our SEMPA work involves studying the effects of size, dimensionality, shape, topography and epitaxial substrate on magnetic microstructures. The photoemission experiments focus on understanding magnetic phenomena in novel epitaxial systems through measurements of spin resolved band structure. Our STM measurements investigate the electronic structure of atoms, molecules, clusters, and microstructures on surfaces. The STM allows us to study the growth of microstructures with atomic resolution. It also permits us to verify, for example, that the novel epitaxial structures we grow have the physical structure we planned and that their observed magnetic phenomena results from our tailoring of the physical structure.

This year, we have also begun new experimental efforts in magnetic scanning tunneling microscopy and the optical control of metal atom beams. In order to permit these new activities, we are phasing out our work on inverse photoemission and temporarily limiting our involvement at NSLS.

Magnetic Microstructure Research (J. Unguris, M. R. Scheinfein, R. J. Celotta, D. T. Pierce, and M. H. Kelley; M. Aeschilmann, ETH, Zurich)

We are using scanning electron microscopy with polarization analysis (SEMPA) to investigate the micromagnetic structure of ferromagnetic materials. The SEMPA technique was developed at NIST and involves the combination of an ultrahigh vacuum scanning electron microscope (SEM) with electron spin polarization analyzers in order to measure the polarization of secondary electrons emitted from the specimen. In transition metal ferromagnets the spin polarization of the secondary electrons is directly proportional to the polarization of the electrons within the ferromagnet. Polarization analysis of the secondary electrons provides a direct measurement of the magnitude and the direction of the magnetization in the region probed by the incident electron beam. SEMPA can therefore image magnetic structures, such as domains and domain walls, with the highest spatial resolution available of any technique for looking at magnetic structures in reflection. The SEMPA images are quantitative, measuring the magnitude and direction of the magnetization direction at any one point, and the images of the magnetization are independent of specimen topography, which is, however, measured simultaneously. In addition, SEMPA is an ideal probe of surface and thin film magnetism, because the escape depth of the secondaries is only a few nm.

Our new SEMPA facility, which consists of a JEOL model JAMP-30 Auger microprobe fitted with NIST designed gold film polarization analyzers, has been operating flawlessly for the past year. The SEMPA system can image magnetic structures with a measured spatial resolution of 40 nm (0.04 microns). In addition, the Auger microprobe feature enables us to map the chemical composition with about the same resolution and from the same area as the magnetic and topographic images. This provides us with a unique tool to study the relationships between magnetic microstructure, surface composition, and surface topography. A second SEMPA apparatus, the result of a collaboration between the Electron Physics Group and a commercial manufacturer, is scheduled to come on line in February, 1990. In addition to relieving the heavy demand on the current apparatus, the new SEMPA is expected to improve our spatial resolution to less than 10 nm.

We have investigated the surface magnetic domain structure of a large variety of transition metal ferromagnets such as: iron and cobalt single crystals, iron whiskers, ferromagnetic metallic glasses, and NiFe films of various thicknesses and compositions. An especially interesting domain pattern was observed for a cobalt crystal which had its c axis, the easy magnetization direction, perpendicular to the surface. The domain structure had magnetization components both in the surface plane and perpendicular to the surface. <u>This is the first time that anyone using SEMPA has observed a perpendicular magnetization</u>.

We have also used SEMPA to make quantitative, high spatial resolution measurements of surface domain walls and the fine structures within the domain walls. These measurements tested the accuracy of micromagnetic models that were used to calculate surface and bulk magnetization distributions. The agreement between measured and calculated properties, such as domain wall profiles, was excellent. This agreement gives us confidence that the micromagnetic models can be used to predict magnetic properties that cannot be directly measured by SEMPA, such as domain wall structures inside of the ferromagnet or magnetic field distributions inside and outside of the material.

We are beginning to investigate the magnetic structure of thin ferromagnetic films. The surface sensitivity of SEMPA makes it an ideal tool for looking at films that vary in thickness from a monolayer to a few tens of layers. The films can be deposited and analyzed by Auger spectroscopy, reflection high-energy electron diffraction, and SEMPA, all in the same chamber. In this work we will investigate whether domains exist in thin films, how the domain structures vary with thickness, and how the films magnetically couple to other films or magnetic substrates.

In addition to basic research, we have continued to collaborate with private industry by using SEMPA to help solve applied magnetics problems. One example of this is our work with Seagate Magnetics in which we investigated the magnetic structure of written bits in various hard disc memory media. We found that, in noisy recording media, the written bits were not clearly separated by sharp boundaries, but instead were magnetically bridged together, resulting in low signal-to-noise during read-back.

In addition to Seagate Magnetics, we have worked on applied magnetics problems with Digital Equipment Corp., Honeywell Inc., Imprimus, Phillips Research Labs, and Westinghouse Electric Corp. We have also worked on transferring SEMPA technology by consulting directly with university and industrial labs that are in the process of building their own SEMPA systems and by conducting a SEMPA workshop at the IEEE International Magnetics Conference. These collaborative efforts have been scientifically fruitful, intellectually stimulating, and mutually beneficial.

Scanning Tunneling Microscopy (J. Stroscio, R. Dragoset, P. First, D. Pierce, and R. Celotta)

The aim of the scanning tunneling microscopy (STM) program is to investigate novel properties of matter that occur in small size structures on the nanometer scale, and to develop advanced techniques which further the application of scanned electron probe techniques. The STM operates by bringing a sharp probe tip to within atomic dimensions of a specimen. A current flows from the tip to the surface by the quantum tunneling of electrons due to the proximity of the tip to the surface. By scanning the tip over an exposed surface, information is obtained about the structural and electronic properties of the examined specimens. The device operates with a lateral resolution of 2-3 Å, and thus is a natural tool for examining the physics of small scale structures. This is particularly meaningful as microfabrication technology is reaching the ultimate limit (which is one atom) in devices with structures on the order of 100 Å ($0.01 \mu m$) wide.

We have been examining metal structures grown on GaAs(110) surfaces. GaAs is thought to be the semiconductor of the future because of its high speed properties. One of the experiments we have focused on this year is growing epitaxial Fe films on GaAs, with the intention of future studies on the magnetic properties of thin films in coordination with SEMPA experiments. In these experiments we have shown that the Fe grows by initially forming small 3-dimensional clusters instead of a continuous monolayer film. By monitoring how the tunneling current changes with electron energy, we have determined that small clusters are not metallic and larger ones with greater than 35 atoms display fully metallic characteristics. In addition, in this work we have been able to spectroscopically image (by imaging at different electron energies) the gap states that form in the GaAs semiconductor due to the presence of Fe clusters on the GaAs surface. These results are the first to show direct evidence for metal-induced gap states, which have been theoretically predicted in theories of metal-semiconductor interfaces.

In examining ultimate limits in physical properties of small scale structures, we have investigated one-dimensional Cs structures on GaAs(110) which are only two atoms wide and many hundreds of atoms long. These structures thus represent the smallest possible metal-atom lines or "wires" that could be made and offer insight into the physical properties of such small scale structures. Using the STM, we have shown that such narrow "wires" are not metallic, even though bulk Cs is metallic, and hence these atomic "wires" would not conduct electricity if used in devices.

A second STM is currently being completed. It has an advanced design allowing much higher scanning speeds than the previous instrument. The instrument is housed in an ultrahigh vacuum system with sample characterization facilities such as low energy electron diffraction and ion sputtering. The system also has two additional instruments, a field emission microscope to prepare ultra-sharp single atom tips and an electron spin detection system coupled with the STM. The aim of this system is to extend the study of magnetic microstructure to atomic dimensions. The electron spin detector will be used to measure the spin of electrons scattered from the surface during tunneling in the STM. The STM has already demonstrated a scanning ability 10-50 times faster than the older instrument. Detection of spin-polarized electrons from the STM junction will proceed in FY90 with the hope of opening up a new frontier in micromagnetism.

<u>Electron - Atom Collisions Studies</u> (M. Kelley and J. McClelland; S. Buckman, Australian National U.)

Our purpose is to study, in as complete a manner as possible, the interactions important in low energy collisions between electrons and atoms. We use optical state preparation techniques to prepare beams of electrons and atoms in well defined quantum states and perform scattering measurements to determine the dependence of various collision cross sections on the initial state of the incident electrons and atoms. Such state-selected experiments provide substantially more information about the collision than is available from conventional measurements of differential scattering cross sections. We are particularly interested in the influence on the collision of the spin state of the incident electrons and atoms. Determination of this spin dependence provides direct information about both exchange and the spin-orbit interaction, and provides a stringent reliability test for current theoretical scattering calculations.

We have made spin dependent measurements for both elastic and inelastic scattering. The most recent <u>elastic scattering measurements</u> were performed at an incident electron energy of 20.0 eV, at scattering angles in the range from 20 to 140 degrees. Our results show a strong dependence in the scattering cross section on the relative spin orientations of the incident electrons and atoms, indicating that exchange effects are rather important in collisions at this energy. The spin-orbit interaction is seen to play a less important role at this energy. Comparison of state-of-the art electron scattering calculations with these measurements demonstrates the need for further theoretical work on this collision system.

We have also studied <u>inelastic scattering</u> by way of superelastic scattering from the first excited state. Spin-polarized and oriented sodium atoms are prepared in the excited 3P state by optical pumping with circularly polarized light. By detecting only electrons that have de- excited these atoms and gained the 2.1 eV excitation energy of the atoms, we are able to study the 3S - 3P transition with great detail. Our most recent measurements were at an incident energy of 17.9 eV. This incident energy, for superelastic scattering, corresponds to inelastic excitation from the ground to the first excited state at an incident energy of 20 eV. We find that exchange effects, while still significant, play a somewhat less important role in the inelastic collisions at this energy than in the elastic collisions.

A systematic search was also carried out for a spin dependence which requires that both exchange and the spin-orbit interaction play a significant role during the collision. This effect would cause the cross section for scattering to some angle to depend on the spin orientation of the target atom, independent of the spin of the incident electron. In the absence of either exchange or the spin-orbit interaction, this dependence must vanish. We observe both exchange and spin-orbit effects near minima in cross section for elastic scattering at incident energies from 20 eV to 100 eV, but, within our experimental precision, find no evidence of this joint effect.

Our current efforts are directed at extending the energy range in which our elastic and superelastic measurements are possible. We wish to perform elastic scattering measurements at energies below the ionization threshold of 5.1 eV, where theoretical calculations are expected to be quite good. We will then be able provide both elastic and inelastic data over the range of energies from somewhat below to several times the ionization threshold. This is a important energy region for many physical processes, but for which many current scattering calculations have severe difficulties.

Spin Polarized Photoemission at NSLS (D. Pierce and R. Celotta)

We have been participating in an effort at the National Synchrotron Light Source (NSLS) to study novel magnetic systems created in situ by molecular beam epitaxy (MBE). To date, the work has concentrated on the establishment of a spin-polarized, angle and energy resolved photoemission apparatus on the U-5 beamline of the UV storage ring.

This project is unique in a number of ways. First, the research team consists of 10 principle investigators from 8 institutions nationwide. These are national labs (NIST, Argonne, NRL, and NSLS), universities (Rice, Texas at Austin, and Northwestern) and an industrial lab (AT&T Bell). This group functions both as an NSF Materials Research Group as well as an NSLS Participating Research Team. Second, the beamline is the only spin polarized facility in the United States and the only one in the world with a movable spin analyzer to permit angular studies. Third, it is one of the few beamlines in the U.S. to have an MBE capability. Finally, because of the demanding nature of the experiment, we are fortunate to have the highest flux UV beamline at NSLS. It is based on an undulator currently installed in a straight section of the ring. During the next year this same group, acting as an Insertion Device Team, will install a new state-of-the-art undulator now under construction.

The beamline has been used to take spin polarized photoemission data. In the first experiment, our colleagues at NSLS examined the angle resolved spectra of Fe(110) both in a clean state and with adsorbed sulfur. The ability to make both angle and spin resolved photoemission measurements extends greatly previous work and, even in the first experiments, calls into question previous interpretations made in the absence of spin resolved data.

Measurements have begun on the Fe/Cu(100) and Fe/Pd(100) system. The first few layers are thought to grow epitaxially as fcc Fe, as opposed to the normal bcc form. The object of the experiment is to observe the magnetic properties, e.g. anisotropy, Curie temperature, remanence, magnetization, etc., as a function of layer thickness and growth methodology, and to correlate them with the spin dependent electronic structure we measure. The lattice is expanded in going from Cu to Pd, which should promote ferromagnetism. Furthermore, from alloy data Pd is expected to be polarizable, which may lead to interesting electronic and magnetic structure effects for the thin films. Analysis of the data is currently in progress. We expect this facility to greatly extend our ability to study new and interesting magnetic systems.

We have decided to limit our participation in experiments at the facility owing to other priorities. We will maintain our commitment to provide our state of the art spin polarimeters for the experiment. However, we expect to carry out spin polarized photoemission measurements only when we perceive an exceptional scientific opportunity, or when there is a demand for particular information for our experimental program at NIST.

Electron Optics (M. Kelley and M. Scheinfein)

We continue to update our capabilities for the design and characterization of new electron-optical instruments. Sophisticated numerical algorithms are used to compute electrostatic and magnetic lens fields, and improved methods of determining the optical properties of these fields are used. Paraxial and aberration properties can be accurately determined for both electrostatic and magnetic lenses. Non-paraxial, all-order, electrostatic ray-tracing is also used for accurate modeling of novel designs. Furthermore, a third order matrix method has been developed for use in the design and characterization of our electron optical systems.

Significant effort has been spent on the electron optical design of a polarized electron detector for a scanning tip microscope. A tunnelling tip may be pulled away from the surface, and electrons may be extracted by applying a potential between the sample and the specimen. This scanning field emission tip microscope will be used to probe magnetic microstructure of surfaces. The magnetic microstructure is accessible through analyzing the spin-polarization of the electrons excited near the surface of the specimen. It is hoped that this instrument will have 100-Å spatial resolution.

Finally, the electron optical properties of an inhomogeneous field Wien filter were investigated using the matrix method. The inhomogeneous field Wien filter possesses point-to-point focusing. It also may be used as an electron spectrometer, mass-filter, and spin rotator. We plan on using the longitudinal-to-transverse spin-rotation with the point-to-point focusing properties of the Wien filter in future SEMPA implementations to eliminate the need for the 1/4-sphere deflector and one of the electron spin detectors.

Electron Theory (D. Penn)

Our purpose is to study various aspects of electron-electron interactions in solids with application to high T_c superconductivity and surface magnetism.

We have completed the first theory of spin polarized metastable de-excitation spectroscopy. Metastable spin polarized He^* atoms incident on a Ni surface undergo de-excitation in a process which yields electrons from the Ni. The number produced is observed to depend on the relative spin of the Ni and the He^* atoms. The normalized difference in the ejected electron intensity produced by He^* atoms with opposite spin polarizations increases dramatically with increasing kinetic energy of the electrons. We find that the experimental results can be reproduced by theory only with the use of a realistic potential for the Ni electrons in the vacuum region. With such a potential it is found that He^+ ions which result from the He^*-surface interaction are neutralized approximately 4.5 Å from the Ni surface, a much larger distance than given by previous estimates. We also show that the experiment reflects the polarization of Ni electrons at the He ion and it is estimated that the Ni magnetization at the Fermi energy and far from the Ni surface is -20%.

In collaboration with Prof. M.L. Cohen (U.C. Berkeley) the effect of local fields on superconductivity are being studied. We have completed a theory of the total dielectric function which forms the basis for the present work. The total dielectric function approach allows the inclusion of both coulomb and lattice screening in a single dielectric function and thus allows a unified approach to superconductivity that includes local field (lattice) effects. We will proceed by developing a specific model for the dielectric function to examine the interplay between Tc, electron-phonon coupling, local field effects, and lattice stability.

PHOTON PHYSICS GROUP

The Photon Physics Group investigates the interaction of electromagnetic fields on atoms and molecules in various environments in support of radiation measurements and standards programs important to NIST and the outside technical community. This work includes theoretical and experimental studies on the electronic structure of atomic and molecular systems in field-free environments, in crystalline environments (atomic effects in solids), and in strong external fields. The focus is on VUV photoexcitation and photoionization in gases and solids and on multiphoton laser-atom interactions.

Collaborative work is directed toward the laser cooling of atomic hydrogen, laser isotope separation and analysis through resonant multiphoton ionization, and the identification of highly excited states suitable for a soft x-ray laser. For many of the activities, the synchrotron radiation from NIST-SURF-II or Brookhaven-NSLS is used as a source of tunable vacuum ultraviolet and soft x-ray radiation.

Generation of Coherent VUV (P. Lett and T.B. Lucatorto; T.J. McIlrath and Q. Li, U. of Maryland)

Two exciting scientific opportunities have recently arisen within CAMOP: the possibility of laser cooling atomic hydrogen and the possibility of making a precise test of the theory of two-electron QED and relativistic corrections through the measurement of the Lamb shift in ground state He. The cooling of atomic hydrogen will require the efficient generation of coherent radiation at the Lyman-α wavelength, 121.6 nm; the experimental determination of the He ground state Lamb shift requires radiation at 120.4 nm. We shall attempt to generate these two wavelengths by exploiting the recent advances in laser technology represented by the Ti:sapphire laser and the β-barium borate (BBO) non-linear crystal.

The presently proposed upconverison schemes would use tunable Ti:sapphier or dye lasers and BBO non-linear crystals to generate radiation in the range of 205 nm to 208 nm which is then used in resonantly enhanced, four-wave ($2\omega_1 - \omega_2$) mixing schemes in mixtures of Kr:Ar or Xe:Ar. The new capability for efficient generation of radiation in the range 205 nm to 208 nm provided by BBO allows us to effectively pursue these $2\omega_1 - \omega_2$ schemes which should have considerable resonant enhancement of efficiencies as compared to those previously obtained;preliminary estimates based on early experiments with BBO lead us to expect four-wave mixing efficiencies of 10^{-3} (as opposed to 10^{-4}-10^{-5}).

The development of sources to laser cool hydrogen will be done in two stages. First we shall build a 10 Hz source to cool hydrogen confined in a magnetic trap or "bottle". Such traps have been constructed by several of our colleagues. One uses a He dilution refrigerator to cool spin-aligned hydrogen to a temperature of T=80 mK. These atoms can be trapped for a period of many minutes. The application of a pulsed 10Hz laser source of Lyman-α will cool the trapped H to approximately 7.5 mK, which would allow further experimentation on Bose-Einstein condensation and collisions at ultra-cold temperatures to proceed.

The second stage will be the development of a more powerful source to decelerate H formed by dissociation of H_2 at liquid nitrogen temperature (77K). This capability will free us from the need to use a He dilution refrigerator. This source will use either a series of 100 picosecond mode-locked pulses at a 100 MHz repetition rate in a 10 microsecond macro-burst or a single 5 microsecond pulse to decelerate and cool the hydrogen beam. The construction of such a source will advance the state of the art in coherent VUV generation and benefit other areas such as spectroscopy and plasma diagnostics.

The experience gained in developing the Lyman-α source will be applied to developing a 120.285 nm source for the precise measurement of the He ground state energy. Presently the spectroscopy group in the Atomic and Plasma Radiation Division has an ongoing program to provide highly accurate laser spectroscopic measurements (uncertainties of several MHz) of many He excited state energy levels, including the $1s2s^1S$. Because the ground $1s^{2\,1}S$ is over 21 eV from the lowest single-photon allowed excited state, no laser measurement has yet been made of the ground level, and the best present value is derived from conventional grating-based spectrometry with an uncertainty of 4.5 GHz. We plan to measure the $1s^{2\,1}S$--$1s2s^1S$ energy separation by a laser-induced two-photon transition between the two levels with the 120.285 nm source. The preliminary accuracy is expected to be in the range of 150 MH_z, or about 30 times better than the present status. This measurement will be compared to the new theoretical values of the two-electron Lamb shift being calculated by Peter Mohr in the Atomic and Plasma Radiation Division and others.

Soft X-Ray Emission Studies of Advanced Materials (D. Ederer and D. Mueller; T. Callcott, U. Tennessee; J. Rubensson, U. Uppsala)

Soft x-ray fluorescence can provide important information about the electronic states of solid state materials. Fluorescence measurements can be used to study the properties of alloys, impurities, clusters, surface layers, organics, and other fragile compounds. A novel, high sensitivity soft x-ray spectrometer especially deigned for fluorescence measurements has been in operation at the NSLS for almost three years now and is the proud accomplishment of a joint NIST - Tennessee-Oak Ridge National

Laboratory collaboration. Recent experiments have proven it to be one of the best instruments in the world for soft x-ray fluorescence measurements.

The unique capabilities of the instrument have attracted a number of collaborators including scientists from U. Hawaii, U. Connecticut, U. Uppsala, AT&T Bell and Bellcor Laboratories, and the NIST Institute of Materials Science and Engineering (IMSE). The collaboration with AT&T has focussed on studies of thin film and single crystal samples of $YBa_2Cu_3O_{7-e}$ produced at the Bellcor Division. Through collaboration with our IMSE colleagues, we have continued our studies of the $YBa_2Cu_3O_{7-e}$ and Bi-Sr-Ca-Cu-O superconducting ceramics. This last area of research has been funded as part of a DoC initiative on high temperature superconductors.

A few of the highlights of this program are:

a) High Tc Superconductors:

We have made use of soft x-ray emission spectroscopy to examine the electronic structure of bulk $Bi_2Sr_2CaCu_3O_8$ and $Nd_{1.85}Ce_{0.15}CuO_4$ samples, and to compare the electronic structure of thin film $YBa_2Cu_3O_7$, and $Bi_2Sr_2CaCu_3O_8$ samples with the electronic structure of well characterized bulk samples of these materials. Our results are in good accord with current theoretical models. This fact is particularly significant because of the key role theoretical modeling of the electronic density of states has in the development of a physical understanding of the superconducting process. Because soft x-ray emission spectroscopy probes the bulk below the surface, our results were not sensitive to changes due to possible loss of oxygen from the surface region when superconducting cuprates are exposed to ultra high vacuum at room temperature.

b) Electronic Structure of Semiconductor Materials:

Dramatic changes in the silicon $L_{2,3}$ emission spectrum are observed as the excitation energy is varied from the 2p binding energy at 100 eV to 144 eV. It is proposed that a spectator electron, close to the bottom of the conduction band, influences the valence band electrons. The observations indicate that shake up is important in the excitation process and that the population of low-lying levels, via the initial state shake up, influences the high-energy excited silicon L emission spectrum.

c) Instrumentation Improvements:

This year we have put a transmission grating monochromator into service. This device selects a narrow band of the continuum radiation from the storage ring to excite the fluorescence. Fluxes between 10^{12} and 10^{13} photons/sec. are readily obtainable in a band width of about 4 eV. Results have been obtained from the superconductor materials and from silicon samples as described in a) and b), respectively.

A new position sensitive detector that has two orders of magnitude less noise and a factor of two more sensitivity than the old CCD detector has been installed at the soft-x-ray spectrometer at the National

Synchrotron Light Source. This detector system will permit us to obtain higher quality data in a shorter time, and to examine samples that are more dilute or more fragile than those we were able to examine to date. For example, now it will be possible to study structure changes due to radiation damage in polyimides. These polymers are of great importance to the semiconductor industry.

Synchrotron-Laser Hybrid Experiments: Quenching the Fluorescence from a Core-Excitation (D. Ederer and D. Mueller; R. Shuker, Ben Gurion University)

Interest in synchrotron-laser hybrid experiments has been on the increase during the past few years and a number of laboratories have initiated programs to used this new research capability. A number of experiments have been performed with c.w. and low repetition rate laser and synchrotron sources, but no one has synchronized a mode-locked laser to the storage ring frequency, thereby gaining control of the time interval between the laser and synchrotron radiation (SR) pulses at a high rate. We have synchronized a NdYAG mode-locked laser and VUV radiation by locking the laser to the NSLS synchrotron r.f. frequency.

This project is heading in the direction of developing new technology to explore the nanosecond and ultimately the pico and subpicosecond time regime in the VUV and soft x-ray region of the spectrum. In our first attempt to test the feasibility of the technique, synchrotron radiation was used to quench the fluorescence from a core excited solid. The localized electron-hole pair is similar to a Rydberg state. The results of the experiment can be used to infer the radiative lifetime of the exciton. Initial measurements were inconclusive. Another run is planned for FY90.

Resonance Ionization Mass Spectrometry Data Service (E. Saloman)

The techniques of Resonance Ionization Spectroscopy (RIS) and Resonance Ionization Mass Spectroscopy (RIMS) have demonstrated high elemental sensitivity and the potential for almost 100% efficiency. They should become most valuable tools for analytical chemistry. For these techniques to meet their potential, they must be made available to practicing analytical chemists. Presently much of the information needed to apply RIS and RIMS is scattered in several atomic data bases, which contain much more information than the chemists would need. It is the object of this project to organize the available data and supplement it with calculations where the many gaps exist to provide the needed information to permit the application of RIS and RIMS to routine use in analytical chemistry.

We produced the first ten data sheets in an initial simplified format for the new Resonance Ionization Mass Spectrometry Data Service. These sheets were made available for comment by researchers working in the RIS area. The RIS community showed considerable diversity in the types of RIS schemes that they believed were most important to include and as a result an expanded data sheet format was designed which included several schemes per sheet.

We calculated and collected the required information and produced the first ten data sheets for the RIS/RIMS data service in the highly expanded format. Data sheets were prepared for the elements Fe, Pb, B, C, Au, Si, As, Ge, Zn, and Cd. Arrangements were made with the editor-in-chief of the widely read analytical chemistry journal, Spectrochimica Acta Part B, for publication on a continuing basis of the RIS/RIMS data sheets in that journal. The first ten data sheets have been accepted for publication. In addition a data base of RIS/RIMS work has been established.

Resonant Ionization for Isotope Separation and Ultrasensitive Analysis
(T.B. Lucatorto; Q. Li and T.J. McIlrath, U. Maryland)

In most present applications of RIS, the selectivity of the resonantly enhanced ionization is used to distinguish between different elements but not different isotopes of the same element. (A notable exception is the laser isotope separation project at Lawrence Livermore Laboratory.) We have been using high resolution, Doppler-free RIS to explore the potential of using the optical isotope shift to add isotopic selectivity to the ionization process as a means of improving isotope abundance sensitivity in analytical mass spectrometry and of developing viable techniques for producing separated isotopes. We are currently engaged in two experiments: a study of the AC Stark effect in the $5p^5nd$ series in Xe at low n (n=5) and at intermediate n (n>13); and a study of efficient ionization pathways in Ca.

The AC Stark effects causes a shifting and broadening of the resonance in the multiphoton ionization process, a factor that can affect RIS selectivity markedly. We have chosen to look at the AC Stark effects that would arise when an intense IR laser is used to produce efficient ionization of the resonantly excited atoms. The model now used to calculate the AC Stark shifts for Rydberg levels predicts a blue shift nearly equal to the pondermotive potential of a free electron in the laser field. Recent experimental results disagree with these calculations by over a factor of two. Our work is intended to check these experiments and extend the range of the measurements in an effort to resolve the discrepancies.

Research on bone demineralization in weightlessness and in certain diseases has created large demands for samples highly enriched in the rare isotopes ^{46}Ca(0.003% natural abundance) and ^{48}Ca (0.18% natural abundance). Enriched samples are now produced by a Calutron (a large scale electromagnetic isotope separator) at costs ($3000/mg for ^{46}Ca and $260/mg for ^{48}Ca) that seriously limit the level of biomedical research activity in this field. Our goal is to find an effective Doppler-free resonant ionization pathway that will allow efficient laser isotope separation with existing laser technology. Plans are to collaborate in this research effort with Eastern Analytical Inc., a company that is part of the University of Maryland Technology Advancement Program.

Atomic Properties and Data (E. Saloman)

Relativistic multi-configuration Dirac-Fock methods have been applied to the calculation of atomic and ionic energies and transition probabilities. The initial study has been completed, an investigation of the energies and oscillator strengths in the ground state configuration of the sulfur isoelectronic sequence. Results have been obtained for all transitions within this configuration for the 77 ions from sulfur to uranium. They demonstrate striking effects in the f-values corresponding

to atomic numbers where different configurations become important. A report on these effects was published in Physical Review A. The detailed data were published in Atomic Data and Nuclear Data Tables.

This work is a collaboration with the Atomic and Plasma Radiation Division.

Soft X-ray Optics Characterization in the XUV (E. Saloman, J. Kerner)

An existing facility at the SURF-II facility has been used to characterize the transmission of filters and reflectivity of XUV devices such as multilayers, gratings, and grazing incidence optics. Users and samples from many institutions have been accommodated. Samples from U. Arizona, AT&T Bell Labs, IBM, U. Colorado/LASP, Johns Hopkins U., Lawrence Berkeley Labs, Lawrence Livermore Labs, NASA/GSFC, and NIST have been characterized. The possibility of upgrading the capabilities of the characterization facility are being explored.

This work is a collaboration with the Atomic and Plasma Radiation Division.

High Resolution Photoabsorption Cross Sections of Atmospheric Gases in the VUV (T.B. Lucatorto; D.D. Cleary, Naval Postgraduate School, Monterey, CA; R. Morrison, Talladega College; H.P. Morgan and J. Fortna, Univ. of District of Columbia)

In the first set of experiments since being installed at NIST, the 6.65m high resolution spectrometer at the SURF II storage ring was used to perform a high resolution photoabsorption cross section measurement of N_2. The work was motivated by the need of the atmospheric physics community to resolve an inconsistency between plasma density measurements of the F2 region of the ionosphere by various remote sensing techniques.

One of the most practical means of providing real time measurements of the F2 plasma density is to measure the amount of emission in the $O^+(2s2p^4\,{}^4P \text{--->} 2s^2 2p^3\,{}^4S)$ triplet centered around 834 Å. To obtain an accurate measure of the strength of this emission, one must allow for the absorption of the atmospheric N_2 between the F2 layer and the rocket-borne or satellite-borne spectrometer. The previously accepted value of the N_2 photoabsorption cross section around 834 Å was based on measurements that did not have sufficient resolution to separate the tightly spaced N_2 rotational structure in the region. It was hypothesized that instrumental averaging over unresolved features could overestimate the actual cross section at the precise wavelengths of the sharp O^+ triplet and thus lead to the observed discrepancies.

The 6.65m spectrometer at SURF II is one of only two in the world (the other is at Tsukuba, Japan) that has the capability of making accurate photometric measurements at a resolution sufficient to separate the N_2 rotational structure at the positions of the O^+ emission lines. Preliminary measurements made here this past year are consistent with the lower cross section values proposed by Cleary, but further refinements in instrumental resolution (from 0.014 to 0.006 Å) and in background determination are needed before a sufficiently accurate cross section can be provided.

In addition to improving the N_2 photoabsorption measurements at 834 Å, we plan to make other measurements in N_2 and O_2 that are of importance in remote sensing of the atmosphere. This work will be in collaboration with the University of the District of Columbia.

Theoretical Atomic, Molecular, and Optical Physics (C. W. Clark; L. Pan and S. Blodgett-Ford, U. Maryland; S. Buckman, Australian National Univ.)

As in the past few years, theoretical AMO physics in the Photon Physics Group focused on the understanding of high-order multiphoton processes and on core excitation and resonance phenomena in photoabsorption and electron-atom collisions.

(A) The study of high-order multiphoton processes within the past year concentrated primarily on the understanding of high-harmonic generation. This phenomenon, which is under experimental investigation at CEA Saclay (France) and the University of Illinois at Chicago, involves the generation of harmonic radiation in gas samples irradiated by intense lasers, the harmonic order ranging up to 30 in some cases. These observations offer the prospect of generating coherent radiation in the soft x-ray range, controlled by optical techniques applied to a driving laser that oscillates in the visible or infrared. The total yields of high-harmonic radiation that have been obtained to date are still small. However, the experimental observations show, surprisingly, that the yield does not decrease monotonically with increasing harmonic order, but rather exhibits a broad "plateau" region. In other words, in some conditions it is possible to generate 33rd-order harmonic radiation with approximately the same efficiency as 9th-order radiation. This feature obviously holds great promise for practical application, and its elucidation has been a major goal of our theoretical effort.

We have applied the Sturmian function methods developed in the past two years to the computation of the nonlinear frequency-depenedent susceptibilities of hydrogen and hydrogen-like ions for harmonic order up to 70, in the context of lowest-order perturbation theory and, recently, with the next-lowest-order correction included. The principal technical achievements of this work consist of: (1) concise description of low-order susceptibilities over the entire range of frequency by quantum defect techniques; (2) computations of frequency-dependent susceptibilities to the highest order yet reported; (3) the extension of the Sturmian method to treat photoabsorption in the continuum by use of a complex coordinate rotation technique; and (4) the first evaluations of next-order corrections to the nonlinear susceptibilities. The main qualitative conclusions we have derived from this work are as follows:

1) The plateau phenomenon has an analogue in perturbation theory, and the onset of the plateau region observed experimentally in the noble gases occurs at values ofintensity and harmonic order similar to those predicted by perturbation theory for atomic hydrogen.

2) The next-order corrections are large, which implies that perturbation theory for high-harmonic generation fails at much lower intensities than was previously thought.

We have had extensive collaboration in this work with a group at Lawrence Livermore Laboratory, who perform non-perturbative calculations with which we have made critical comparisons, and we have been in regular communication with experimental groups at CEA Saclay and the Princeton Plasma Physics Laboratory.

A new direction of research on this problem was initiated in the summer of 1989, when we began a program of direct numerical integration of the Schrodinger partial differential equation for a hydrogen atom in a time-varying radiation field. Although this work requires much further development, it has resulted to date in a functional computer code that calculates the atomic dipole moment as a function of time. This code gives correct results in the weak-field limit (as judged by comparison to perturbation theory), and exhibits a plateau for harmonic generation in strong fields.

Other related aspects of research in multiphoton processes have dealt with the description of the final state of an electron ejected from an atom by a strong radiation field and with the frequency-dependent polarizabilities of systems bound by short-range forces.

(B) Theoretical work on photoabsorption and electron collisions was done largely in collaboration with experimental groups. The most successful venture consisted of a description of the electron energy loss spectrum (EELS) associated with 4d excitation of Ba in the ceramic $YBa_2Cu_3O_{7-x}$, as measured at Innsbruck (Austria), and York U. (England). Comparison of these spectra with the total photoyield spectra acquired by the Far Ultraviolet Physics Group (as described in last year's Annual Report) showed that, even at primary electron energies of 2 keV, major EELS features were not present in the photoyield spectrum. A quantitative theoretical analysis showed that these features could be accounted for by non-dipole transitions allowed in the Bethe-Born approximation. A simple statistical model was invoked to explain the EELS spectrum at low primary energy, so that the Ba 4d loss spectra may now be considered to be understood over the full range of experimental practice. The appreciable strength of octupole 4d - 4f excitation observed in Ba suggested that the corresponding feature in Cs might exhibit high sensitivity to the valence state, as was suggested in our previous work. Experiments at Innsbruck undertaken in the summer of 1989 appear to have confirmed this, in that a strong line associated with a $4d^9 4f\ ^1F_3$ state is found in CsO but not in Cs metal.

Work with Guest Scientists from Dublin City University (Ireland) and U. of Hamburg, West Germany, led to striking new results in the absorption spectra of transition metals. The anomalous 3p absorption spectrum of Cr was thought to be fairly well understood through our previous year's study of isoelectronic Mn^+. Our interpretation suggested that Cr^+ would provide a critical test of the overall picture. The anomalous spectrum of Cr derives from a strong mixing of $3p^5 3d^6 4s$ valence and $3p^5 3d^5 4snd$ Rydberg states; simple Hartree-Fock calculations indicate that this mixing should be more pronounced in Cr^+ which lacks a 4s electron. The measured absorption spectrum of Cr^+ does indeed show a significant transfer of oscillator strength into the Rydberg region; the transition between Cr and Cr^+ is thus much unlike the transition between Mn and Mn^+, in which the absorption spectrum is essentially the same. Analysis of all of the sharp 3p - ns features in the Cr^+ spectrum has been completed, and has resulted in an accurate value of the ionization limit. Interpretation of the broader 3p - nd features is not yet complete.

Contributions were made to studies of the effect of negative ion resonances on electron-stimulated desorption of atoms from surfaces, in collaboration with groups from U. of Pittsburgh and the Surface Science Division. Their conclusions are summarized in the Surface Science Division's contribution to this report. A long-standing project with a group at the Australian National University on critical evaluation of atomic negative ion resonances continued apace. The main original work done by our group on this project consisted of computations of energies and widths of shape resonances in electron scattering by noble gases, and the discovery of similar (yet to be observed) features in electron scattering by halogens and halogen negative ions. Some of these features have been verified by independent calculations undertaken by a group at Johns Hopkins University.

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Pierce, D.T., Spin-Polarized Electron Microscopy, Physica Scripta, Vol. **38**, 291-296, (1988).

Scheinfein, M.R., Unguris, J., Celotta, R.J. and Pierce, D.T., The Influence of the Surface on Magnetic Domain Wall Microstructure, Phys. Rev. Lett., **6316**, 668 (1989).

Scheinfein, M.R., Definition of Ultimate Spatial Resolution, Ultramicroscopy **28**, 359 (1989).

Scheinfein, M.R., Pierce, D.T., Unguris, J., McClelland, J.J., Celotta, R.J. and Kelley, M.H., Improved Low-Energy Diffuse Scattering Electron-Spin Polarization Analyzer, Rev. Sci. Instrum. **60**(1), 1 (1989).
Scheinfein, M.R., Second Order Transfer Matrices for Inhomogeneous Field Wein Filter Including Spin-Precession, OPTIK, **82**(3), 99 (1989).

Stroscio, J.A., Kavanagh, K.L., Capano, M.A., Hobbs, L.W., Barbour, J.C., Maree, P.M.J., Schaff, W., Mayer, J.W., Pettit, D., Woodall, J.M. and Feenstra, R.M., Asymmetries in dislocation densities, surface morphology, and strain of GalnAs/GaAs single heterolayers, J. Appl. Phys. **64**(10), 4843 (1988).

PUBLICATIONS IN PREPARATION

Division 571, Electron and Optical Physics

Canfield, L.R., Kerner, J. and Korde, R., Stability and Quantum Efficiency Performance of Silicon Photodiode Detectors in the Far Ultraviolet, (to be published in Applied Optics)

Canfield, L.R., Korde, R. and Kerner, J., Silicon Photodiodes with Stable Near-Theoretical Quantum Efficiency in the Soft X-Ray Region, (to be published in Proc. of Technical Program on X-Ray Instrumentation in Medicine and Biology, Plasma Physics, Astrophysics and Synchrotron Radiation; International Conference on Optical Science and Engineering, Paris, 1989).

Canfield, L.R., Ogawa, H.S., McMullin, D. and Judge, D.L., Sounding Rocket Measurement of the Absolute Solar EUV Flux Utilizing a Silicon Photodiode, (to be published in the Journal of Geophysical Research).

Clark, C.W., Pan, L.W. and Taylor, K.T., High-order Harmonic Generation by Hydrogenic Ions, in Proceedings of the Third International Laser Science Conference, edited by W.C. Stwally 1989.

Clark, C.W., Matthew, J.A.D., Ramsey, M.G., and Netzer, F.P., Electron-excited 4d → 4f Ba Resonances in $YBa_2Cu_3O_{7-x}$: Selection Rules at Intermediate Energy (to be published in Phys. Rev. A).

Clark, C.W., and Demkov, Y.N., Making Zone Plates with a Laser Printer, (submitted to American Journal of Physics).

Clark, C.W., The frequency-Dependent Polarizability of an Electron Bound by a Zero-Range Potential, (submitted to J. Opt. Soc. Am B).

Cutkosky, R.D., Versatile Scan Generator and Data Collector For Scanning Tunneling Microscopes, (to be published in Rev. of Sci. Instrum.).

Ederer, D.L., Densities of States in LiAl From Soft X-ray Emission Spectra (to be published in Phys. Rev. B).

Hughey, L.R., Record Capture and Acceleration Efficiency in the SURF-II 300 MEV Circular Storage Ring, (to be published in the proceedings of 1989 Particle Accelerator Conference).

Kelley, M.H., Unguris, J., Scheinfein, M.R., Pierce, D.T. and Celotta, R.J., Vector Imaging of Magnetic Microstructure, In Proceedings of Microbeam Analysis Society Meeting, Asheville, N.C., July 1989, edited by P.E. Russell, p. 391 (to be published).

Kelley, M.H., Spin-Polarization, Orientation and Alignment in Electron-Atom Collisions, in _Electronic and Atomic Collisions_, (to be published).

Kerner, J., Slaughter, J.M., Burkland, M.K., Kearnery, P.A., Lampis, A.R., Milanovic, Z., Schulze, D.W., Falco, C.M., Roberts, J., Saloman, E.B., Multilayer Mirrors for 182A, Phys. Scrip., special issue (to be published).

Lett, P.D., Phillips, W.D., Rolston S.L., Tanner, C.E., Watts, R.N., and Westbrook, C.I., Optical Molasses, J. Opt. Soc. Am. B. (to be published November 1989).

Lett, P.D., Westbrook, C.I., Watts, R.N., Rolston, S.L., Tanner, C.E. Phillips, W.D., and Gould, P.L., Heterodyne Spectrum of the Fluorescence from Optical Molasses, (to be published in Coherence and Quantum Optics 6, Edited by J. Eberly, L. Mandel and E. Wolf, Plenum, 1990)

Madden, R.P., Hughey, L.R., Hamilton, A., Furst, M.L., SURF II Progress and Opportunities, In Proceedings of the Sixth U.S. Conference on Synchrotron Radiation Instrumentation, Berkeley, CA., August 1989 (to be published).

McClelland, J.J., Progress on Spin Detectors and Spin-polarized Electron Scattering from Na at NIST, in Proceedings of the Symposium on Polarization and Correlation in Electronic and Atomic Collisions, Stevens Institute of Technology, August 1989 (to be published).

McClelland, J.J., Kelley, M.H. and Celotta, R.J., Superelastic Scattering of Spin-polarized Electrons from Sodium, (to be published in Physical Review A, September 1989).

Mueller, D., Stockbauer, R.L., Robey, S.W., Kurtz, R.L., Shih, A., Singh, A.K., Toth, L. and Ogofsky, M., Resonant Photoemission and Chemisorption Studies of Tl-Bu-Ca-Cu-O, (to be published in AIP Conference Proceedings of AVS Topical Conference on Thin Film Processing and Characterization of High-Temperature Superconductors).

Mueller, D., Kurtz, R.L., Robey, S.W., Stockbauer, R.L., Shih, A., Toth, L., Singh, A.K. and Ogofsky, M., Electron Structure of High Tc Superconductors Studied Using Photoelectron Spectroscopy, (to be published in Vacuum).

Mueller, D., Ederer, D.E., Rubensson, J.E., Shuker, R., Wallace, J., Zhang, C.H., Tai, J., Callcott, T.A., Dong, Q.-Y., Toth, L.E., Ragne, R. and Ogofsky, M., A Soft X-Ray Emission Spectroscopy Investigation of Bi2Sr2CaCu2O8, (to be submitted to Physica Scripta).

Pan, L.-W., Treatment of Continuum-Continuum Coupling in the Theoretical Study of Above-Threshold Ionization, (to be published in Atoms in Strong Fields, NATO ASI series, ed. C. Nicolaides, C.W. Clark and M. Nayfeh (Plenum, New York, 1989).

Penn, D.R., Tanuma, S. and Powell, C.J., Inelastic Mean Free Paths in Solids at Low Energies, (to be published in J. Elec. Spect.).

Penn, D.R. and Apell, P., Spin Polarized Metastable Atom De-excitation; Theory, (submitted to Phys. Rev. Letts.).

Penn, D.R. and Apell, P., Theory of Spin Polarized Metastable Atom De-excitation, Phys. Rev. B, (to be published).

Phillips, W.D., Westbrook, C.I., Watts, R.N., Rolston, S.L., Tanner, C.E., Lett, P.D., and Gould, P.L., A Heterodyne Measurement of the Fluorescence Spectrum of Optical Molasses (to be published in Laser Spectroscopy 9, 1990).

Pierce, D.T., Scheinfein, M.R., Unguris, J. and Celotta, R.J., Magnetic Microstructure of Thin Films and Surfaces: Exploiting Spin Polarized Electrons in the SEM and STM, (to be published Materials Research Society Symposium Proceedings).

Scheinfein, M.R., Unguris, J., Celotta, R.J. and Pierce, D.T., Magnetic Length Scales at Surfaces, (to be published in Vacuum).

Scheinfein, M.R., Unguris, J., Pierce, D.T. and Celotta, R.J., Surface Magnetic Microstructure, in Magnetism in Low Dimensional Systems, ed. by L. Falicov, (Springer Verlag, Berlin, 1989) (in press).

Scheinfein, M.R., Unguris, J., Kelley, M.H., Celotta, R.J. and Pierce, D.T., Scanning Electron Microscopy with Polarization Analysis, (to be published in Rev. Sci. Inst.).

Scheinfein, M.R., Unguris, J., Pierce, D.T. and Celotta, R.J., Micromagnetic Length Scales at Surfaces, (to be published in Journal Applied Physics).

Stroscio, J.A., First, P.N., Dragoset, R.A., Whitman, L.J., Pierce, D.T. and Celotta, R.J., Dispersion of Evanescent Band Gap States in Fe Clusters on GaAs(110), J. Vac. Sci. and Tech., (in press).

Unguris, J., Scheinfein, M.R., Celotta, R.J. and Pierce, D.T., Scanning Electron Microscopy with Polarization Analysis Studies of Ni-Fe Magnetic Memory Elements, in Proceedings of International Magnetics Conference, Washington, D.C., March 28-31, 1989, (to be published November 1989).

Unguris, J., Scheinfein, M.R., Celotta, R.J. and Pierce, D.T., The Magnetic Microstructure of the (0001) Surface of hcp Cobalt, (to be published in App. Phys. Lett.).

Unguris, J., Scheinfein, M.R., Celotta, R.J. and Pierce, D.T., Scanning Electron Microscopy with Polarization Analysis Studies of Magnetic Microstructure, (book chapter to be published in Chemistry and Physics of Solid Surfaces VIII, Springer-Verlag).

INVITED TALKS

Division 571, Electron and Optical Physics

Celotta, R.J., "Scanning Tunneling Microscopy," American Physical Society, St. Louis, Missouri, March 21, 1989.

Celotta, R.J., "Magnetic Microstructure," Naval Research Laboratory, Washington, DC, March 2, 1989.

Celotta, R.J., "Magnetic Microstructure," University of Indiana, Bloomington, Indiana, Feb. 15, 1989.

Clark, C.W., "High Harmonic Generation in Hydrogenic Ions," International Laser Science Conference, Atlanta, GA, Oct. 3, 1988.

Clark, C.W., "Computational Studies of Atoms in Strong Fields," International Laser Science Conference, Atlanta, GA, Oct. 3, 1988.

Clark, C.W., "Weak-Field Limits and Asymptotic Behavior," North Atlantic Treaty Organization Advanced Study Institute, Kos, Greece, Oct. 10, 1988.

Clark, C.W., "Laser Isotope Separation at JAERI," Japan Atomic Energy Research Institute, Nov. 3, 1988.

Clark, C.W., "Atomic Physics in the Solid State: Giant Resonances, Excitons, and High T_c Superconductivity," University of Maryland Baltimore County, Catonsville, MD, Nov. 9, 1988.

Clark, C.W., "Highly Excited Atoms," Twentieth Reunion of the Physics Club of Montgomery College, Takoma Park, MD, Dec. 2, 1988.

Clark, C.W., "High Harmonic Generation in Hydrogenic Ions,", X-Ray Laser Group Seminar, Princeton Plasma Physics Laboratory, March 3, 1989.

Clark, C.W., "High-Harmonic Generation in Hydrogen Ions: Comparison of Perturbative and Non-Perturbative Calculations," University of Rochester, Rochester, NY, June 29, 1989.

Clark, C.W., "The Frequency-Dependent Polarizability of an Electron Bound in a Zero-Range Potential in N Dimensions," Conference on Super-Intense Laser-Atom Physics, University of Rochester, Rochester, NY, June 30, 1989.

Clark, C.W., "The Frequency-Dependent Polarizability of an Electron Bound by a Zero-Range Potential in N Dimensions," Gordon Conference on Atomic Physics, Brewster Academy, Wolfeboro, NH, July 5, 1989.

Clark, C.W., "Electron-Excited 4d--->4f Resonances in $YBa_2Cu_3O_{7-x}$: Selection Rules at Intermediate Electron Energy," Gordon Conference On Atomic Physics, Brewster Academy, Wolfeboro, NH, July 6, 1989.

Clark, C.W., "Photoabsorption and Electron Energy Loss Spectroscopy of $YBa_2Cu_3O_{7-\delta}$," Fifth NIST Superconductivity Information Exchange Meeting, Boulder, CO., September 21, 1989.

Dragoset, R.A., "High-resolution Scanning Tunneling Microscopy: Metal Clusters and Thin Films on Galium Arsenide," Symposium for Innovation in Measurement Science '89, Hobart & William Smith Colleges, Geneva, NY, August 8, 1989.

First, P.N., "Scanning Tunneling Microscopy of Metals on Semiconductor Surfaces," Physics Dept. Colloquium, Georgia Institute of Technology, Atlanta, GA, May 24, 1989.

First, P.N., "Scanning Tunneling Microscopy of Metals on Semiconductor Surfaces," Solid State Seminar, Brown University, Providence, RI, February 28, 1989.

Hart, M.W., "The Use of Spin-Labeling Techniques in Metastable Atom De-excitation Spectroscopy," Lawrence Livermore National Laboratory, Livermore, CA., September 25, 1989

Hart, M.W., "The Use of Spin-Labeling Techniques in Metastable Atom De-Excitation Spectroscopy," Sandia National Laboratories, Albuquerque, NM, August 28, 1989.

Hart, M.W., "The Use of Spin-Labeling Techniques in Metastable Atom De-Excitation Spectroscopy," IBM Almaden Research Center, San Jose, CA, June 22, 1989.

Hart, M.W., "Spin Polarized Inverse Photoemission Study of Ultrathin Co Films on Cu(111)," American Physical Society Meeting, March 20, 1989.

Hughey, Lanny, "Record Capture and Acceleration Efficiency in the SURF II 300 MeV Circular Storage Ring," 1989 Particle Accelerator Conference, Chicago, IL, March 21, 1989.

Kelley, M.H., "Spin Polarization, Orientation, and Alignment in Electron-Atom Scattering," XVI ICPEAC Conference, New York, NY, July 26, 1989.

Kelley, M.H., "Vector Imaging of Magnetic Microstructure," 1989 Microbeam Analysis Society Meeting, Asheville, NC, July 18, 1989.

Kelley, M.H., "Measuring the Shapes of Atoms," Sigma Xi Lecture, National Institute of Standards and Technology, Gaithersburg, MD, March 21, 1989.

Kelley, M.H., "Electron-Atom Collision Studies Using Optically State-Beams," NIST Staff Research Seminar, National Institute of Standards and Technology, Gaithersburg, MD, February 2, 1989.

Lett, P.D., "Laser Cooling, Optical Molasses and the Coldest Gas in the Universe," Electrical Engineering Department, University of Wisconsin, Madison, WI, February 23, 1989.

Lett, P.D., "Laser Cooling, Optical Molasses and the Coldest Gas in the Universe," Physics Department, Marquette University, Milwaukee, WI., February 24, 1989.

Lett, P.D., "Laser Cooling to MicroKelvin Temperatures," Applied Physics Laboratory, Johns Hopkins University, Laurel, MD., March 10, 1989.

Madden, R.P., SURF II Progress and Opportunities," Conference on Synchrotron Radiation Instrumentation, Berkeley, CA., August 1989.

Madden, R.P., "UV-VUV Radiometry at NIST," Committee on Optical Radiation Measurements (CORM) Meeting, NIST, May 1989.

McClelland, J.J., "Progress on Spin Detectors and Spin-Polarized Electron Scattering from Na at NIST," Fifth International Symposium on Polarization and Correlation in Electronic and Atomic Collisions, Hoboken, NJ, August 2, 1989.

Ott, William, "Radiometry at NIST," Arnold Engineering Defense Center, Nashville, TN., February 14, 1989.

Pan, Liwen, "Treatment of Continuum-Continuum Coupling in the Theoretical Study of ATI," North Atlantic Treaty Organization Advanced Study Institute, Kos, Greece, Oct. 10, 1988.

Pan, Liwen, "High Order Harmonic Generation in Hychrogenic Ions," John Hopkins University, Baltimore, MD, Dec. 1, 1988.

Pan, Liwen, "Computation of High-order Multiphoton Processes in Atomic Hydrogen," Royal Holloway and Bedford New College, Univ. of London, Egham, Surrey, England, March 31, 1989.

Pan, Liwen, "Computation of High-Order Multiphoton Processes in Atomic Hydrogen," Theoretical seminar, JILA, University of Colorado, Boulder, CO, June 15, 1989.

Pan, Liwen, "The Coulomb-Volkov State and Its Application in the Study of Multiphoton Ionization," University of Rochester, Rochester, NY, June 29, 1989.

Pan, Liwen, "The Coulomb-Volkov State and Its Application in the Study of Multiphoton Ionization," Gordon Research Conference on Atomic Physics, Brewster Academy, Wolfeboro, NH, July 6, 1989.

Pan, Liwen, "High Harmonic Generation in Hydrogenic Ions,", Atomic Physics Seminar, The Johns Hopkins University, Baltimore, MD, Dec. 2, 1988.

Penn, D.R., "Total Dielectric Function, Algebraic Sign and Superconductivity," NIST Conference on High Tc, Boulder, CO., September 20, 1989.

Penn, D.R., "Total Dielectric Function, Algebraic Sign, Electron-Lattice Response, and Superconductivity," University of CA at Berkeley, Berkeley, CA, May 29, 1989.

Penn, D.R., "Electron Correlations in High Tc Materials," Visiting Committee on Advanced Technology, NIST Boulder, Boulder, CO, May 2, 1989.

Pierce, D.T., "Surface Magnetic Microstructure," Seventh International Conference on Solid Surface, Cologne, West Germany, September 25, 1989.

Pierce, D.T., "Imaging Magnetic Microstructure with High Spatial Resolution," International Workshop on Monolayer Magnetism, Berkeley Springs, WV, August 15, 1989.

Pierce, D.T., "High Resolution Imaging of Magnetic Microstructure in Thin Magnetic Layers," American Vacuum Society, Murray Hill, NJ, June 14, 1989.

Pierce, D.T., "Magnetic Microstructure of Thin Films and Surfaces: Exploiting Spin-Polarized Electrons in the SEM and STM," Materials Research Society Symposia, San Diego, CA, April 28, 1989.

Pierce, D.T., "Surface Magnetic Microstructure," 2nd International Workshop on Magnetism in Low-Dimensional Systems, San Luis Potosi, Mexico, May 22-26, 1989.

Pierce, D.T., "Probing Magnetic Microstructure on the Nanometer Scale," American Vacuum Society 35th National Vacuum Symposium and Topical Conference, Atlanta, GA, October 3-7, 1988.

Scheinfein, M.R., "Surface Magnetic Microstructure Using SEMPA," Symposium Eastman Kodak Research Lab., Rochester, NY, July 1989.

Scheinfein, M.R., "Scanning Electron Microscopy with Polarization Analysis," Symposium, Cornell University, Ithaca, NY, June 1989.

Scheinfein, M.R., "Surface Magnetic Microstructure," 2nd International Workshop on Magnetism in Low-Dimensional Systems, San Luis Potosi, Mexico, May 22,26, 1989.

Scheinfein, M.R., "Observation of the Surface Domain Structure of an hcp (0001) Co Crystal," American Physical Society Mtg., St. Louis, Missouri, March 1989.

Stiles, M.D., "Inelastic Gas-Surface Scattering," Technical University of Denmark, Lyngby, Denmark, May 9, 1989.

Stroscio, J.A., "Scanning Tunneling Microscopy of Small Metal Structures on GaAs(110)," International STM '89 Meeting, Oarai, Japan, July 9, 1989.

Stroscio, J.A., "Scanning Tunneling Microscopy of Metal Clusters on GaAs(110)," Electrotechnical Laboratory, Tsukuba, Japan, July 18, 1989.

Stroscio, J.A., "Scanning Tunneling Microscopy of Metal Atom Structures on GaAs(111) Surfaces," Institute for Solid State Physics, Tokoyo, Japan, July 17, 1989.

Stroscio, J.A., "Scanning Tunneling Microscopy of Small Metal Particles," Condensed Matter Physics Seminar, College Park, MD, April 13, 1989.

Unguris, J., "SEM with Polarization Analysis: Studies of Magnetic Microstructure," International Summer Institute on Surface Science, Milwaukee, WI, August 21, 1989.

Unguris, J., "Magnetic Microstructure Imaging Using Spin Polarized SEM," Western Pennsylvania Chapter of the American Vacuum Society, Pittsburgh, PA, June 28, 1989.

Unguris, J., "Scanning Electron Microscopy with Polarization Analysis Studies of Ni-Fe Magnetic Memory Elements," International Magnetics Conference, Washington, DC, March 31, 1989.

Unguris, J., "Scanning Electron Microscopy with Polarization Analysis Tutorial," International Magnetics Conference, Washington, DC, March 29, 1989.

JOURNAL EDITORSHIPS

Division 571, Electron and Optical Physics

C.W. Clark, Topical Editor for Atomic Spectroscopy, Journal of the Optical Society of America B.

K.T. Taylor, M.H. Nayfeh, and C.W. Clark, eds., Atomic Spectra and Collisions in External Fields, (Plenum, New York 1989).

SPONSORED SEMINARS AND COLLOQUIA

Division 571, Electron and Optical Physics

Bucksbaum, Phillip, Bell Labs, "The Molecular Bond in Intense Fields: Photodissociation of H_2," April 12, 1989.

Buncick, Milan, University of Wisconsin-Madison, "Polymer Applications to the Microelectronics Industry," February 17, 1989.

Carre, Bertrand, IRF, France, "Resonant Photoionization of Excited Sodium, Studied by Laser and Synchrotron Radiation Excitation," August 11, 1989.

Codling, Keith, Reading University, England, "Processes Using Covariant Mapping," April 28, 1989.

Cohen, Marvin L., University of California at Berkeley, "Some Perspectives on High Temperature Superconductivity," May 19, 1989.

Crance, Michele, Laboratoire Aime, France, "Multiphoton Ionization of Hydrogen Atom in Strong Field," May 5, 1989.

Della Torre, Edward, George Washington University, "Micromagnetics of Small Particles," October 14, 1988.

Demkov, Yurii, Leningrad State University, "James Clerk Maxwell and the Mendeleev Periodic Table," February 7, 1989.

Eyler, Edward, Yale University, "Precise Laser Spectroscopy of Two-Electron Systems," October 17, 1988.

Fink, Manfred, University of Texas at Austin, "Toward Accurate Measurements of Electron Spin Polarization," October 20, 1988.

Florescu, Viorica, University of Bucharest, "Perturbed Wavefunctions for the Hydrogen Atom in a Uniform Harmonic Electric Field and Applications," September 15, 1989.

Gailite, Erna K., Latvian Academy of Sciences, "Multiphoton Ionization and Above-Threshold Ionization in Hydrogen: Experiment and Theory," September 29, 1989.

Gluskin, Efim S., Institute of Nuclear Physics, Novisibirsk, U.S.S.R., "Synchrotron Radiation Research in Novisibirsk, USSR," July 7, 1989.

Kamiya, Itaru, University of Tokyo, "Development of a Field Ion-Scanning Tunneling Microscope and Its Applications," March 30, 1989.

Kennedy, Eugene, N.I.E.H.D., Dublin, Ireland, "XUV Photoabsorption Studies of Atoms and Ions," September 7, 1989.

Kumar, Vijay, Physical Research Laboratory, Ahmedabad, India, "Atomic Physics at PRL," August 3, 1989.

L'Huillier, Anne L., CEA Saclay, France, "Harmonic Generation in Strong Laser Fields: Influence of Ionization and Propagation," July 24, 1989.

Long, James, Naval Research Lab, "Combined Laser-Synchrotron Radiation Experiments on the NSLS X-Ray Ring," February 15, 1989.

Lorentz, Steven, University of Oklahoma, "Low-Energy Electron Scattering on Sodium," August 9, 1989.

Meier, Felix, ETH, Zurich, Switzerland, "Epitaxial Magnetic Films and Laser Induced Photoemission From Fe," August 11, 1989.

Morgan, John D., Harvard University, "Precise Variational Calculations for Atomic Helium," February 17, 1989.

Miller, John C., Oak Ridge National Laboratory, "Nanosecond and Picosecond Multiphoton Ionization of Weakly Bound Molecules," March 16, 1989.

Nicolaides, Cleautles, National Hellenic Research Foundation, Athens, Greece, "Many-Electron, Many-Photon Theory of Atoms in Strong Fields," December 15, 1988.

Puntajer, Anna K., University of Innsbruck, Austria, "Asymmetries in Intense Laser-Free Electron Scattering," October 3, 1988.

Rife, Jack C., Naval Research Lab, "Soft X-ray, Multilayer-Coated Gratings-Performance and Applications," March 29, 1989.

Standage, Max C., Griffith University, Brisbane, Australia, "Electron-Photon Coincidence Experiments Using Laser Excitation Techniques," April 3, 1989.

Sundaram, Bala, Johns Hopkins University, "Localization Theory for RF Floquet States," January 24, 1989.

Taylor, Kenneth, Royal Holloway and Bedford New College, Surrey, England, "Rydberg States of Molecular Hydrogen in a Magnetic Field," December 16, 1989.

Tonner, Brian P., University of Wisconsin-Milwaukee, "Photoemission Microscopy of Surfaces Using Synchrotron Radiation," February 13, 1989.

Walker, J.C., Johns Hopkins University, "Inter-Layer Interaction in Magnetic Superlattices," April 17, 1989.

Weiss, Paul S., Pennsylvania State University, "Tunneling Scanning Microscopy at 4K," June 21, 1989.

Williams, J.F., University of Western Australia, "(e,2e) Coincidence Studies of Atomic Hydrogen," October 26, 1988.

Wong, Tamae M., University of Pennsylvania, "The Electronic Structure of CsAs and GaAs," September 22, 1989.

Wuilleumier, Francois, Laboratoir Pour l"Utilization du Rayonnement Electromagneque, Orsay, France, "New Facilities for Atomic Physics at Super ACO," October 28, 1989.

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Division 571, Electron and Optical Physics

Robert J. Celotta

Member, General Committee, International Conference on the Physics of Electronic and Atomic Collisions.

Charles W. Clark

Chairman, National Academy of Sciences/National Research Council Committee on Line Spectra on the Elements - Atomic Spectroscopy.

Co-Director, NATO Advanced Study Institute, "Atoms in Strong Fields".

Co-Chairman, Conference on Lasers in Science and Technology.

David L. Ederer

Organized a session on the industrial and scientific application of third generation synchrotron radiation facilities at the Conference for the Industrial Application of Accelerators, Denton, TX., October 1988.

Program Committee for the 6th Synchrotron Radiation Conference, Lawrence Berkeley Labs, August 1989.

Lanny R. Hughey

Member, Design Review Board for Title I Design of the Vacuum System of the Argonne National Laboratory Advanced Photon Source 7 GeV Electron Storage Ring.

Thomas B. Lucatorto

Co-chairman, 1989 International Conference on the Physics of Electron and Atomic Collisions (ICPEAC XVI).

Member, Program Committee, 5th International Symposium on Resonance Ionization Spectroscopy and Its Applications, 1990.

Robert P. Madden

Member, Optical Society of America Nominating Committee.

Member, Calibration and Stability Working Group of the Ozone Trends Panel.
Coordinator, International Radiometric Intercomparison of Solar Irradiance Monitoring Experiments.

Member, International Committee for the International Conference on Vacuum Ultraviolet Radiation Physics.

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 at Brookhaven National Laboratories.

Member, Advisory Committee for the U.S. National Synchrotron Radiation Instrumentation Conference.

William R. Ott

Member, DoD Panel on Optics Technology Applications, October 1989.

DoD Liaison, SDI-Related Metrology at NIST.

Daniel T. Pierce

Member, Editorial Board, Journal of Electron Spectroscopy.

Program Committee and International Advisory Committee, Fourth International Conference on Electron Spectroscopy, Honolulu, Hawaii, July 10-14, 1989.

MAJOR CONSULTING AND ADVISORY SERVICES

Division 571, Electron and Optical Physics

L.R. Canfield advised and consulted with numerous people from industry, academia and Government agencies on applications of detectors and standard detectors in the far ultraviolet.

L.R. Canfield consulted with Raj Korde of the United Detector Technology on matters involving semiconductor photodiodes in the far ultraviolet.

L.R. Canfield consulted with H. Ogawa and D. Judge concerning narrow-bandpass detector systems for solar flux determinations in rocket flight experiments.

R.J. Celotta and D.T. Pierce consulted on the production and detection of polarized electrons with researchers from Brookhaven, AT&T Bell Labs, Bell Communications Corporation, University of Texas, MIT, Argonne National Laboratory, Perkin Elmer Corporation, and the Naval Research Laboratory.

C.W. Clark advised the X-ray Laser Group at Princeton Plasma Physics Laboratory on atomic physics problems associated with x-ray laser development.

D.L. Ederer consulted with Rupert Perera at Lawrence Berkeley Labs in the study of property of multi-layers.

D.L. Ederer consulted with staff at Bell-Corp. to obtain thin film super conductors.

L.R. Hughey consulted with Design Review Board for Title I design of the Vacuum System at the Argonne National Laboratories.

R.P. Madden consulted for NASA by serving on the "Spacecraft Instrument Calibration and Stability" Working Group of the "Ozone Trends Panel" contributing to the report to Congress entitled "Present State of Knowledge of the Upper Atmosphere 1988: An Assessment Report" as required under the Clean Air Act Amendments of 1987. Public Law 95-95.

R.P. Madden, at the request of the Director of the Earth Science and Applications Division of the Office of Space Science and Applications, NASA, is coordinating an international round-robin intercomparison of solar irradiance monitoring space experiments.

R.P. Madden is on the DARPA Advisory Committee for the Brookhaven X-Ray Lithography Synchrotron Source Program.

R.P. Madden is on the Program Review Committee for the BNL National Synchrotron Light Source.

W.R. Ott consulted with staff from the Lawrence Livermore Labs, Lawrence Berkeley Labs, U. Arizona, Lockheed, and AT&T Bell Labs on XUV optical properties of multilayer devices and measurement services and research opportunities available at NIST/SURF-II.

W.R. Ott consulted with staff at the Arnold Engineering Development Center, Tennessee, on radiation measurements involving infrared, ultraviolet, and soft x-ray radiation.

W.R. Ott participated in a DoD review panel on Optics Technology Applications.

SPONSORED WORKSHOPS

Division 571, Electron and Optical Physics

C.W. Clark was co-director of a NATO Advance Study Institute, "Atoms in Strong Fields," Kos, Greece, October 9-21, 1988.

R.A. Dragoset organized and chaired the Surface Analysis session of the Symposium for Innovation in Measurement Science '89, Hobart and William Smith Colleges, Geneva, NY, August 8, 1989.

M.H. Kelley organized, jointly with Kurt Becker of City College of New York and Paul Neill of University of Nevada-Reno, the 5th International Symposium on Polarization and Correlation in Electronic and Atomic Collisions, Stevens Institute of Technology, Hoboken, NJ on August 2-4, 1989.

T.B. Lucatorto organized and chaired the Research Advisory Committee Symposium on Gas Phase Pump and Probe Experiments, NIST, Gaithersburg, MD., February 10, 1989.

D.T. Pierce was co-chair (with Prof. Leo Falicov, Department of Physics, University of California, Berkeley) of Department of Energy Council on Materials Sciences Panel On "Surface, Interface and Thin-Film Magnetism", Santa Fe, NM, June 18-21, 1989.

J. Unguris organized the Scanning Electron Microscopy with Polarization Analysis workshop at the International Magnetics Conference, Washington, DC on March 29, 1989.

CALIBRATION SERVICES PERFORMED

Division 571, Electron and Optical Physics

Type of Service	Customer Type*	SP 250 Item No.	Number Calibration or Tests
Far UV radiometric transfer standard detectors (photodiode calibrations)	1,4-8	N.A.	26
Spectrometer calibrations using SURF as an absolute source	5-7	N.A.	16
Totals			42

* Column 2: 1, calibration labs; 2, hospitals; 3, nuclear energy establishments; 4, industry; 5, US government labs; 6, DoD labs; 7, universities; 8, foreign governments.

ATOMIC AND PLASMA RADIATION DIVISION

FISCAL YEAR 1989 TECHNICAL ACTIVITIES

The Atomic and Plasma Radiation Division carries out a broad range of experimental and theoretical research on atomic structure and atomic radiation in plasmas. The Division determines a large variety of atomic radiation and collision data, encompassing wavelengths of spectral lines, atomic energy levels, ionization potentials, atomic transition probabilities, plasma line broadening parameters, and ionization and excitation cross sections. Two data centers located in the Division critically evaluate and compile atomic energy levels, wavelengths, and transition probabilities.

Since in most cases atomic radiation originates from plasmas, we are also engaged in research on the effects of the plasma environment on atomic radiation, such as studies of spectral line broadening and line shifts. We explore these effects in order to gain an understanding of atomic processes in plasmas as well as to use them for developing new measurement techniques. We use well-defined atomic radiation sources as VUV radiometric standards and wavelength standards.

Our activities, which support many areas of science and technology, have undergone significant changes in direction, in response to changes in the external forces that drive our priorities. Demand for detailed understanding of atomic processes in cool plasmas, both for modelling purposes and diagnostics, has increased. These needs have arisen mainly from materials processing by plasmas, such as the widely used plasma etching of semiconductors, as well as 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. Also, process monitoring and modelling in plasma chemistry, spectrochemistry and medical applications can be achieved on a fundamental level only with reliable atomic radiation and collision data. For these technologies, heavy neutral and singly ionized atoms, including some rare earths, are of principal interest.

Different demands arise from VUV and x-ray laser physics. In this research area, transition energies and lifetimes (or radiative decay rates) of highly stripped ions are essential for the selection and testing of potential laser systems. VUV and x-ray laser research has not only assumed importance for defense applications, but also for biological and bio-medical studies (e.g. the "water window"). We are active both in generating atomic data and in the development of lasing schemes.

The Nation's research program on magnetic fusion energy is steadily progressing, and the atomic data we produce for highly stripped heavy ions are needed for modelling the cross-field ion transport for estimating the effects of impurities on the plasma energy balance, and for plasma diagnostics, such as the measurement of ion temperatures. Beyond this, there is also the fundamental scientific quest for an experimentally

well-tested, fully relativistic atomic structure theory that accurately describes the properties of highly ionized as well as heavy atoms, including quantum electrodynamic (QED) effects.

Finally, our vacuum ultraviolet radiometry work with plasma sources is now providing miniaturized calibrated radiation source packages to allow radiometric calibrations on board spacecraft. These are used, for example, on the space shuttle for accurate monitoring of the solar ultraviolet radiation, and are part of the Hubble Space Telescope instrumentation.

The Division consists of three technical groups: Atomic Spectroscopy, Atomic Radiation Data, and Plasma Radiation. It currently has 13 professional physicists, among them 12 Ph.D.s. During 1989 the Division had 21 guest scientists, from Germany (2), Austria (2), China (2), India (2), Sweden (1), Israel (1) and U.S.A. (11).

Some of our significant accomplishments during the past year are:

- We have extended knowledge of the energy levels and wavelengths for 67 atomic ions belonging to 5 isoelectronic sequences and ranging from Cu^{12+} to Sn^{30+}; our results for the sodium sequence revealed the necessity for including of quantum-electrodynamic contributions for n = 3 electrons in theoretical calculations.

- We began a collaboration with NIST researchers in the Dental and Medical Materials Group to investigate the kill mechanism of bacteria on dental tools placed in a simple microwave-excited plasma. We hope to develop a simple and fast sterilization method for application in the dental and medical fields.

- We completed major compilations of critically evaluated energy-level data for the 16 spectra of sulfur and for the 29 spectra of copper.

- We applied a nonperturbative theory to calculate the vacuum polarization contribution to the Lamb shift of K- and L-shell electrons. This contribution is one of the major QED corrections for energy levels of heavy atoms. A comprehensive study of various terms that affect the Lamb shift and other relativistic effects, such as two-photon exchange Feynman diagrams, screening of self energy, and self energy of excited levels, continues in collaboration with visiting scientists from the U. S., Germany, and France.

- Two major books on atomic transition probabilities of Sc, Ti, V, Cr, Mn, Fe, Co, and Ni have been published as supplements to the Journal of Physical and Chemical Reference Data. These two volumes are about 500 pages each and contain critically evaluated transition probabilities for about 18,000 transitions for neutral through hydrogenic ions of the above elements.

- We have established a soft x-ray characterization facility on the NIST electron storage ring, SURF II. We have measured reflectivities of numerous multilayer samples and collaborated with many laboratories, including AT&T Bell Labs, Johns Hopkins University, University or Arizona, NASA/Goddard, University of Colorado/LASP, Lawrence Livermore, Lawrence Berkeley, and IBM.

These and other activities are discussed in the following sections, where the principal work of the three technical groups during the past year is described.

I. Atomic Spectroscopy Group

(a) Highly Ionized Atoms

The energy levels and wavelengths for spectra of highly ionized atoms are of basic interest for testing theoretical descriptions of atomic properties, which are affected by large relativistic and quantum-field (QED) contributions. They are also necessary data for the modeling and diagnostics of high-temperature plasmas occurring in x-ray laser research, solar flares, tokamaks and other fusion-research machines. We have excited highly charged ions in several sources: the highest temperatures obtained so far were in plasmas produced by the OMEGA laser at Rochester, and we have also used plasmas generated in the TEXT tokamak at the University of Texas, and sliding-spark, vacuum-spark, and laser-generated plasmas at NIST.

The spectra of Na-like ions are generally prominent in high-temperature plasmas. J. Reader and several collaborators from the Naval Research Laboratory have just extended knowledge of the energy levels and wavelengths for eleven such ions from Y^{28+} to Sn^{39+}. The spectra were obtained from laser-produced plasmas by using large lasers at Los Alamos and Rochester. Comparisons of the experimental 3s-3p excitation energies with values calculated with Desclaux's Dirac-Fock code revealed the necessity for including QED shifts for n=3 electrons in the calculations. QED contributions obtained from a $1/n^3$ scaling of Mohr's results for n=1,2 electrons gave much improved agreement with experiment. These accurate measurements will be used for calibration and diagnostics of plasmas in x-ray laser and controlled-fusion research.

J. Sugar and collaborators completed analyses of spectra of Mg-like, Si-like, S-like, and Cl-like ions of the elements Cu to Mo. This includes wavelengths and energy levels for 56 ions of 14 elements in ionization stages from Cu^{12+} to Mo^{30+}. The spectra were excited in laser-generated plasmas in our laboratory and in the TEXT tokamak at Austin. The energy levels were compared with Dirac-Fock and Hartree-Fock calculations to test the theory and to use the smooth variation of deviations from experiment for interpolations along the isoelectronic sequences. The new experimental wavelengths will be used as standards in high-temperature plasma research.

J. Reader and U. Feldman (NRL) carried out a complete analysis of the spectrum of the Mo^{6+} ion after finding that a previous analysis from another laboratory was totally erroneous. They have also continued experiments to test their proposed scheme to produce lasing in a Mo^{6+} transition at 600 Å by photopumping the upper level with a Mo^{11+} line.

During the coming year we plan to visit the Rochester OMEGA laser facility (and possibly also the NOVA facility at Livermore and the large KMS Fusion laser) to excite higher-temperature spectra of heavy elements. One of the planned experiments is to extend our work on Na-like spectra to the rare-earth region of the periodic table--50 to 60 electrons stripped from the atoms.

(b) <u>Laser Spectroscopy and High-Accuracy Determinations of Atomic Energy-Level Structures</u>

A basic objective of our laser spectroscopy program is to test experimentally the most accurate theoretical calculations for selected atoms. The development of theoretical methods that treat electron-correlation, relativistic, and QED energy contributions accurately and consistently is one of the fundamental goals of atomic physics. Helium is of special importance because the electron-correlation contributions can be calculated to almost arbitrary accuracy in a non-relativistic approximation, and the inclusion of two-electron relativistic and QED effects is simpler than for atoms having more electrons. Our measurements for helium contribute to a broad effort towards increased understanding of this system.

C. Sansonetti and J. Gillaspy are ready to begin measurements of the $2\ ^1S - n\ ^1P$ wavelengths in helium including both low levels and highly-excited Rydberg states. The atomic beam apparatus constructed for this experiment is producing a suitable flux of atoms excited to the metastable $2\ ^1S$ level, and the transition $2\ ^1S - 3\ ^1P$ at 5015 Å has been observed with a signal-to-noise ratio of better than 500. Higher members of the series will be excited with a frequency-doubled dye laser. Sansonetti and Gillaspy expect that measurements for the entire series will determine the $2\ ^1S$ ionization energy with an accuracy approaching a part in 10^9. They are also considering the possibility of direct frequency measurements for the transitions $2\ ^1S - 16\ ^1S,^1P,^1D$. The greatly improved ionization energy for $2\ ^1S$ will permit new tests of the most accurate theoretical calculations for helium, including two-electron QED contributions.

In related work, C. Sansonetti and Gillaspy have been conducting stringent tests of the Fabry-Perot wavemeter to determine the wavelength accuracy that can be obtained in the helium experiment. The limits of the optical system and computer algorithms used to determine the laser wavelength are being explored by measuring the wavelength of a laser shifted from the reference laser with an accousto-optic modulator. This provides a test source whose actual wavelength is known to high accuracy.

To test the accuracy of the system at wavelengths far from the reference laser, they have locked a dye laser to well-known transitions of $^{120}Te_2$ around 4860 Å. Here they use FM sideband techniques to observe the Doppler-free saturated-absorption resonances and to implement the dye laser lock.

Also in support of the helium beam experiment, Sansonetti and K. Deilamian have used intracavity frequency doubling to obtain 2-3 mW of tunable laser power in the vicinity of 3200 Å. The tuning range of the current system will allow excitation of the He 2 ^1S - n ^1P transitions for n=6-13. Other dyes and doubling crystals will permit excitation to levels having still higher n values.

Improved measurements of transitions not accessible with the metastable-beam apparatus are required to establish the energies of a number of low-lying helium levels. Some of these transitions have been observed using Doppler-free laser methods in a low-pressure discharge. Accurate measurements of their wavelengths are planned. Other transitions are not readily accessible to tunable lasers. Sansonetti has recorded emission spectra of low-pressure rf discharges in helium by Fourier transform spectroscopy. These spectra include all lines from 4000 Å to 2.5 μm. Although the results of these emission measurements are less accurate than the laser measurements, they represent a large improvement over previous values for such important transitions as 2 ^1S - 2 ^1P and 2 ^3S - 2 ^3P.

(c) Platinum Ultraviolet Reference Wavelengths

The spectrum of a platinum hollow-cathode discharge will be used for on-board wavelength calibration of the High-Resolution Spectrograph (HRS) for the Hubble Space Telescope. Since the absolute wavelength accuracy of this instrument will be the limiting factor in a number of important planned observations, during the past several years we measured the Pt spectrum from 1032 to 4100 Å with our 10.7-m normal incidence vacuum spectrograph. Some 3000 lines of Pt I and Pt II have been determined with an average uncertainty of ±0.002 Å. These measurements have been incorporated into the calibration codes for the HRS and are also now used in the reduction of data obtained with the still active (11 years old) International Ultraviolet Explorer (IUE) satellite. Our Pt measurements will also be used extensively for calibrations in high-resolution laboratory UV and VUV spectroscopy.

We have also made scans of the Pt spectrum using photon-counting detection. Computer reduction of these scans has given accurate relative intensities (±20%) and allowed production of an atlas showing more than 6000 lines. A paper giving wavelengths and relative intensities for the 3000 stronger lines mentioned above, is in press. The atlas will be published separately and will include wavelengths and intensities for more than 6000 lines and energy-level transitions for all classified Pt I and Pt II lines in the 1128-4000 Å region (J. Reader, N. Acquista, C. J. Sansonetti, and J. Sansonetti).

(d) Atomic Energy Levels Data Center

This center critically evaluates and compiles data on energy levels and spectral lines of atoms and atomic ions. We monitor the literature in this area and maintain bibliographic files with references classified according to spectra and types of data. We answer many individual requests for information on atomic spectroscopic data and supply separate lists of references of special interest for fusion-plasma research, for astronomy, and for spectrochemistry. We also publish complete bibliographies on atomic spectra from time to time.

During the past year W. C. Martin, R. Zalubas, and A. Musgrove completed new compilations of critically evaluated data on the energy levels for all 16 spectra of sulfur (S I - S XVI), and Sugar and Musgrove completed similar work for all 29 spectra of copper (Cu I -Cu XXIX).

Together with the Data Center on Atomic Transition Probabilities and staff of the Standard Reference Data Program, we have begun work on a computer-readable spectroscopic database intended eventually to cover all atoms and atomic ions for which acceptable data are available. We plan to include wavelengths, energy levels, transition probabilities, and full bibliographic files of references keyed to the data. The system will allow sorting and retrieval according to spectrum, wavelength region, etc., and will cover all wavelengths from about 1 Å to the mm region. G. R. Dalton (OSRD) and Musgrove have developed the energy-level entry and retrieval programs and loaded our evaluated energy-level data for all 235 iron-group spectra and for all sodium through sulfur spectra into the system (25,000 levels for 300 spectra). Computerized bibliographic files have been entered into a newly designed database that will be linked to the numerical database.

The database will include wavelengths with their energy-level classifications, and during the past year we have added significantly to our compilations of such data. Sugar and collaborators from JAERI (Japan) have completed their wavelengths compilations for the copper spectra Cu X through Cu XXIX. Similar work was completed for the silicon spectra Si I through Si VI, and work on the sodium, magnesium, and aluminum spectra is underway (V. Kaufman, W. C. Martin, A. Musgrove).

II. Atomic Radiation Data Group

The group (a) studies atomic structure and collision theories and (b) critically evaluates and compiles atomic transition probability and spectral line shape data. The latter activity is carried out in the Data Center on Atomic Transition Probabilities.

(a) Theoretical Studies

(1) A set of computer codes to calculate relativistic energy levels and transition probabilities for atoms has been developed and is being used to provide atomic data for comparison with experiments carried

out by NIST spectroscopists as well as to assist ssientists in other research institutions. Some of the codes have been transferred to Lawrence Livermore National Laboratory and Los Alamos National Laboratory to be used in their x-ray laser studies. Simpler versions of the codes are being shared with scientists in universities with lesser computing capabilities. The latest version of these codes includes extensive estimates of the Lamb shift corrections and is able to handle highly excited states of principal quantum numbers up to about 15.

(2) Many corrections must be applied to existing estimates of the Lamb shift in heavy atoms, because current theoretically sound predictions are based on a one-electron hydrogenic model with a point nucleus. A comprehensive effort is under way to provide a solid theoretical basis for these corrections that includes the self energy for electrons with principal quantum numbers 3 or higher, the self energy for an extended nucleus instead of a point nucleus, higher order relativistic effects that result from Feynman diagrams that exchange two or more photons, and screening of the Lamb shift due to other bound electrons in an atom. Our emphasis in this study is to develop theoretical methods that can provide reliable data for heavy atoms. This requires using nonperturbative methods, because in these systems $Z\alpha$ (Z=nuclear charge, α=fine structure constant) is not small, while perturbative theories assume that $Z\alpha$ is small.

(3) In parallel with the relativistic atomic structure codes mentioned in (1) above, a set of general purpose codes for nonrelativistic atomic structure and transition probabilities has been developed and is being used to provide accurate atomic data for light atoms. One advantage of these nonrelativistic codes is that they can represent electron correlation, which dominates energy levels of light atoms, to high accuracy, far better than the relativistic codes. For super accurate calculations of energy levels, predictions of electron correlation corrections from these nonrelativistic codes must be combined with the predictions of the relativistic codes (including the QED corrections) mentioned above. This combined approach was taken to provide accurate energy levels and f values of Be-like ions. This combination can predict energy levels to an accuracy of 0.1% or better, but f values may still elude our goal of a few percent accuracy. The 3s-3p array f values of the nitrogen atom calculated with elaborate correlated wave functions still disagrees with experimental data by 10-15%.

(4) Relativistic distorted-wave Born cross sections for excitation and ionization of ions by electron impact can be calculated using a set of cross section codes recently developed and the relativistic wave functions generated by the codes mentioned above. The cross section codes are being improved so that they can be used for neutral atoms and lightly charged ions as well. Introduction of correlation orbitals to improve the target atom description brings an undesirable side effect in the case of neutral or lightly charged target. Methods to prevent this side effect are being studied. For medium to highly charged ions, the current code can provide reliable excitation cross sections for arbitrary electron configurations, with the possibility of using elaborate

correlated wave functions if necessary. The cross section codes are providing benchmark data for other codes designed for mass production of cross section data.

(b) Data Center for Atomic Transition Probabilities

(1) Two major books, "Atomic Transition Probabilities--Scandium through Manganese," and "Atomic Transition Probabilities--Iron through Nickel," were published in December 1988. Each book is about 500 pages, and together they contain about 18,000 transition probabilities. We actively advertised the books directly to astronomers, chemists, and physicists in the U.S., Canada, Europe and Asia and have sold 500 books as of August 1989.

(2) The literature on f values is continuously monitored and an up-to-date bibliography is maintained. Work to put the bibliography into a computer database is in progress, and all new references are being directly entered into the database now. We will eventually include all references in bibliographies published by this Data Center in the past, thus providing a totally integrated bibliography on transition probabilities and line shape data. References collected for our bibliography are also provided every 6 months to the International Atomic Energy Agency in Vienna to be included in the "International Bulletin on Atomic and Molecular Data for Fusion" published by the IAEA.

III. Plasma Radiation Group

The plasma measurements program provides essential data and measurement techniques for the analysis and characterization of plasmas, mainly for temperature and density determinations, for VUV source radiometry, plasma processing, and for VUV lasing schemes. The determination of collisional rate coefficients is of critical importance in plasma modeling, especially for VUV laser schemes and fusion-type plasmas. Determination of atomic transition probabilities and plasma line broadening parameters has provided many of the data needed for measurements of plasma densities and temperatures of low temperature plasmas widely used for technological applications, such as in semiconductor and materials processing, spectrochemistry and plasma chemistry. Characterization of rf plasma sources with optical emission spectroscopy provides a key to understanding and controling processes in semiconductor plasma reactors as well as the mechanism for sterilizing medical artifacts. Radiometric measurements of high intensity VUV and x-ray sources have led to advances in source development for x-ray lithography. Our studies of population inversion in the theta pinch have led to a better understanding of recombination mechanisms for possible VUV laser schemes. Pulsed plasma source studies have produced promising new VUV radiometric sources. Our portable radiometric standards have been used for many spacecraft calibrations and are in increasing demand for that purpose.

(a) Soft X-ray Reflectometry on SURF II

The emerging technology of devices that efficiently reflect radiation in the wavelength range from 40 to 600 Å has recently been applied to enhance the output of x-ray lasers, to take unprecedented high resolution, single wavelength pictures of the entire solar disk, and to observe single biological cells in their natural environment. Soft x-ray lithography may also be an application of such devices. These optical components include multilayer mirrors fabricated on large substrates ($> 35\ cm^2$) used at near normal incidence reflection allowing large optical apertures and stigmatic imaging. Because of the phenomenon of Bragg diffraction, their reflectivity is substantially enhanced at a specific wavelength of the incoming radiation. Measurement of the reflectivity of this type of optical component is essential to optimize and enhance this technology.

We have made measurements of the reflectivity of multilayer mirrors on the NIST storage ring, SURF II for the wavelength region between 100 and 500 Å. The present capabilities include a grazing-incidence, scanning monochromator and a reflectometer attached to a beamline on SURF II. This instrument operates in the wavelength range from 80 to 600 Å. Samples from different laboratories, including the University of Arizona, the University of Colorado, Johns Hopkins University, NASA, Lawrence Livermore, Lawrence Berkeley, IBM, Princeton University, and Ovonics Corporation have been measured. Collaborations with some of these and other institutions, including Bell Labs, have been set up for future experiments in lithography and biological microscopy. (J. Roberts, E. Saloman)

(b) Characterization of R. F. Plasmas

One of the most serious problems in the manufacturing of semiconductor devices with plasmas is the precise control of the various stages of the process. Commercial fabricators of complicated semiconductor devices have no real-time control with present plasma reactors to allow for immediate adjustments or curtailment of the plasma processing. In collaboration with the SEMATECH Corporation, we have undertaken to characterize of a prototype and reference rf plasma source using optical emission spectroscopy to "calibrate" a commercial electric probe. This probe will be incorporated in production line rf plasma reactors on assembly lines at SEMATECH as a process control tool. The reference R. F. plasma source will also be available to the industry as a means of recalibrating this probe or any other characterizing tool.

The calibration procedure will entail the measurement of the excited state densities of atoms, ions and molecules to determine the deviation, if any, of the plasma electron temperature from a pure Boltzmann distribution. Certain parameters of the discharge will be varied, such as gas pressure, gas constituents, flow rate and rf power, and the changes in the density distribution will then be correlated with the changes in the electric probe observations. This will quantify the probe measurements allowing the source to be used as a process control device for semiconductor fabrication. (J. Roberts)

(c) Vacuum Ultraviolet Radiometry with Plasmas

The argon mini-arc has proven to be a useful standard radiometric source in the near UV and VUV spectral regions. Like all secondary standards, the arcs must be calibrated against primary standards; each arc is individually calibrated. During the past year however, work was started to establish the mini-arc as a standard source by "prescription." By better standardization and demonstration of the equality in output between individual arcs, the need for a separate calibration for each could be eliminated. For this purpose five arcs were identically constructed and accurately intercompared in the near UV (200-335 nm). They were found to differ by at most 2.3% in absolute spectral irradiance, and 0.2% in relative spectral distribution. This result represents a significant improvement in the arc as a radiometric source.

A paper presenting the results of the characterization of the Pt-Ne sealed hollow lamp has been completed and will be published in Applied Optics. This paper contains data obtained in the calibration of several of these lamps for the throughput test of the Hubble Space Telescope.

The project to develop a body of atomic branching ratios for use in vacuum ultraviolet radiance calibrations is continuing. Collections of branching ratios for the hydrogen, helium, lithium, and beryllium isoelectronic sequences have been obtained from existing data, and a paper presenting these results has been accepted for publication in the Journal of Quantitative Spectroscopy and Radiative Transfer. In addition, a project is being initiated to make these data available on computer disks. Work will continue to update the existing body of data and to develop branching ratios for additional isoelectronic sequences.

(d) Microwave Plasma Sterilization Source

During the past year, staff of the Dental and Medical Materials Group at NIST demonstrated a fast sterilization technique for dental tools by placing them in a simple microwave-excited plasma. We are now cooperating in this project by performing some studies that we hope will lead to understanding of the sterilization mechanism. Planned studies are designed to characterize the plasma and find out which plasma properties are important or essential to the sterilization. So far, a device has been assembled using a standard microwave oven. Spectral emission studies have been initiated extending from the visible to the vacuum ultraviolet regions. Tests are underway that should demonstrate the importance of UV radiation in the sterilization process.

(e) Low Density Plasmas

We are developing methods for determining the physical properties of low density plasmas. Most of these methods are spectroscopic and laser-based. Low density plasmas have been gaining in importance, particularly in the semiconductor-processing and analytical industries. The current area of focus is in the developing "collisional redistribution" methods in plasmas. They appear promising because they are well-suited to low density environments and can provide a wealth information. The carefully determined and cross-checked physical quantities can then be used to calibrate simple probes that are useful in an industrial setting. The newly constructed laboratory includes a specially designed spectrograph with negligible coma, a pulsed dye laser, and a gated OMA data-collection system.

We are also continuing a theoretical effort to calculate collisional line shapes of hydrogenic species in low density plasmas. Hydrogenic species are important because they are by far the most sensitive. However, particularly at moderately low densities, the same physics that gives rise to their sensitivity also makes dynamical many-body effects important, so that the above calculations are uniquely difficult. Our current results are promising but show the need for building in an adiabatic limit.

(f) Experimental Tests of the Spin-Statistics Theorem and the Pauli Exclusion Principle (PEP)

Quantum mechanics allows many symmetries of multi-particle states. Why does nature choose only two, those which are either symmetric or anti-symmetric with respect to interchange of particle coordinates? The restriction to these two symmetries is the content of the symmetrization postulate. It remains a postulate since it can only be proven with the help of several assumptions, some of which are rather ad-hoc in nature. The spin-statistics theorem associates antisymmetry with half-integer spin particles, and symmetry with integer spin quanta particles. PEP is a special case of antisymmetry states, in which the probability of more than one identical half-integer spin particle occupying the same state is zero.

The above symmetries are among the few that remain "absolute" in physics: without PEP, atoms, nuclei, and neutron stars would collapse. Yet other symmetries could occur in nature at a small level (as large as about one part in about 10^6) without our having detected them thus far. We are designing and constructing an experimental apparatus that will be sensitive to "forbidden" symmetries at a level of one part in 10^{11}, with a long term possibility of extending this sensitivity considerably. The pump laser, tunable laser, vacuum system, detection electronics, and optics and light-collection system have been designed and are under test. Initial experiments will search for symmetric states in helium. An observed violation of any of the above symmetry principles would have a profound impact indeed, easily on the order of parity violation, which was first observed at NIST.

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Sugar, J., Kaufman, V., Indelicato, P., and Rowan, W. L., "Analysis of Magnesiumlike Spectra from Cu XVIII to Mo XXXI," J. Opt. Soc. Am. B 6, 1437 (1989).

Wiese, W. L. and Fuhr, J. R., "On the Accuracy of Atomic Transition Probabilities". Proceedings of Conference: "Lecture Notes in Physics" (1988).

Wiese, W. L., Brault, J. W., Danzmann, K., Helbig, V. and Kock, M. "A Unified Set of Atomic Transition Probabilities for Neutral Argon," Phys. Rev. A 39, 2461, 1989.

Wiese, W. L., "The Spectroscopic Data Base for Carbon and Oxygen," Physica Scripta T28, 10 (1989).

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PUBLICATIONS IN PREPARATION

Division 572, Atomic and Plasma Radiation

Datla, R. U., J. Roberts, J. and Bhatia, A. K., "Magnetic Dipole Line Intensity Measurements for Si-like Ions in the TEXT Tokamak and Comparison to Theoretical Predictions," (submitted).

Datla, R. U., Eshhar, S. and Roberts, J. R., "Excited Level Populations in CIV in a rcombining θ-pinch Plasma," (submitted).

Elton, R. C., Datla, R. U., Roberts, J. R.and Bhatia, A., "Neonlike AR and Cl 3p-3s Emission from a θ-pinch plasma," Phys. Rev. (in press).

Hahn, T., and Wiese, W. L., "Oscillator Strength Ratios Between 4s-5p and 4s-4p Lines of Neutral Argon" (submitted).

Kelleher, D. E., "On Quadrupole Moments from Term Energy Separations of High Angular Momentum States: Halogen-like Ions" (submitted for publication in Nist Journal of Research).

Kelleher, D. E., Gillaspy, J., Deilamian, K., "Proposed Search for States of Forbidden Permutation Symmetry" (to be published in Nineth International Conference on Laser Spectroscopy by Springer Verlag).

Klose, J. Z. and Wiese, W. L., "Branching Ratio Technique as Applied to Vacuum UV Radiance Calibration: Extensions and an Expanded Data Set" (Submitted to J. Quant. Spectrosc. Radiat. Transf.).

Martin, W. C., Zalubas, R. and Musgrove, A. "Energy Levels of Sulfur, S I through S XVI," J. Phys. Chem. Ref. Data 19 (1990 to be published).

Mohr, P., Blundell, S. A.. Johnson, W. R. and Sapirstein, J., "Evaluation of Two-Photon Exchange Graphs for the Helium Isoelectronic Sequence" (submitted).

Mohr, P., "Computational Aspects of Precision Bound-State QED," lecture given at the Summer School of Computational Atomic and Nuclear Physics at Sewanee, TN (submitted).

Mohr, P., "Quantum Electrodynamics of High-Z Few-Electron Atoms," in Atomic Physics of Highly-Ionized Atoms, ed. by R. Marrus (Plenum, New York, to be published).

Reader, J., Feldman, U., "Spectrum and Energy Levels of Six-Times Ionized Molybdenum Mo (VII)" (submitted).

Reader, J., Acquista, N., Sansonetti, C. J., and Sansonetti, J. E., "Wavelengths and Intensities of a Platinum/Neon Hollow Cathode Lamp in the Region 1100 to 4000 Å," (submitted to Astrophysical Letters, Supplement Series).

Sansonetti, C. J., "Precise laser wavelength measurements: What can we learn from classical spectroscopy?," Proceedings of the 4th International Laser Science Conference (submitted).

Sugar, J., Kaufman, V., and Rowan, W. L., Spectra of the Si I isoelectronic sequence from Cu XVI to Mo XXIX (submitted).

Sugar, J., Musgrove, A., Energy Levels of Copper, Cu I through Cu XXIX, J. Phys. Chem. Ref. Data (in press, 1989).

Zhu, Q., Bridges, J. M., Hahn, T. D. and Wiese, W. L., "Atomic Transition Probability Measurements for Prominent Spectral Lines of Neutral Nitrogen," Phys. Rev. A (in press).

INVITED TALKS

Division 572, Atomic and Plasma Radiation

Bridges, J. M., "Standard Source Radiometry in UV & VUV," Arnold Engineering Center, Nashville, Tennessee, February, 1989.

Kelleher, D. E., "The Interplay Between Experiment and Theory in Stark Broadening", Plasma Spectroscopy Symposium, University of Maryland, April 7, 1989.

Kelleher, D. E., "Proposed Search for States of Forbidden Permutation Symmetry," Nineth International Conference on Laser Spectroscopy, Bretton Woods, New Hampshire, June 18-24, 1989.

Kim, Y.-K., Univ. of Western Ontario, Canada: Physics Dept. Colloquium on "Relativistic Effects in Atoms and Molecules," Oct. 19, 1988.

Kim, Y.-K., Univ. of Windsor, Canada: Physics Dept. Colloquium on "Relativistic and QED Effects in Atoms," Oct. 21, 1988.

Kim, Y.-K., Korea Advanced Energy Research Institute (KAERI): A Short Course on "Quantum Defect Theory," June 12-16, 1989.

Kim, Y.-K., KAERI: Theoretical Physics Colloquium on "Relativistic Hartree-Fock Method," June 19, 1989.

Kim, Y.-K., KAERI: Institute Colloquium on "Cold Fusion," June 20, 1989.

Mohr, P. J., "Quantum Electrodynamics of High-Z Atoms" Theory Seminar, Oak Ridge National Laboratory, November 28, 1988.

Mohr, P. J."Quantum Electrodynamics of High-Z Atoms" Physics Department Colloquium, University of Tennessee, Knoxville, November 29, 1988.

Mohr, P. J., "Quantum Electrodynamics Effects in High-Z Few-Electron Atoms" Atomic and Plasma Radiation Division Seminar, National Institute of Standards and Technology, June, 13, 1989.

Mohr, P. J.,"Computational Aspects of Precision Bound-State QED" Invited lecture presented at the 1989 Summer School on Computational Nuclear and Atomic Physics, Sewanee, TN, June 26 - July 7, 1989.

Martin, W. C., "Review of Data on Atomic Wavelengths, Energy Levels, and Transition Probabilities" October 2, 1989, Chicago, Ill., Annual Meeting of the Federation of Analytical Chemical and Spectroscopy Societies.

Sansonetti, C. J., "Precise Laser Wavelength Measurement: What Can We Learn from Classical Spectroscopy?," Fourth International Laser Science Conference, Atlanta, GA, October 2-6, 1988.

Sugar, J., "Spectroscopy of the $3s^2 3p^n$ Shell from Copper to Molybdenum," Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysics and Fusion, Amsterdam, The Netherlands, August, 1989.

Wiese, W. L., "Progress and Problems in the Measurement of Transition Probabilities", Physics Colloquium, Jugellonian University, Krakow, Poland, October 3, 1988.

Wiese, W. L., "A Unified Set of Atomic Oscillator Strengths for Neutral Argon", Pedagogical University Opole, Poland, October 4, 1988.

Wiese, W. L., "Plasma Broadening of Isolated Heavy Lines", Workshop on Plasma Line Broadening, University of California, Berkeley, July 18, 1989.

Wiese, W. L., "New Transition Probability Results for Atomic Nitrogen, Third Atomic Data Workshop, Mendon, France, September 6, 1989.

Wiese, W. L., "Spectroscopic Data for Tokomak Edge Plasmas - The Second to Fifth Spectra", Second Specialists Meeting on Fusion Plasma Edge Studies, International Atomic Energy Agency, Vienna, September 13, 1989.

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Division 572, Atomic and Plasma Radiation

Daniel E. Kelleher

Member, International Organizing Committee of the Conference on Spectral Line Shapes.

Yong-Ki Kim

Organizer and Program Committee member of the 7th APS Topical Conference on Atomic Processes in Plasmas, Oct. 2-5, 1989, at NIST.

Arlene Robey

Equal Employment Opportunities Counselor, NIST, collateral duty assignment (1989).

William C. Martin

Chairman, Working Group on Atomic Spectra, International Astronomical Union.

Member, IAEA Network of Atomic Data Centers for Fusion.

Member, Optical Society of America. W. F. Meggers Award Committee.

Jack Sugar

Chairman, OSA Fellows and Honorary Members Committee.

Wolfgang L. Wiese

Member of Organizing Committee, International Astronomical Union, Commission on Fundamental Spectroscopic Data.

Chairman, Working Group on Atomic Transition Probabilities, International Astronomical Union.

Vice President, Commission on Fundamental Spectroscopic Data, International Astronomical Union.

Member, Network of Atomic Data Centers for Fusion, coordinated by the International Energy Agency

Member of Organizing Committee, International Astronomical Union, Commission on Fundamental Spectroscopic Data.

Chairman, Working Group on Atomic Transition Probabilities, International Astronomical Union.

Wolfgang L. Wiese

Vice President, Commission on Fundamental Spectroscopic Data, International Astronomical Union.

Member, Network of Atomic Data Centers for Fusion, coordinated by the International Atomic Energy Agency.

Peter J. Mohr

Member, NAS/NRC Committee on Line Spectra of the Elements - Atomic Spectroscopy.

Invited Session Chairman, Meeting of the Division of Atomic, Molecular, and Optical Physics, American Physical Society, Windsor, Ontario, Canada, 17-19 May 1989.
Member of International Advisory Committee, conference series on Physics of Highly-Ionized Atoms.

SEMINARS ORGANIZED

Division 572, Atomic & Plasma Radiation

Wolfgang L. Wiese, NIST, Atomic & Plasma Radiation Division, "Impressions of a Trip to Yugoslavia and Poland--Scientific and Otherwise," November 1, 1988.

P. W. J. M. Boumans, Philips Research Laboratories, Eindhoven, Netherlands, "Measurement of Pseudo Physically Resolved Rare Earth Spectra Emitted from an ICP and Simulation of Effective Spectra for Interference Predictions in Analysis," November 9, 1988.

Anil K. Pradhan, Joint Institute for Laboratory Physics, Boulder, Colorado, "The Opacity Project," December 1, 1988.

Paul Indelicato, NIST and CNRS, "MCDF Calculations of Relativistic Effects in Two- and Three-Electron Atoms," January 10, 1989.

Jack Sugar and Joe Reader, NIST, "Two Soft X-Ray Lasr Schemes," January 24, 1989.

M. Finkenthal, Hebrew University, Jerusalem, Israel, "XUV Spectroscopy in Tokamak Plasma Physics Research," January 31, 1989.

Yong-Ki Kim, NIST, "Relativistic Hartree-Fock Theory: Past, Present, and Future," February 14, 1989.

A. W. Weiss and W. L. Wiese, NIST, "Atomic Oscillator Strengths for Nitrogen--Some New Calculations, Measurements, and Old Puzzles," February 28, 1989.

Gerhard Soff, Gesellschaft für Schwerionenforschung - GSI, Darmstadt, Federal Republic of Germany, "The GSI Positron Peaks - Recent Investigations," March 7, 1989.

S. Suckewer, Princeton University, "Quenching of the Einstein A-Coefficients," March 9, 1989.

Richard Pratt, National Science Foundation and University of Pittsburgh, "The Relativistic Atom and Relativistic Processes," March 21, 1989.

Joseph Sucher, University of Maryland, "The Concept of Potential in Quantum Field Theory," March 29, 1989.

H. J. Kunze, Ruhr Universität, Bochum, West Germany, "Plasma Sources for the X-Ray Region," April 4, 1989.

Nikola Konjevic, Institute of Physics, Beograd, Yugoslavia, "Plasma Broadening and Shift: Experiment Versus Theory," April 11, 1989.

John G. Conway, Lawrence Berkeley Laboratory, "Lifetimes and Oscillator Strengths in Neutral Cerium," April 12, 1989.

R. U. Datla, NIST, "Neon-Like 3s-3p X-Ray Laser Transitions Studied in a Theta-Pinch Plasma," April 18, 1989.

Alfred Maquet, JILA, Université Pierre et Marie Curie, Paris, "Theory of Electron-Atom Collisions in the Presence of a Laser Field," April 25, 1989.

Ann-Marie Mårtensson-Pendrill, University of Göteborg, Sweden, "Beryllium Discrepancy-Comparison Betwen Accurate Calculations and Experiment," May 16, 1989.

Bill Conner, University of Wisconsin, "Microwave Absorption Spectroscopy in Low Density Plasmas, August 1, 1989.

Karl Welge, Bielefeld University, West Germany, "Chaos in Atoms?," August 3, 1989.

G. von Oppen, Technische Universität, Berlin, RF Spectroscopy of Impact-Excited Helium Atoms," August 8, 1989.

K.T. Lu, Atomic Engineering Corporation, "Atomic Engineering Database Management System: Application to VUV New Laser Materials," September 19, 1989.

Liwen Pan, NIST, University of Maryland, "Application of High-Order Perturbation Theory to Atomic Processes," September 26, 1989.

JOURNAL EDITORSHIPS

Division 572, Atomic and Plasma Radiation

J. Reader, Editor, Line Spectra of the Elements, Handbook of Chemistry and Physics, CRC Press.

W. L. Wiese, Associate Editor, Journal of Quantitative Spectroscopy and Radiative Transfer

W. L. Wiese, Editor, Atomic Transition Probabilities, Handbook of Chemistry and Physics, CRC Press.

MAJOR CONSULTING AND ADVISORY SERVICES

Division 572, Atomic and Plasma Radiation

1. The Data Centers on Atomic Energy Levels and Transition Probabilities routinely fill requests for atomic data or literature information submitted by scientists in a wide range of research areas. The requests average about 30 per month. Periodically, special reports are prepared for particular user groups. Thus, W. C. Martin and W. L. Wiese have written updates on atomic data of interest for the astrophysical community for the Transactions of the International Union (IAU), covering the three year period September 1984 through August 1987, and give review reports at the General Assemblies of the International Astronomical Union. J. R. Fuhr and A. Robey submit literature reference lists every six months to the International Atomic Energy Agency (IAEA) for inclusion in the IAEA semiannual Bulletin of "Atomic Data for Fusion."

2. J. M. Bridges consulted with NASA-Goddard scientists on tests and calibrations to be performed for the Shuttle Solar Backscatter Ultraviolet experiment.

3. J. M. Bridges consulted with NRL scientists on calibration work to be performed for the Solar Ultraviolet Spectral Irradiance Monitor.

4. J. M. Bridges and J. R. Roberts consulted with SEMATECH and Motorola on ultraviolet radiometry of semiconductor photoresist exposure.

5. J. Reader continues to consult with members of the x-ray laser program at Lawrence Livermore National Laboratory about the spectra of highly ionized atoms in laser-produced plasmas and the wavelength calibration of such spectra.

6. J. R. Roberts consulted with members of Bell Labs on characterization of x-ray optics for lithography.

7. J. R. Roberts and R. U. Datla continue to consult with staff of the Naval Research Laboratory on population inversion experiments and recombination mechanisms in UV lasers.

8. J. R. Roberts consulted with the University of Arizona, Johns Hopkins University, Stanford University, Lawrence Livermore National Laboratory, Lawrence Berkeley National Laboratory, NASA, IBM, Lockheed, and the University of Colorado/Laboratory for Atmospheric and Space Physics, on the characterization of x-ray optics.

9. J. R. Roberts continues to serve as a member of the TEXT Users Organization (TUO). TEXT stands for Texas Experimental Tokamak and is a national plasma users facility.

10. J. R. Roberts continues to consult with members of Bell Labs on population inversion experiments in C^{+3} on the NIST theta pinch.

11. W. C. Martin and J. Reader consult and advise NASA scientists and other astronomers on standard wavelengths for calibration of the High-Resolution Spectrograph for the Space Telescope.

12. J. Sugar and W. L. Wiese consulted and advised the Japan Atomic Energy Research Institute (JAERI) on the compilation of spectral lines.

13. J. Sugar consulted with KMS Fusion scientists on the development of x-ray lasers.

14. Y.-K. Kim consulted with the Lawrence Livermore National Laboratory on x-ray laser development.

15. Y.-K. Kin advised the Los Alamos National Laboratory on relativistic atomic structure calculations.

CALIBRATION SERVICES PERFORMED

Division 572, Atomic and Plasma Radiation

Type of Service	Customer	SP 250	Tests	No. of Income
Radiometer	IBM	40040S	1	$ 1.3k
Radiometer	IBM	40040S	1	1.3k
Argon Mini-Arc	SERI	40040S	1	1.9k
Argon Mini-Arc	Martin-Marietta	40010C	1	2.9k

SURFACE SCIENCE DIVISION

FISCAL YEAR 1989 TECHNICAL ACTIVITIES

1. INTRODUCTION

A. Background

Over the last decade, there has been a dramatic growth of surface science and its applications. This growth and its significance have been documented in two major reports, the Pimental report to the National Academy of Sciences on "Opportunities in Chemistry" (National Academy Press, Washington, D.C. 1985) and the Brinkman report to the National Academy of Sciences on "Physics Through the 1990's" (National Academy Press, Washington, D.C., 1986). Both reports describe in some detail the pervasive role of surfaces, interfaces, and thin films in frontier scientific research and in major technological applications. The scientific opportunities range from studies of the dynamical processes involved when atoms and molecules interact with surfaces to heterogeneous catalysis, physical and chemical properties of clusters, fabrication and characterization of novel thin-film and superlattice materials, and surface critical phenomena, among many other topics. A principal goal of investigations in these areas is to obtain knowledge at a fundamental atomic and molecular level of surface and interface properties and processes. The technological applications include microelectronics, information processing, catalysis, corrosion, coatings, adhesion, wear, and biomaterials as well as areas of national concern such as energy generation, transportation, environmental pollution, space technology, and national security. A strong driving force in both the scientific and technological sectors is the need for improved U.S. economic competitiveness; in a 1987 analysis, the U.S. Department of Commerce has identified surfaces and thin films as having major significance for the development of new technologies.

Many measurement techniques are used to characterize surface properties (such as composition, atomic structure, electronic structure, defects, and topography) and surface processes (such as reactions, diffusion, segregation, and exposure to beams of ions, neutrals, photons, and electrons). A choice of one or more techniques is made typically on the basis of the property to be measured, the specimen material, and the specific needs (e.g., spatial resolution, chemical information, sensitivity, degree of difficulty, and cost). New techniques are also being developed to characterize the properties of thin-film materials and the dynamics of molecule-surface interactions. Many of the techniques are continually being refined and extended, as are the concepts on which they are based. The concepts and techniques that have proven successful for surface characterization are also being applied to the characterization of interfaces and thin films. In many such applications, surface material is removed by ion sputtering or other means to expose an interface or other region of interest. While useful, artifacts can generally be introduced by the removal process and there is now a growing need for non-destructive techniques for interface characterization, particularly with the sensitivity, elemental specificity, and spatial resolution of current surface-characterization methods.

The most common type of surface measurement is the determination of surface composition. Most surface analyses now are qualitative but there is a growing demand for quantitative analyses with improved accuracy. At the present time, there are few standard procedures and limited reference data and reference materials. A variety of techniques are used for determining of surface atomic structure, surface electronic structure, and for investigating surface processes such as reactions, diffusion, segregation, etc. Theories of the measurement process need to be developed for the newer techniques. For all techniques, there is a need for relevant procedures, tests to establish measurement reliability, and applicable reference data. In most cases, the measurement science needs to be developed since knowledge of the key concepts and parameters is often extremely limited. Some concepts and data are synthesized and developed from those of disciplines such as atomic and molecular physics, chemistry, and materials science.

B. Goal, Objectives and Division Programs

The goal of the Surface Science Division is to improve the quality of existing surface-characterization measurements and to extend the present capability. Specific objectives of the Division are:

(1) Perform experimental and theoretical research in surface science to provide a scientific base for surface-measurement methodology;

(2) Develop measurement methods and provide properties data for the physical and chemical characterization of surfaces and surface processes to meet identified needs of industry, government, and other groups;

(3) Develop reference procedures, reference data, and reference materials in cooperation with national and international standards organizations; and

(4) Develop expertise in selected new areas of surface science in order that NIST can provide measurement services where needs are expected in the near future.

While the Division has a broad mandate, its resources are limited and it has to concentrate its activities in areas considered to be of high priority. The Division is now organized into three Groups (Surface Dynamical Processes, Thin Films and Interfaces, and Surface Spectroscopies and Standards) which represent the three principal directions of the current program.

Descriptions are given in the following pages of technical work performed over the past year. These are followed by lists of publications, patent actions, invited lectures, seminars held at NIST, external conferences organized, involvement with professional groups, and collaborations with other scientists. In addition to a regular series of Division seminars on surface science topics, the Division has been active in establishing a NIST-wide series of seminars on interface science. A successful series of discussion meetings was also held within the Division on scattering phenomena.

Some technical highlights of the past year are listed below; further details of these accomplishments are given in the indicated sections of this report.

- Studies of laser-induced desorption of NO from a Si(111) surface have shown the importance of thermalized band-edge carriers in the desorption process (section 2.A)

- The ellipsoidal-mirror analyzer has been installed at SURF-II; initial tests indicate that the analyzer is operating within design expectations (section 2.B)

- X-ray photoelectron spectroscopy has shown how fully chlorinated silanes can be used to prepare silicon films by chemical vapor deposition; the chlorinated silanes are much safer to handle than silane (section 2.C)

- Adsorbed gases can be used as surfactants to modify the morphology of epitaxial films and thereby to permit a new degree of control at the atomic level on thin-film microstructures (section 3.A)

- The technique of grazing-angle x-ray diffraction has been used to determine the roughness spectrum of a germanium surface (section 3.B)

- Calculations of ballistic electron transport have shown the transmission probability for the two structural forms of silicon-nickel disilicide interfaces is too low to be useful for a proposed new type of transistor (section 3.C)

- Atom-probe field-ion microscopy studies have shown that the surface layers of europium 1-2-3 superconducting oxides lose oxygen at room temperature but not at 85 K or below (section 3.D)

- A new theory has been developed that successfully accounts for a giant enhancement in electron-resonance-assisted desorption (section 4.A)

- A new scanning scattering microscope has been developed (and a patent application filed) to measure surface roughness with a height sensitivity of about 1 nm (section 4.B)

- New calculations of inelastic mean free paths of low-energy electrons in solids show substantial differences amongst materials in the 50-200 eV range (section 4.C)

2. SURFACE DYNAMICAL PROCESSES GROUP

As greater control and predictability of physical properties of surfaces are sought, the surface science community is increasingly turning to a molecular level understanding of surface probes, surface properties and surface reactions. Within the Surface Dynamical Processes Group, a variety of approaches are used to obtain information on the microscopic behavior of surfaces. The techniques range from laser probes of surface reactions to synchrotron based measurements of surface electronic structure and reactivity. Systems of interest have ranged from small molecules adsorbed on metal and semiconductor single crystals, to compositionally controlled high temperature superconductors and chemical etching of electronic materials.

A. Laser Probes of Surface Dynamics (R. R. Cavanagh, J. D. Beckerle, S. A. Buntin, and L. R. Richter together with M. P. Casassa, E. J. Heilweil, D. S. King, and J. C. Stephenson of the Molecular Spectroscopy Division)

Lasers have emerged as extremely powerful tools for unraveling the complex properties of molecular processes at surfaces. By exploiting both the short pulse duration and the narrow spectral linewidths characteristic of lasers, it is possible to follow and/or induce adsorbate-specific surface processes. The prospects for capitalizing on the accompanying non-thermal behavior in such transient events has made this an extremely active area of surface science. Within the present program, two distinct aspects of laser/surface interactions are addressed. The first area of the program involves the complete characterization, using quantum-state-specific techniques, of the desorbed molecules in laser-induced desorption. These studies provide insight into the potential energy surfaces relevant to desorption, and the pathways for optical excitation. In a second area of the program, the time-resolved response of clean and adsorbate-covered surfaces is examined. The excited state lifetimes of vibrationally excited adsorbates are measured in an infrared pump-probe configuration. These experiments provide direct information on the rate at which selectively excited molecular populations decay.

Laser Induced Desorption (R. R. Cavanagh, S. A. Buntin and L. J. Richter together with D. S. King of the Molecular Spectroscopy Division).

Experiments examining laser-induced desorption (LID) of NO from platinum (111) have recently been completed. Laser-induced fluorescence (LIF) was used to probe the partitioning of energy between the various degrees of freedom of the desorbed NO. The desorption-laser wavelength dependence of the kinetic energy and vibrational state distributions has been examined at 1906, 1064, 532 and 355 nm. Combined with measurements of the desorption yield as a function of angle of incidence of the desorption laser beam, these results provided the first unambiguous proof of the role of "hot" carriers in the chemistry of molecules bound to metal surfaces. Recent theoretical modeling in collaboration with J. W. Gadzuk suggests that a short lived (10^{-15} s) negative ion resonance could account for the observed desorption yield. The experimental studies determined that the spin-orbit populations were strongly inverted, and that the rotational population exhibited a pronounced low J plateau. Our present understanding of the desorption process indicates that these non-Boltzmann internal-state populations are characteristic of the molecular ejection pathway. The site-specific nature of this desorption process, and the highly non-Boltzmann populations associated with this channel, suggest the sensitivity of surface excited states to subtle details of gas/surface interactions. More significant, however, was the clear demonstration that the short-lived transients associated with hot carriers on metal surfaces can dominate chemical events.

Similar LIF studies of the LID of NO/Si(111) have been undertaken in order to better characterize the role of carrier-induced surface reactions. We have discovered that there is a strong coverage dependence in the LID signals (yield per incident photon, relative yield at different wavelengths, internal state populations, etc.). For instance, the relative NO population in the first excited vibrational state increases by a factor of three as the NO coverage increases from a dilute limit to saturation ($v=1/v=0$: 0.19 ± 0.09 and 0.64 ± 0.24, respectively). Data acquired to date indicate that the kinetic energy of the desorbed NO greatly exceeds the peak surface temperature (1000 K vs. 100 K) and that the kinetic energy increases with increasing rotational energy. Figure 1 shows the internal state population for a low coverage of NO. While under population of the F_2 levels compared to the F_1 levels is apparent, within the F_1 level the rotational state population can be described by a Boltzmann distribution with T_{rot} = 200 K. By increasing the NO coverage, the population of the F_1 and F_2 states becomes equilibrated with the nuclear rotations, and the population can be described as T_{rot} = 600 K. The details of the coverage dependence of the internal states are still under study. The lack of a marked wavelength dependence in the desorption dynamics at low coverage has suggested that the desorption is driven by thermalized band-edge carriers. At higher coverages, the dynamics become wavelength sensitive, an effect that is currently under study. Future work is expected where the influence of crystal face and excitation below the gap (Si(100) and GaAs(110), respectively) will be investigated.

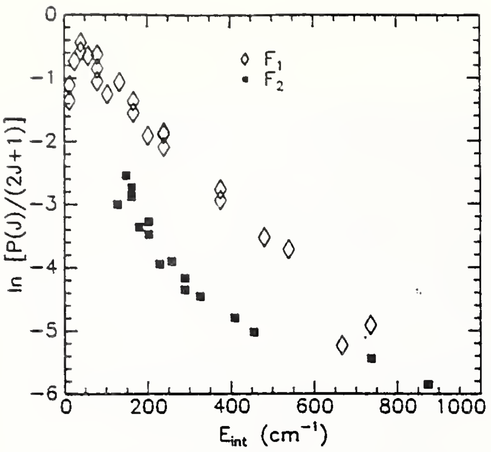

Fig. 1. Internal state distribution for NO in v = 0 produced via laser-induced desorption of low coverages of NO on Si(111) at 95 K with 355 nm radiation. The high-energy spin-orbit state F_2 has significantly less population than the ground spin-orbit state F_1 for NO with comparable internal energy (E_{int} ≡ spin-orbit + rotational energies).

Extension of existing state-specific detection techniques to include the detection of gas-phase CO are in progress. The generation of narrow-band vacuum ultraviolet (VUV) laser radiation in the spectral region of 140-155 nm is necessary to detect CO by LIF. The method of choice is two-photon resonance-enhanced four-wave sum-frequency generation in Mg vapor. In this nonlinear frequency conversion process, three photons from two dye lasers are combined in a heat pipe to generate a single VUV photon ($\omega_{VUV} = 2\omega_1 + \omega_2$). The lasers and heat pipe facilities were procured during the past year. In addition, a VUV test apparatus has been constructed and detector optimization (for both VUV signal and CO LIF) is currently underway for frequency tripling in Xe. It is expected that the first tests using Mg vapor for VUV generation will take place in the fall of 1989, with desorption studies beginning shortly thereafter. In these experiments, CO desorption will be investigated for a number of systems. Specifically, probing the dynamics of laser heating and carrier-driven desorption for metal-based systems such as CO/Pt(111) and CO/K/Pt(111) will clarify the influence of adsorbate properties (eg. electronic structure, binding energies, etc.) on these processes. In addition, studies of the photofragmentation/photodesorption of CO from $Mo(CO)_6$/Si(111) will provide insight into adsorbate-moderated energy relaxation at surfaces. This work was supported in part by the U.S. Department of Energy.

Time-Resolved Vibrational Relaxation at Surfaces (R. R. Cavanagh and J. D. Beckerle together with M. P. Casassa, E. J. Heilweil, and J. C. Stephenson of the Molecular Spectroscopy Division)

Vibrational relaxation times (T_1) have been measured for CO on Rh and Pt particles supported on SiO_2. By configuring a 2 ps tunable infrared system for pump-probe measurements, it has been possible to characterize the temperature, polarization, and wavelength dependence of T_1 for these CO/Metal/SiO_2 specimens. Comparison with model metal carbonyl compounds in solution and supported on SiO_2 indicated that rapid (≈ 7±2 ps) new decay processes were involved. Comparison with existing theories and frequency domain experiments on single-crystal surfaces has suggested that relaxation through low-lying electron-hole (e/h) pair excitations could be responsible for the observed time scale. In collaboration with Gadzuk, theoretical modeling of the electronic levels of the metal clusters as a function of particle size has demonstrated that the present particles (≈30 Å) fall near the size threshold for infrared excitation of e/h pairs.

Work in the area of vibrational relaxation has now shown that experiments on well-characterized single-crystal surfaces are essential for establishing the site selectivity and the role of e/h pairs in vibrational relaxation. Based on the expertise acquired over the past several years, it is now apparent that single-reflection picosecond infrared experiments are technologically feasible. An ultra high vacuum (UHV) system dedicated to these experiments is now operational. Conventional surface diagnostics have been applied to platinum and palladium surfaces in order to prepare specimens for Fourier Transform Infrared (FTIR) spectral measurements and for transient picosecond infrared experiments. Initial measurements of the coverage and temperature dependence of the CO/Pt(111) system were made using a commercial FTIR spectrometer with a resolution of 0.125 cm^{-1}. The results of these experiments have confirmed previously published reports of both the coverage- and temperature-dependent perturbations of the spectral widths and positions.

Initial tests of the UHV system with the 2 ps infrared laser are in progress. Optics have been configured for the single-reflection experiments, and tests of pulse-to-pulse stability and random noise sources are well underway. The picosecond laser system has recently been used to record the infrared spectrum of CO/Pt(111), indicating a peak position and signal strength in good agreement with the FTIR results. Preliminary data indicated a weak transient (signal/noise ≈ 1) in the pump-probe measurements of vibrational relaxation for this system at 2105 cm^{-1} for θ_{CO} = 0.5 ML. Work is presently underway to further reduce the background noise and increase the dynamic range in this system.

These experiments will provide the first time-resolved characterization of energy transfer for a molecule directly bound to a well characterized site of a metal surface. It is at these short molecule-metal distances where not only classical electrodynamic theories break down, but where surface chemistry takes place. The knowledge gained in this generation of time-resolved experiments should greatly aid in the development of new measurement technologies capable of directly determining the dynamics of molecular energy-transfer processes at surfaces. This work was supported in part by the Air Force Office of Scientific Research.

<u>B. Studies of Surfaces Using Synchrotron Radiation</u> (R. L. Kurtz, D. R. Mueller, S. W. Robey, R. L. Stockbauer, T. E. Madey, E. L. Roman-Garcia,* A. Shih,* and Q. Wang*)

The major goals of this effort are to determine the electronic structure of surfaces, thin-films, and adsorbates using variable-wavelength photoelectron spectroscopy and to identify the electronic excitations that lead to ion desorption. Synchrotron radiation provides the incident photons for both types of experiments with its tunability being its greatest asset. In the photoemission experiments, the tunability allows us to probe resonances which can be used to identify peaks in the valence-

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*Guest Scientist

band spectra as well as to increase sensitivity to minority states on the surface. In the ion yield measurements, the tunability allows us to obtain ion yield data (ion intensity as a function of photon energy) which are correlated with photoemission results to identify the excitations that initiate the ion desorption process.

Photoemission Studies of High-T_c Superconductors (S. W. Robey, R. L. Kurtz, R. L. Stockbauer, D. R. Mueller,* and A. Shih*)

One of the basic questions concerning the new high-T_c superconductors is the nature of the electronic interactions that lead to the superconductivity. The answer to this question lies in knowing the electronic structure of the new material. Photoemission spectroscopy is a powerful technique for elucidating electronic properties and has provided data that can be compared directly with band structure calculations.

Our effort over the past year has been directed towards the design and construction of a research scale molecular-beam epitaxy system for the production of thin films of these materials by coevaporation. This system will be coupled to facilities for resonant photoemission studies (at the NIST SURF II synchrotron) and to various other electron spectroscopies and characterization techniques for studies of the growth and epitaxy of the superconducting oxides, as well as for investigations of the electronic structure of well-characterized thin films. Detailed investigations of the factors affecting the epitaxial growth on different substrates, the effects of substrate interactions and the effects of buffer layers (e.g., barium fluoride) can be pursued. It is also expected that important information will be gained in the area of surface interactions of the high-temperature superconducting materials with other materials, such as metals, information which is of importance for the realization of devices from these complex oxides.

The necessary ultra-high vacuum chamber has been designed and constructed and will provide for the installation of up to six different deposition sources at one time. Each source will be individually monitored and controlled by means of electron impact emission sensors for measurement of evaporation rates for different materials. Evaporation sources have been constructed and tested and the implementation of control by means of a MacIntosh II PC is currently underway. This work has been supported in part by the Office of Naval Research.

Molecular Adsorption on Oxide Surfaces (R. L. Kurtz, R. L. Stockbauer, E. L. Roman-Garcia,* and T. E. Madey)

Our long-term interest in the electronic structure and chemistry of oxide surfaces continues with a synchrotron-radiation photoemission study of the interaction of molecules with defective and nearly-perfect $TiO_2(110)$ surfaces at temperatures between 160 and 300 K. This work is performed as part of a co-operative agreement between the United States and Spain and involves a collaboration with the Instituto Ciencia de Materiales, CSIC, Madrid. Typically, preliminary photoemission and thermal desorption studies are performed in Spain while the resonant photoemission studies are performed in a surface analysis chamber at the NIST SURF II storage ring.

We have completed a study of H_2O adsorption on $TiO_2(110)$ which has suggested a new model for dissociative adsorption on oxide surfaces at low temperatures. The work has continued with a recent investigation of low-temperature adsorption and dissociation of NH_3 on $TiO_2(110)$.

Electron Attenuation Lengths in Condensed Molecular Solids (R. L. Kurtz, R. L. Stockbauer, and Q. Wang*)

Values of electron attenuation lengths (ALs) in different materials and at different electron energies are needed for quantitative surface analyses by Auger-electron spectroscopy and x-ray photoelectron spectroscopy. We have continued to improve a method developed earlier for measuring ALs in condensed molecular solids, materials for which the AL data base is extremely sparse.

Films of water, methanol, ethanol, and acetone have been condensed on a substrate at liquid-nitrogen temperature. The attenuation of photoelectrons from the substrate valence band has been measured as a function of film thickness to obtain AL values over the electron energy range 28-180 eV. We have examined the effects of several parameters in our experiments. First, we have substituted nickel for the copper substrate used previously. Second, the effect of the measurement geometry was studied by comparing and contrasting results obtained with various masking arrangements for our cylindrical-mirror analyzer. Finally, we have explored different methods for depositing the overlayer film and found that continuous dosing with a microcapillary array during the acquisition of photoemission spectra resulted in data of improved quality.

Ellipsoidal-Mirror Analyzer (R. L. Kurtz and R. L. Stockbauer)

Our group has played a strong role in developing techniques and instrumentation for studies of both electron- and photon-stimulated desorption processes. Our interests range from studies of desorption and fragmentation of small molecules adsorbed on clean metallic substrates to desorption from more complex oxide surfaces where ejection of both substrate and adsorbed species are of interest. These studies provide basic information on bonding and structure of these surfaces as well as on the dynamical effects occurring during the stimulated desorption process. Toward this end, a large effort has been devoted to developing an ellipsoidal-mirror analyzer (EMA) based on the design of Eastman. The instrument has now been installed on beam line 1 at the NIST SURF-II synchrotron light source. Initial testing indicates that the analyzer is operating generally within design expectations. Extensive software development has been completed which allows the analyzer to be used for a variety of electron and ion spectroscopies and to provide control of auxiliary functions. Initial studies on clean and NH_3-covered Ru(0001) have been initiated and preliminary angle-integrated photoelectron and photon-stimulated ion desorption spectra have been obtained.

The next phase in making the instrument fully operational will involve the refinement of the angle-resolving capabilities. This will provide us with the ability to measure desorbed ion kinetic energy distributions as a function of desorption angle giving information on substrate dynamic response and reneutralization effects. Such measurements together with time-of-flight techniques will permit studies of the angular distributions of ions of different masses and comparative studies of yields for positive and negative ions. In contrast with measurement techniques used to date, this analyzer will permit simultaneous measurement of desorbing ion mass, and the kinetic energy and angular distribution as a function of the incident photon or electron energy that stimulates the desorption process. Measurements of this type should result in a more complete description of the systems of interest than has been realized previously.

This instrument will be our primary research instrument in the near future and, in addition to the ion desorption studies, will be used for angle-integrated photoelectron studies of a wide range of materials ranging from semiconductors to high-temperature superconductors.

Molecular Dynamics Studies of Ion Desorption Phenomena (R. L. Kurtz)

Through experimental results obtained on oxide surfaces, our group has proposed that surface structures of complex materials such as steps and local site defects may be elucidated by studies of ion desorption angular distributions. In order to further investigate this possibility, we have extended the work of Walkup by producing software to calculate ion desorption trajectories for ionic materials. This allows us to investigate a wide range of surface structures and defects and calculate the resulting ion desorption trajectories. This modeling will allow us to determine the connection between proposed models of surface structure and actual measured ion desorption images. Presently, trajectories are being run for a range of surface structures for TiO_2 and MgO. In the future, effects of image charge and reneutralization will be included to provide a connection to the measurements of ion kinetic energy vs. desorption angle measured on such systems using the ellipsoidal-mirror analyzer.

C. <u>Studies of Molecular Structure and Surface Reactions</u> (J. A. Yarmoff, S. A. Joyce, L. J. Whitman, and T. E. Madey)

We have used a variety of experimental techniques to study the structure of adsorbed molecules on surfaces and to determine the mechanisms of surface reactions. The systems chosen for study are of interest in catalytic surface chemistry, semiconductor processing, and tribology.

Coadsorption of PF_3 and K on Ru(0001) (S. A. Joyce, J. A. Yarmoff, and T. E. Madey)

We have studied the coadsorption of PF_3 and K on a Ru(0001) surface using both positive- and negative-ion electron stimulated desorption ion angular distributions (ESDIAD), thermal desorption spectroscopy, low-energy electron diffraction, and soft x-ray photoemission. In the absence of coadsorbed potassium, positive and negative-ion images ESDIAD show highly anisotropic, off-normal fluorine ion emission from PF_3, demonstrating that the P-F bonds are oriented away from the surface normal. However, in the presence of K, both the positive- and negative-ion ESDIAD images show large amounts of normal emission indicating some reorientation of the P-F bonds along the surface normal. The photoemission results indicate that the chemistry of the PF_3 adsorption is significantly altered by the presence of K. In addition to changes in the desorbed-ion angular distributions, we observe dramatic changes in the yields of the positive and negative ions as a function of potassium coverage, as well as the emergence of a species that we identify as a metastable, neutral fluorine. Qualitatively similar changes in desorption yields have also been observed from coadsorbed HF and K. This work has been supported in part by the U.S. Department of Energy.

Chemisorption of Chlorosilanes on Silicon (L. J. Whitman, S. A. Joyce, and J. A. Yarmoff)

Motivated by the desire for a safer alternative to SiH_4 and SiH_2Cl_2 for Si thin-film growth via chemical vapor deposition (CVD), a number of studies have demonstrated that films can be efficiently deposited with the fully chlorinated silanes, $SiCl_4$ and Si_2Cl_6, which are relatively stable liquids under ambient conditions. Little is known, however, about the basic chemical interactions between chlorosilanes and Si surfaces. We have studied the chemisorption of $SiCl_4$, Si_2Cl_6 and chlorine on single-crystal Si surfaces in ultra-high vacuum using soft x-ray photoemission spectroscopy, thermal desorption spectroscopy, and Auger electron spectroscopy. We find that $SiCl_4$ dissociatively chemisorbs at room temperature on Si(111)-7x7 with an extremely low sticking coefficient, forming only SiCl moieties on the surface. In contrast, Si_2Cl_6 chemisorbs with near-unit probability, partly dissociating into SiCl, $SiCl_2$, and $SiCl_3$. Upon heating, most of the adsorbed Cl desorbs near 650°C as $SiCl_2$ with no appreciable Cl_2 desorption. This result implies that without an additional reactant (e.g., hydrogen) to remove adsorbed Cl, these fully chlorinated silanes will etch silicon. Similar results are observed with Si(100)-2x1.

Photon-Stimulated Desorption of Fluorine from Silicon (S. A. Joyce and J. A. Yarmoff)

We have continued our investigations into the photon-stimulated desorption (PSD) of fluorine from silicon surfaces. Our previous work on monolayer amounts of fluorine adsorbed on silicon had shown how the PSD onsets at the Si 2p edge provide a measure of the unoccupied density of states of the bonding silicon atoms. We have extended this technique to measurements of the Si 2p edge for surfaces that had been subjected to steady-state etching by XeF_2. Photoemission measurements of this surface show a thick reaction layer comprised of both silicon monofluoride (SiF) and trifluoride (SiF_3), and a small amount of difluoride (SiF_2). Photoemission, however, is unable to measure the spatial distributions within this layer. With PSD, we see strong signals at the 2p edge due to both silicon monofluoride and trifluoride, which indicates that the spatial distribution of the layer is relatively homogeneous. We have also made further measurements of the PSD of fluorine at the F 1s edge. By comparison of the near-edge x-ray absorption fine structure (NEXAFS) signal to the PSD yield, we have determined the relative PSD yields of fluorine originating from SiF versus SiF_3 surface sites.

Near-Edge Studies of CaF_2 Surfaces and CaF_2/Si(111) Interfaces (J. A. Yarmoff)

In collaboration with Dr. F. Himpsel of the IBM Watson Research Center, we have investigated the near-edge structure at the Ca 3p edge in CaF_2 with NEXAFS and PSD. CaF_2 grown on Si is a good model system of a semiconductor/insulator interface, since the lattice match (of 0.6%) allows for the growth of an atomically abrupt interface. There are a variety of transitions that occur at the Ca 3p edge that arise from crystal-field splitting in the bulk material. There are additional features which are due to the bonding at the Si interface, states localized at the CaF_2 surface, and defect sites. We have performed a thorough investigation of this system and identified the origin of each observed feature.

Resonant Photoemission from MoS_2 Surfaces (J. A. Yarmoff)

MoS_2 is an important tribological material because of its layered crystal structure. This crystal structure also leads to some interesting chemical properties at its surface. MoS_2 is an extremely inert material with respect to light elements, but does react vigorously with some adsorbed metals. In addition to previous studies of ion-beam damage effects and metal adsorption in collaboration with Dr. J. R. Lince of the Aerospace Corporation, we have performed some new measurements of the resonant photoemission of this material. These measurements will help to understand the valence electronic structure of MoS_2.

3. THIN FILMS AND INTERFACES GROUP

In recent years it has become clear that thin films and interfaces not only can have novel physical properties but are also of considerable technological importance. Structure at the atomic level is the key to many properties and to the performance of solid-state materials and devices. The Thin Films and Interfaces Group is concerned with the structural aspects of epitaxial growth of thin-film systems, artificially structured or atomically engineered novel materials, electron transport across interfaces, and buried interfaces. As much as possible, the structural parameters are related to specific properties of interest. Examples of recent work are the achievement of improved magnetic properties of Fe-Cu sandwich structures, the prediction of a novel x-ray mirror to detect the Bragg condition, the prediction of a silicon-silicide interface with improved ballistic-electron transport properties, and the observation that the europium 1-2-3 superconducting material retained its surface stoichiometry on exposure to vacuum only when cooled to liquid-nitrogen temperature.

A. Novel Two-Dimensional Materials (W. F. Egelhoff, Jr.)

There exist major gaps in current understanding of the fundamental principles that govern the chemical and physical properties of layered structures in the two-dimensional limit. We plan to synthesize and determine the fundamental properties of ultrathin layered materials with layers so thin (a few atoms thickness) that they exhibit two-dimensional behavior. Knowledge of the factors influencing the growth and properties of ultrathin layered systems is expected to allow optimization of desired chemical and physical characteristics and will thus benefit a number of scientific fields ranging from magnetism to novel semiconductor devices.

Determination of Surface Structure by X-Ray Photoelectron and Auger Electron Diffraction

Over the past several years this project has been developing the technique of x-ray photoelectron (XPS) and Auger (AES) forward scattering as a structural probe for the study of surfaces and interfaces. In previous years, the work of this project demonstrated that XPS and AES intensities are strongly enhanced along next-nearest-neighbor axes of a crystal. The angle-resolved XPS and AES spectra thus act like "searchlights" pointing out the bond directions in the top few atomic layers of the sample. As a probe of short-range order, this searchlight effect is useful for studying the structure of epitaxial films, especially the growth mode in the early stages, and for observing surface segregation and interdiffusion phenomena.

In the past year this technique has been used to investigate the growth of epitaxial films of Fe on the Cu(111) surface. It was found that at room temperature and below the Fe grows in a bcc lattice with the close-packed bcc(110) plane parallel to the close-packed fcc(111) plane of Cu, but with the interface out of registry. Upon annealing this Fe structure above 100°C, or if the growth temperature is above 100°C, the Fe takes an fcc(111) form (pseudomorphic with the Cu substrate). These results demonstrate how XPS and AES forward scattering allow us to follow in detail the structural transformations that occur in epitaxial films.

One of our plans for the coming year is to investigate how this structural transformation affects the magnetic properties of the Fe. We expect major changes since ultrathin Fe films generally exhibit magnetic properties that are structure-sensitive.

The Use of Surfactants in Epitaxy

The technique of molecular beam epitaxy holds considerable promise as a source of novel materials and devices. However, to fulfil this promise continuous progress will have to be made in our ability to control, at the atomic level, the exact arrangement of atoms in the epitaxial structure. The use of adsorbed gases as a tool for modifying the structure of epitaxial films has been an occasional topic of investigation in this project for the past four years. The initial results have been rather promising, particularly in the area of trying to induce high-surface-free-energy metals to wet the surface of low-surface-free-energy substrates. This is a generic problem in epitaxy since such free-energy differences are a common driving force behind unwanted effects such as agglomeration or interdiffusion. These effects often prevent the growth of atomically sharp interfaces (a common goal in epitaxy, as well as one of the most elementary examples of a structural arrangement of atoms over which we would like to gain control).

Figure 2 illustrates one aspect of how adsorbed gases provide a degree of control. A monolayer (ML) of Fe or Ni, deposited on clean Cu(100) at room temperature, tends to agglomerate; at higher temperatures interdiffussion occurs. However, if half a monolayer of oxygen is preadsorbed on the Cu(100), the Fe or Ni will wet the substrate in order to maximize the bonding between the transition metal and oxygen, as in Fig. 2b. Since Fig. 2b is the ground state of the system, annealing does not produce interdiffusion. The oxygen is thus acting as a surfactant to modify the balance of surface and interface free energies that control the epitaxial growth mode. In addition, we have found that adsorbed oxygen has a strong tendency to float out onto the surface of a subsequently deposited film without significantly affecting the epitaxial order. Similar adsorbate-induced wetting and adsorbate floating-out have been observed for a variety of other adsorbates and metal-metal systems; these effects should therefore be of general applicability in facilitating epitaxial growth.

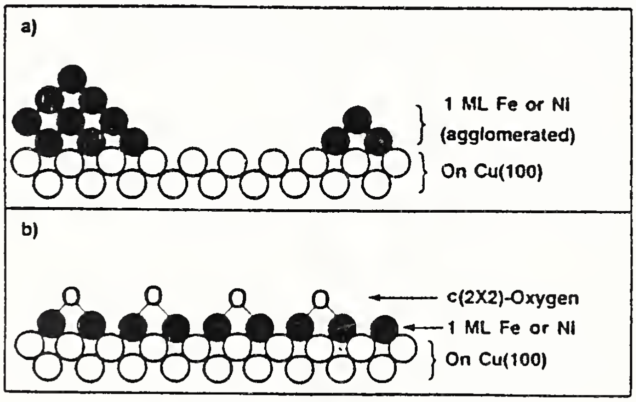

Fig. 2. An illustration of (a) the agglomeration that occurs when 1 ML of Fe or Ni is deposited on Cu(100) around room temperature and (b) how a pre-adsorbed oxygen layer induces the 1-ML Fe or Ni to lie flat to maximize its bonding with the oxygen.

Magnetic Properties of Atomically-Engineered Thin-Film Materials

The connection between the structure of epitaxial films and their magnetic properties is currently one of the most intensively investigated topics in the field of magnetism. The reason for this is that such films are expected to lead to new generations of commercial products such as computer discs for information storage and magnetoresistance detectors for disc reading heads. Since these are multi-billion dollar-a-year industries, a worldwide race is on to develop these products which are a key to supremacy in the next generation of information technology.

In attempts to synthesize novel thin-film materials, the critical ingredients for success are determinations of film structure, an understanding of the relationship between structure and properties, and the ability to control the structure during growth. These three topics are the focus of the present effort in magnetic thin films. In the past few years, major progress has been made in this project in developing XPS and AES forward scattering as a tool for structural determinations. More recently, this work has been combined with measurements of intensity oscillations for reflection high-energy electron diffraction (RHEED) to gain still deeper insights into epitaxial growth modes.

This combination of techniques has allowed improved growth and processing methods to be developed for optimizing the magnetic properties of epitaxial films. During this year, the properties of Fe-Cu sandwich structures produced by us using these methods have been investigated in collaboration with groups at Simon Fraser University in Canada and Cambridge University in England. It has been found that the magnetocrystalline anisotropy (a measure of sample quality and a technologically important parameter) is much greater when these sandwich structures are prepared by our methods rather than by the methods used by others in this field. We also have been able to achieve the theoretically predicted high-spin, or high-moment, state of fcc-Fe in these structures. This work thus represents a vindication of our approach of, first, developing methods for studying the structure, second, investigating the relationship between structure and properties, and finally, developing growth and processing techniques to allow us to gain control of the growth morphology to optimize the properties.

Our research plans for the future consist of extending these studies to other systems such as Co, Ni, Mn, and Cr films on substrates such as Ag, Au, and Pt. We hope to install an in situ magnetic probe such as the magneto-optical Kerr effect to get a more rapid turn-around in information on how processing affects magnetic properties. We also plan to use our existing base of expertise to move into the area of magnetoresistance effects in superlattice structures comprised of magnetic and non-magnetic metals. A giant magnetoresistance effect in such samples has been recently discovered and we are well positioned to make important contributions since there is expected to be a strong structure-properties relationship in these materials. We plan to grow epitaxial films of several metals on high-perfection silicon or germanium substrates; these films will be characterized by the x-ray standing wave technique (see below) and then used as substrates on which to grow superlattice structures.

B. Structural Analysis of Interfaces (T. Jach)

The objective of this project is to determine accurate positions and distributions of atoms, particularly at interfaces. This information and related data are used to analyze the energetics of solid surfaces in order to understand and predict epitaxy, reconstructions, and related interface phenomena. Emphasis is placed on the development of techniques that use x-ray diffraction and reflection at the interfaces, and which look at the de-excitation spectra of the atoms involved. The experiments require intense focussed or collimated x-ray beams available only at synchrotron light sources. A goal is to study and control interface formation to the point that it is predictable, with particular attention to semiconductor-metal interfaces.

Grazing Angle X-Ray Diffraction and Surface Roughness

In collaboration with Dr. D. Novotny of the NIST Semiconductor Electronics Division and Drs. M. B. Bedzyk and Q. Shen of the Cornell High Energy Synchrotron Source, grazing-angle diffraction has been used to study the surface roughness of germanium. A new phenomenon was directly observed--the superficial wave. This is a diffracted wave trapped at an interface where a change occurs in the dielectric susceptibility of the medium. The wave is scattered back out of the interface by roughness. It is potentially more sensitive to roughness than x-ray reflectivity measurements because the superficial wave is capable of propagating along the interface for millimeters. Roughness of samples on a scale of a few hundred angstroms was clearly evident, leading to the conclusion that roughness of a scale of ten angstroms or less should be detectable. A kinematical theory of rescattering was combined with the dynamical theory of diffraction to give qualitative understanding of the scattering process.

Back-Reflection X-Ray Standing Waves and Surface Relaxation

X-ray standing waves (XSW) originating from diffraction can be used to determine adsorbate position with respect to the bulk lattice, as long as the lattice is nearly perfect. When combined with nearest-neighbor distances obtained from measurements of the surface x-ray absorption fine structure, the relaxation of the surface atoms in the presence of the adsorbate is obtained. When the bulk crystal has a high density of defects, such as occurs in a metal, the lattice strain may be compensated by going to a Bragg angle of 90°, but an alternative requirement of high energy resolution (< 0.4 eV) is imposed. The focused NIST beamline X-24A at the Brookhaven National Synchrotron Light Source satisfies these requirements adequately to observe relaxation of the surface of copper in the presence of adsorbed sulfur and chlorine. In the case of chlorine, a relaxation of 0.07 Å was observed, the first such direct measurement. This work was performed in collaboration with Drs. J. R. Patel, D. W. Berreman, F. Sette, P. H. Citrin, and J. E. Rowe of AT&T Bell Laboratories, Dr. P. L. Cowan of the NIST Quantum Metrology Division, and Mr. B. Karlin of Brookhaven National Laboratory.

Reflection-Electron Microscopy Studies of Surface Diffusion in Thin Films

Reflection electron microscopy was used to study the development of columnar growth in metal films during deposition on amorphous substrates. Dimensions, orientation, and structure were obtained for crystallites that evolved on substrates held at various temperatures during gold vapor deposition. These data, when compared with theoretical calculations for surface free energy, diffusion, nucleation and growth, led to general predictions on the orientation and growth of fcc films, and a possible new mechanism for explaining whisker growth. This work was done in collaboration with Dr. G. Hembree of Arizona State University and Dr. L. B. Holdeman of COMSAT, Inc.

Future work in this project will concentrate on XSW measurements of atomic positions and point defects at interfaces when metal films are deposited on high-perfection semiconductor substrates. This work will contribute to the project on magnetic properties of superlattice structures described above.

C. Ballistic Transport Through Interfaces (M. D. Stiles)

Recent developments in growth capabilities of layered materials make possible the use of abrupt, coherent interfaces to make novel devices. To predict the behavior of such devices it is necessary to understand how electrons transmit from one material to another through these sharp interfaces. In collaboration with Dr. D. R. Hamann of AT&T Bell Laboratories, a method has been developed for calculating transmission probabilities for abrupt coherent interfaces between arbitrary materials. The method is based on first-principles electronic-structure calculations so that it is only necessary to know the geometry of the interface to predict the transmission probability.

This past year we completed the first calculation using this method for an interface of technical interest. Nickel disilicide is a metal that has a lattice constant very close to that of silicon so that even though the crystal structures are quite different they can be grown on top of each other with highly ideal interfaces. These ideal interfaces have led to a proposed metal-base transistor using nickel disilicide as the base between silicon. For the device to be useful it is necessary that the transmission probability for electrons scattering from the interfaces should be high. Using the method mentioned above we found that the transmission probability is too low for the proposed device to work as hoped. In addition we found that there is a large difference in the transmission probability for the two possible interfaces that will form depending on the growth kinetics. This prediction should make it possible to test the method we have developed.

We are currently working to extend the method so that it is capable of treating III-V compound semiconductors. The modifications are of a technical nature and not in the basic method itself. We will apply this method to proposed devices that rely on highly ideal interfaces between the different semiconductors, in particular those that make use of tunneling though narrow layers of these semiconductors. In addition we will apply this method to interfaces between III-V semiconductors and group III-transition metal bimetallic systems that are being studied for use in novel devices.

D. Micro-Structural and Micro-Compositional Characterization of Novel Materials (A. J. Melmed, P. P. Camus, and H. B. Elswijk*)

The techniques of field-ion microscopy (FIM) and atom-probe (AP) mass analysis can be applied to a wide range of novel materials to give real-space determinations of surface structure and qualitative bulk atomic structure, information that is complementry to results from other microscopies and diffraction techniques. The unique capability of specimen dissection by controlled field evaporation enables elemental composition determinations to be made with sub-nanometer spatial resolution. These techniques have been used for micro-structural and micro-compositional characterization of two types of novel materials, high-temperature superconductors and magnetic thin films.

High-T_c Superconductors (A. J. Melmed, P. P. Camus, and H. B. Elswijk*)

The superconducting critical temperature, T_c, is highly dependent upon the oxygen concentration in the 1-2-3 ceramic oxide materials. Because the most oxygenated material is not a stable compound, oxygen out-diffusion may occur, thereby modifying the electrical properties, especially in the near-surface region. This possibility has significant implications, especially for the interpretation of data obtained with surface-sensitive techniques. Therefore, the effect of vacuum exposure on the near-surface composition of ceramic superconductors was studied. Based upon the number of detected ions per surface layer, it was determined that the only type of atom probe capable of measuring statistically significant differences in the surface composition was a wide-angle atom probe with which circular regions of diameter typically 170 Å can be examined.

Atom-probe field-ion microscopy specimens were fabricated from Eu 1-2-3 superconducting material using the method of sharp shards. Initial surface composition measurements after imaging showed a non-stoichiometric, oxygen-depleted layer. A "deep-cleaning" procedure was then employed whereby field evaporation was used to remove approximately 5-10 nm of material. Subsequent composition analyses confirmed that this treatment was sufficient to remove the non-stoichiometric layer and to reveal a surface consisting of the expected 1-2-3-7 material. Various vacuum exposures at 85 K and room temperature were performed followed by composition analyses of the near-surface region.

For vacuum treatments of three hours at 85 K, no measurable change in the oxygen or metallic content was observed. For vacuum treatments of approximately 18 hours at room temperature, no change was measured in the metallic contents; however, a significant change was observed for the oxygen content. These results indicate that data obtained from freshly cleaved samples at or below 85 K by surface analysis techniques should be characteristic of material consisting of the expected composition, in contrast to samples exposed for longer periods of time at room temperature. Tℓ-based ceramic superconductors were also analyzed in an attempt to determine changes in the oxygen concentration in the near-surface region.

However, the material was found to be too inhomogeneous in composition for reliable measurements.

Investigations of the diffusivity of electrical-contact metals (Au, Ag, etc.) into ceramic superconductors are planned. It is hoped that the results will lead to a better understanding of the mechanical strength and interdiffusion properties of metal/superconductor contacts.

Magnetic Thin Films (P. P. Camus and A. J. Melmed)

Unique magnetic properties are obtained from composite thin films consisting of non-magnetic and magnetic components, Ag and Fe_3O_4 for instance. Mossbauer spectroscopy indicated that the magnetic contributions are a function of the Ag content, diffraction studies identified the phases as pure Ag and pure Fe_3O_4 particles, and transmission electron microscopy (TEM) determined the particle size to be in the range 3-30 nm (as a function of Ag content). But the chemical distributions of the elements have not been obtained. Therefore, a study was commenced whereby the field ion microscope was used to observe the microstructure and atom-probe microanalysis was used to measure the distribution and concentration of the elements.

The TEM studies indicated that conventional specimen preparation techniques produced artifacts; therefore, the method of sharp shards was used for specimen fabrication. The electrical conductivity of the thin films, which consist of a large volume fraction of Fe_3O_4, could be expected to be dominated by the (at best) semi-conducting properties of the Fe_3O_4. As FIM requires a finite conductivity at 85 K, a success at imaging the material was not guaranteed. However, it was found that field-ion images and AP analyses could be obtained. Brightly imaging regions in a dimly imaging matrix indicative of particles and dark regions indicative of voids were observed. AP analyses were more difficult than for metals or ceramic superconductors. The preliminary results indicate that the Ag is not homogeneously distributed, but there exist Ag-enriched and Ag-depleted regions, which is consistent with the previous studies.

The current plan is to extend the work by characterizing the composition of the brightly imaging regions and the matrix, and by quantifying the extent and amplitude of the Ag-enriched regions in a few of the available sample compositions. It is hoped that a better understanding of the effect of the Ag on the microstructure will be useful in optimizing the commercially important magnetic properties of these composite thin films. This work has been performed in collaboration with Dr. R. D. Shull of the NIST Metallurgy Division.

Simulation of Field-Ion Microscope Images for Icosahedral Materials (A. J. Melmed and H. B. Elswijk*)

A complete description of the atomic structure for the icosaehdral phase of Al-Mn has not yet been found and, in fact, there is still no general consensus on the most appropriate structural model to describe the phase. Accordingly, new models have been explored with regard to their agreement with the various experimental observations. The results of computer simulations, using the new structural models, with field ion microscopy observations have been compared.

The overall visual appearance of the experimental FIM images was best matched by a model having a large cubic unit cell (3.32 nm) containing a Mackay icosahedral motif. This interesting result clearly indicates that, for a unit cell which is large on the scale of the FIM specimen, the dominant symmetry features of the FIM image are due to the internal atomic motif (icosahedral) of the unit cell rather than to the crystal symmetry (cubic).

4. SURFACE SPECTROSCOPIES AND STANDARDS GROUP

Many different spectroscopies are used for the characterization of surfaces. Emphasis is placed here on the development of a conceptual understanding of important emerging spectroscopies and results, on the provision of needed information and data for widely used spectroscopies and related techniques, the development of new surface-characterization methods, the development of needed standard reference materials, and involvement with national and international standards committees concerned with surface analysis.

A. Theory of Dynamical Molecular Processes at Surfaces (J. W. Gadzuk and E. Blaisten-Barojas*)

This project is part of a continuing effort directed to understanding both the static and dynamic behavior of atoms, molecules, solids, surfaces, radiation and their mutual interactions. This understanding comes from consideration of the microscopic atomic-scale statistical properties of ensembles. Based upon our studies, phenomenological model theories and numerical simulations are constructed which relate to the chemical physics and statistical-mechanical behavior and to the intrinsic properties of relevant physico-chemical systems. In addition, a significant effort is invested in the study of the role of an actual measurement process in determining observed quantities in different surface spectroscopies. Ways in which measurement-process-specific quantities such as line shapes, satellite structures, etc. provide additional information on system dynamics are of considerable interest.

Resonance-Assisted Electron-Stimulated Desorption (J. W. Gadzuk)

Recent experiments have shown giant enhancements in the stimulated desorption of adsorbates from a surface under bombardment by electrons of a certain energy. These enhancements appear to be due to the electron being trapped in a temporary negative-ion shape resonance. In collaboration with Dr. C. W. Clark of the NIST Radiation Physics Division, a theory has been developed for the resonance enhancement in terms of time-dependent wavepacket propagation. This theory accounts for the large resonance-enhanced desorption yields observed for oxygen adsorbed on palladium surfaces.

Vibrational Relaxation of Molecules on Finite Metal Clusters (J. W. Gadzuk and E. Blaisten-Barojas*)

Picosecond pump-probe experiments are being carried out (see section 2.A) to determine the vibrational relaxation times associated with intramolecular vibrationally excited states of diatomic molecules adsorbed on metal surfaces. For experimental reasons, the initial measurements have been made with small metal clusters, thus opening up the possibility that finite quantum-size effects could influence the vibrational relaxation rate due to cluster electron-hole pairs and thus the measured absorption spectrum or lineshape. We have developed an exactly solvable theory for such relaxation and lineshapes in which the cluster electron-gas is treated within the random-phase approximation. The resulting absorption lineshapes are extremely cluster-size dependent when the cluster size increases from ~ 5 to >> 50 Å, as illustrated in Fig. 3. Due to quantum-size effects, the absorption spectrum is a series of sharp delta functions clothed in a Lorentzian-type envelope whose width is the inverse of the measured vibrational relaxation time. The spacing of the delta functions varies inversely with cluster size. In this way, such measurements may also be useful diagnostic probes of cluster properties.

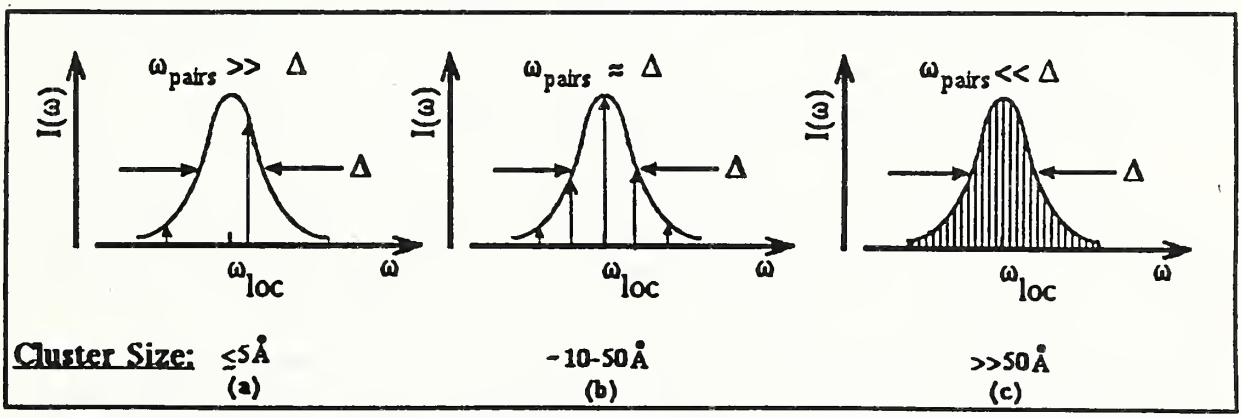

Fig. 3. Model absorption spectra for localized oscillator on metallic cluster of varying characteristic dimension and thus electron-hole pair excitation energy, as labelled.

Chaos and Fractals in Molecule-Surface Collisions (J. W. Gadzuk)

In collaboration with Dr. N. Sathyamurthy of the Indian Institute of Technology, numerical simulations of molecule-surface scattering events have shown two qualitatively different classes of behavior. One class exhibits simple and smooth scattering characteristics such as translational to internal-state energy redistribution while the other shows the formation of long-lived trapped-molecule-surface resonances. Under some circumstances, the energy redistribution patterns of these resonances displayed a self-similarity indicative of an inherent fractal structure within the dynamics. We have been the first to note and study such behavior, within the context of non-linear chaotic dynamics at surfaces. We have also succeeded in quantifying earlier apparent random results, thus opening the door to a new approach to analysis of numerical surface dynamics.

We plan to continue work in the area of surface reaction dynamics with near-term emphasis on the determination of self-consistent reaction trajectories, and the determination of energy-redistribution patterns amongst translational, vibrational, rotational, and electronic degrees of freedom of "reactant" molecules and electron and phonon modes of surfaces. Analyses are made for controllable dynamic and reactive conditions with synthesis of the various components of the elementary reaction theories into theories of experimentally realizable processes. Special emphasis will be placed on the phenomenon of dissociative surface processes and on the role of non-linear dynamics. In addition, analysis will be made, whenever possible, of novel experimental results. Current interest includes laser-assisted surface processes and state-to-state analysis, high-resolution surface vibrational spectroscopy, picosecond pump-probe studies of molecular vibrational relaxation times in the presence of small metal clusters showing quantum-size effects, and other experimental probes of non-adiabatic effects.

B. Ion-Surface Interactions (J. Fine, G. P. Chambers,* D. Marton,* M. H. Mintz* and M. H. Shapiro*)

Ion beams are used to bombard surfaces in order to measure surface composition (e.g., by secondary-ion mass spectrometry or ion-scattering spectroscopy) and to remove surface layers so that the composition of the exposed surface can be measured as a function of depth (i.e., a depth profile). Many physical phenomena occur during ion bombardment that are poorly understood, amongst them the nature of excitation events during the collision cascade, the energy states of ejected ions and neutrals, and ion-induced effects such as diffusion or segregation. Much of the available literature describes the ion-surface interactions in macroscopic terms such as the sputtering yield but these is a growing need for fundamental understanding at the microscopic level. In addition, there are needs for evaluated sputtering yield data, for standard reference materials to allow convenient determination of sputter-removal rates and other purposes, and for characterization of the changing topography of ion-bombarded surfaces.

Laser Spectroscopy of Sputtered Atoms and Ions (J. Fine and M. H. Mintz*)

In collaboration with Dr. J. D. Fassett of the NIST Inorganic Analytical Research Division, a series of experiments has been designed to determine the kinetic energy distributions of specific sputtered atoms and ions and their states of excitations. Resonance multiphoton laser-ionization schemes have been developed to detect sputtered atoms in specific excited states.

Measurements have been recently made of the kinetic energy (KE) distributions of collisionally ejected ions and neutrals from polycrystalline Mg by 3 keV argon ions. The measured Mg^+ KE distributions depend on extraction potential and indicate for our time-of-flight analyzer that the ion angular distributions are energy dependent. At higher energies (30-100 eV), the angular distributions are less cosine-like (more forward peaked) and more shifted to the specular direction. A one-color (285.2 nm), two-photon ionization scheme has been used to detect Mg^o. The Mg^o KE distributions show an enhanced number of high-energy neutrals for our 55° angle of incidence compared to what would be expected for a normal-incidence ion beam.

We are currently developing a laser ionization scheme to detect collisionally excited Mg^o in the 3s3p metastable state and to determine its KE distribution. Following that, we plan to investigate the KE distributions and state populations of sputtered Mg^+ by means of ultraviolet two-color resonance methods.

Detection of Atom Vaporization from Solid Surfaces by Laser Resonance Ionization (J. Fine and M. H. Mintz*)

Many surface growth mechanisms and the manner in which they evolve are often difficult to characterize. One possible way to monitor the coverage-dependent development of processes that affect surface-atom vaporization is to actually measure the change in the surface vapor pressure. We have used the single-atom detection capability of resonant multiphoton ionization techniques to observe directly the vaporization of Mg atoms from a partially oxidized polycrystalline Mg surface. By investigating the submonolayer oxidation regime, we have been able to show that two different chemisorption mechanisms can be experimentally distinguished: an initial random chemisorption stage followed by an island growth stage that dominates this process.

The possibility for the direct detection of changes in atom vaporization from surfaces that have low vapor pressures ($\sim 10^{-17}$ Torr) suggests that this type of measurement could have application to the study of a variety of surface processes involving both single and multiphase systems - many of which were previously not considered experimentally feasible. Examples of such process in addition to chemisorption include monolayer film growth modes, interdiffusion at sputter-profiled interfaces, and surface segregation.

Simulation of Ion-Surface Collisions (M. H. Shapiro* and J. Fine)

Multiple-interaction calculations have been performed to simulate ion-surface collisions occurring for typical sputtered conditions and to investigate the dynamical phenomena occurring in the resulting collision cascades. We have been particularly interested in investigating collisional-ion/surface-excitation processes which lead to the ejection of excited atoms from single-crystal solids. This past year we have completed an analysis of multiple-interaction calculations for 5 keV Ar^+ collisions with Aℓ. Collisional mechanisms, trajectories, and their dependence on atom geometry in the target have been explored. In contrast to most previous studies, we find that essentially all ejection of core-excited atoms results from asymmetric collisions (an incident ion colliding with a target atom). Analysis of the trajectories indicates that the excitation/ejection collision can be of two general types, depending on whether the incident ion is coming in along a low- or a high-index direction. We have just begun to make a computer movie of these trajectories and of the excitation/ejection encounters so that these results can be more effectively explained and understood. Our calculations also agree nicely with measurements of the azimuthal dependence of the bombarding ions on the Auger-electron de-excitation of atoms sputtered from Aℓ(100) performed recently in collaboration with scientists at the Centre d'Etudes Nucleaires, Saclay, France.

Sputtering-Induced Surface Microroughness (J. Fine and D. Marton*)

Changes in surface microtopography which often occur during ion bombardment can significantly affect the measured depth resolution of interfaces in sputter depth profiles. To better understand the importance of this roughening effect on interface analysis, we have developed a new type of microscope, the Scanning Scattering Microscope (SSM), for which a patent application is being filed.

The SSM makes use of a finely focused laser beam (632 nm) to scan the surface being examined. Almost all of the non-specularly reflected light is collected with a hemispherical mirror to give a roughness image of the surface as the laser beam is scanned. The light signal is determined by the local roughness of the surface, not by the shape or changes of height that other methods provide. We have evaluated the SSM by examining a number of test specimens: sputter-profiled thin-film interfaces, an integrated circuit linewidth test pattern, NIST SRM 475 optical microscopy standard, and a polished silicon surface. We find that the SSM can give a quantitative measurement of rms surface roughness (for roughness less than 100 nm) and a height sensitivity of about 1 nm. We also find that the surface roughness of ion-bombarded Ni/Cr and Ag/Ni thin-film systems correlate with depth-resolution (interface-width) measurements on the same specimens by Auger depth profiling.

Compilation of Ion Sputtering Yield Data (J. Fine and G. P. Chambers*)

We are preparing a compilation of evaluated sputtering-yield data for those parameters that will have specific use in surface analysis and depth profiling. Our compilation will be in tabular form for those ion species (Ne, Ar, Kr, Xe, O_2, N_2. Cs) and energies (0.5 to 20 keV) and angles of incidence used in surface characterization. The compilation will contain sputtering yields for elemental targets only.

Sputtering yield data have been evaluated using a method based on target surface reactivity, surface oxide formation, and sputter removal rates. Limits were established for determining which data were more consistent than others. Based on the setting of such limits and on the total ion dose used to obtain the measurement, we have been able to show that subsets of the yield data exist which are quite reasonable in the scatter of the data and which have the expected dependence on ion energy. We have also found the preferred yield data could be fitted to curves generated from the Sigmund sputtering theory and Ziegler-Biersack-Lindhard nuclear stopping cross sections. These fitted curves will be used to generate recommended values of sputtering yields for ion energies from 0.5 to 20 keV. We anticipate that our evaluated yield data (recommended values) will be much more useful and reliable than the unevaluated data compilations that are now available. This work is supported by the NIST Office of Standard Reference Data.

Development and Production of Standard Reference Materials for Sputter-Depth Profiling (J. Fine and D. Marton*)

Standard reference materials (SRMs) are needed for the convenient determination of ion-beam sputter-removal rates, for optimization of ion-sputtering conditions to achieve high depth resolution, for calibration of surface analysis instrumentation, and related functions. Our development of SRMs has been supported by the NIST Office of Standard Reference Materials.

(i) NIST SRM 2135

We have previously developed, fabricated, and certified SRM 2135, a multilayered Ni/Cr thin-film structure for calibrating sputter depths and erosion rates, for monitoring ion beam stability, and for optimizing sputtering conditions. The total sales of SRM 2135 is now more than 160 but the stock has been depleted. Work is now in progress on the fabrication of a large additional stock (600-900 pieces) of SRM 2135. Because the fabrication facility used previously is no longer available, we are developing new fabrication techniques at the Comsat Laboratories in Germantown, MD. Using rf planar-magnetron sputter-deposition techniques, prototype materials have been developed with properties similar to those of the previous SRM 2135. These properties include sharpness of interfaces, film-thickness uniformity from sample-to-sample, and layer-thickness uniformity from layer to layer. We believe that the uncertainty in all layer thicknesses can be kept to ± 2%. Production of stock is now proceeding.

(ii) NIST SRM 2136

A new "marker-type" SRM has been under development along with improved Auger profiling techniques necessary for its characterization. This Cr/Cr_2O_3 multilayered thin-film structure consists of 7 well-defined, thin oxide-marker layers (about 3 monolayers thick) separated by Cr films which are about 30 nm thick. The uniformity of the marker layer spacing is about 3% (one standard deviation); it should be useful both as a depth profile standard for secondary-ion mass spectrometry analysis as well as a sensitivity standard for Auger analysis. The new SRM has been certified for total Cr thickness by differential pulse polarography and inductively coupled plasma spectroscopy. This total Cr thickness is 175.3 ± 6.4 $\mu g/cm^2$ where the uncertainty corresponds to two standard deviations. The individual Cr layer thicknesses have been certified from the total Cr thickness and from Auger sputter-depth-profile measurements.

(iii) New SRM for the Calibration of Energy Scales of Auger-Electron and X-Ray Photoelectron Spectrometers

We are developing a new SRM consisting of Cu, Ag, Au, and Si for the convenient calibration of the energy scales of Auger-electron and x-ray photoelectron spectrometers. Prototype single-element specimens have been fabricated by rf planar-magnetron sputter deposition; work is proceeding on their evaluation for diffraction effects.

C. Electron Spectroscopy of Surfaces (C. J. Powell, N. E. Erickson, and S. M. Thurgate*)

Electron-spectroscopic techniques are extensively used for different types of surface characterization, particularly to attain surface sensitivity. Two techniques, Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS), are in widespread use for measurements of surface composition. The objective of this project is to provide needed reference data to enhance the utility of the techniques in common use.

Inelastic Mean Free Paths of Low-Energy Electrons in Solids (C. J. Powell)

Values of inelastic mean free paths (IMFPs) of low-energy (≈ 50-2000 eV) electrons are needed for quantitative surface analyses by AES and XPS. Information is particularly desired on the dependences of the IMFP on material and electron energy.

In a collaboration with Drs. D. R. Penn of the NIST Electron Physics Group and S. Tanuma of the Nippon Mining Company, calculations have been made of IMFPs for 200-2000 eV electrons in 27 elemental solids and 4 compounds. From these IMFP values, we developed a general formula to predict IMFPs for other materials in terms of several material parameters. We have now extended the calculations to lower energies by avoiding an approximation in the algorithm used previously. Substantial differences are found in the shapes of the IMFP versus energy curves in the 10-200 eV range for different materials. Figure 4 shows examples of these curves for aluminum and gold which are illustrative of the data for free-electron-like and non-free-electron-like materials, respectively. The minimum IMFP value is found about 40 eV for Al while that for Au occurs at 120 eV. These differences can be understood in terms of the different inelastic scattering mechanisms in the two metals. The differences in the shapes of the IMFP-energy curves at low energies also indicate a serious limitation in the widely used formula of Seah and Dench for a related quantity, the electron attenuation length. We have found that our IMFP results could be adequately represented by a modified form of the Bethe equation over the 50-2000 eV range; this new formula should be a useful means of predicting the IMFP dependences on material and energy. We are currently extending the IMFP calculations to other materials for which optical constants (needed typically over a range of about 1-1000 eV) are available.

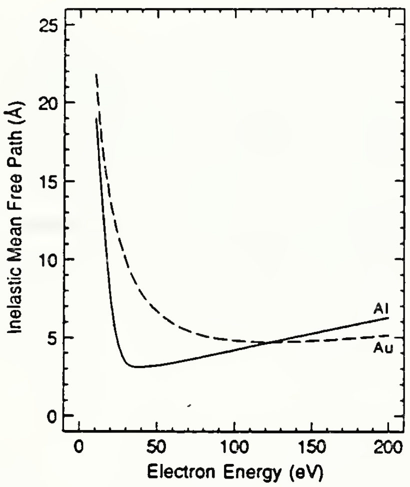

Fig. 4. Plots of the calculated inelastic mean free paths for aluminum (solid line) and gold (dashed line) as a function of electron energy.

Uncertainties in Quantitative Surface Analyses by AES and XPS (C. J. Powell)

In a collaboration with Dr. M. P. Seah of the UK National Physical Laboratory, an extensive review has been made of the individual steps in AES and XPS analyses and of the varius sources of uncertainty for each step. Quantitative analyses are difficult to perform on account of the many options available and the morphological complexity of many specimens, lack of adequate knowledge of instrumental performance, and to limitations of current methodology and data. While there are many pitfalls, there has been substantial progress in recent years in recognizing the more serious problems and in providing solutions, procedure, and data. It is believed that the review will be a useful source of guidance for the many users of AES and XPS instruments.

Characterization of Oxide Layers on InP (N. E. Erickson and S. M. Thurgate*)

Indium phosphide is an important compound semiconductor yet little is known of its surface composition after different preparation procedures. One of the difficulties in the use of a technique such as XPS coupled with argon-ion bombardement to get composition information as a function of depth is that the ion bombardment can modify the chemical compounds present.

We have measured XPS data for InP samples prepared in different ways as a function of ion bombardment time. From an analysis of the "chemical" shifts of the core-electron lines and of changes of lineshapes, we have been able to deduce the nature of the initial oxide surface and the changes in composition with depth for the different samples.

D. Surface-Analysis Standards Committees (C. J. Powell and J. Fine)

The Division is active in ASTM Committee E-42 on Surface Analysis and with two international groups, the Surface Chemical Analysis Technical Working Party of the Versailles Project on Advanced Materials and Standards (VAMAS) and the Subcommittee on Surface Analysis of the International Union of Pure and Applied Chemistry (IUPAC). These groups provide reference procedures, needed reference data, and characterization of reference materials for the techniques of surface analysis in common use. The groups also sponsor symposia and workshops and conduct laboratory intercomparisons of particular types of measurements.

5. PUBLICATIONS

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(b) Publications in Progress

Balasubramanian, V., Sathyamurthy, N., and Gadzuk, J. W., "Fractals in Molecule-Surface Collisions, Surface Sci. Lett. (in press).

Buntin, S. A., Richter, L. J., King, D. S., Cavanagh, R. R., "State-Resolved Evidence for Hot Carrier Driven Surface Reactions: Laser-Induced Desorption of NO from Pt(111)," J. Chem. Phys. (in press).

Camus, P. P., "Atom Probe Field-Ion Microscopy Applications," High Temperature Science (in press).

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Demmin, R. A., Kurtz, R. L., Stockbauer, R., Madey, T. E., Mueller, D. R., and Shih, A., "Photoemission Studies of Pt Overlayers on W(110)," J. Chem. Phys. (submitted).

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Kurtz, R. L., Stockbauer, R. L., Madey, T. E., Roman, E., de Segovia, J. L., and Chen, H. H., "H_2O Chemisorption on TiO_2 Surfaces: The Role of Defects," Proceedings of the Symposium on Chemically Modified Oxide Surfaces (in press).

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Marton, D. and Fine, J., "Ion Bombardment Induced Diffusion: A Case Study on a Sputtered Ag/Ni Layered System," Periodica Polytechnicia Chemical Engineering (in press).

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Nenadović, T., Popović, N., and Fine, J., "Mechanical Sputtering of Structural Stainless Steels," J. Mat. Sci. (in press).

Perera, R. C. C., Cowan, P. L. Lindle, D. W., LaVilla, R. E., Jach, T., and Deslattes, R. D., "Molecular-Orbital Studies via Satellite-Free X-Ray Fluorescence: Cℓ K-Absorption and K-V Emission Spectra of Chlorofluoromethanes," Phys. Rev. A. (submitted).

Powell, C. J., "The Surface Sensitivity of Electron Spectroscopies," Current Contents, Physical, Chemical, and Earth Sciences (submitted).

Powell, C. J., "Progress and Pitfalls in Quantitative Surface Analysis by Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy," in New Developments and Trends in Surface Science (submitted).

Powell, C. J. and Seah, M. P., "Precision, Accuracy, and Uncertainty in Quantitative Surface Analyses by Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy," J. Vac. Sci. Tech. A (submitted).

Schwarzacher, W., Allison, W., Willis, R. F., Penfold, J., Ward, R. C., and Egelhoff, Jr., W. F., "Variation in Magnetic Properties of Cu/fcc Fe/Cu(001) Sandwich Structures," Solid State Commun. (in press).

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Tanuma, S., Powell, C. J., and Penn, D. R., "Material Dependence of Electron Inelastic Mean Free Paths at Low Energies," J. Vac. Sci. Tech. A (submitted).

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Thurgate, S. M. and Erickson, N. E., "XPS/Ar^+ Ion Profile Study of Thin Oxide Layers on InP," J. Vac. Sci. Tech. A (submitted).

Whitman, L. J., Joyce, S. A., Yarmoff, J. A., McFeely, F. R., and Terminello, L. J., "Summary Abstract: The Chemisorption of $SiCl_4$, Si_2Cl_6, and Chlorine on Si(111) 7x7," Vacuum (submitted).

(c) Recent Publications of New Staff Members Resulting From Previous Positions
(Beckerele and Whitman)

Beckerle, J. D., Johnson, A. D., and Ceyer, S. T., "Collision Induced Dissociation and Desorption: CH_4 on Ni(111)," Springer Series in Surface Sciences Vol. 14, Solvay Conference on Surface Science, F. W. de Wette, ed., (Springer-Verlag, Berlin, 1988), p. 109.

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Beckerle, J. D., Yang, Q. Y., Johnson, A. D., and Ceyer, S. T., "Adsorption of CO and O_2 on Ni(111) at 8K," Surface Sci. 195, 77 (1988).

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Mieher, W. D., Whitman, L. J., and Ho, W., "A Time Resolved Electron Energy Loss Spectroscopy Study of CO on Pt(111): Adsorption Site Occupations Versus Coverage and Temperature," J. Chem. Phys. 91, 3228 (1989).

Richter, L. J., Mieher, W. D., Whitman, L. J., Noonan, W. A., and Ho, W., "Improved Multidetector for Time-Resolved Electron Energy Loss Spectroscopy,." Rev. Sci. Instrum. 60, 12 (1989).

Whitman, L. J. and Ho, W., "Dissociation Kinetics on an Alkali Metal-Promoted Surface: NO and K on Rh(100)," Surface Sci. 204, L725 (1988).

Whitman, L. J. and Ho, W., "The Kinetics and Mechanisms of Alkali Metal-Promoted Dissociation: Adsorption and Reaction of NO on Potassium-Precovered Rh(100)," J. Chem. Phys. 89, 7621 (1988).

Whitman, L. J. and Ho, W., "Desorption Kinetics on an Alkali Metal-Precovered Surface: CO and K on Pt(111)," J. Chem. Phys. 90, 6018 (1989).

Whitman, L. J., Richter, L. J., Gurney, B. A., Villarrubia, J. S., and Ho, W., "CO Adsorption Site Occupations on Fe(111) vs. Coverage and Temperature: The Kinetics of Adsorption and Reaction," J. Chem. Phys. 90, 2050 (1989).

6. PATENT ACTIONS

Patent Application: "Diffraction Device Which Detects the Bragg Condition," T. Jach and J. C. Geist, G. P. Carver, and D. B. Novotny of the NIST Semiconductor Electronics Division, U.S. Ser. No. 17/232.243.

Patent Disclosure: "Amorphous Silicon X-Ray Normalizing Detector," T. Jach and J. C. Geist of the NIST Semiconductor Electronics Division.

Patent Disclosure: "Scanning Scattering Microscope," J. Fine and D. Marton.

7. INVITED TALKS

Buntin, S., "Photogenerated 'Hot' Electron Induced Desorption of NO from Pt(111)," Chemistry Department, Argonne National Laboratory, Argonne, IL, January 23, 1989.

Buntin, S., "Photogenerated 'Hot' Electron Induced Desorption of NO from Pt(111)," Department of Chemical Physics Seminar, Aerodyne Corporation, Department of Chemical Physics, Billrica, MA, March 23, 1989.

Buntin, S., "Dynamics in Laser-Induced Desorption of NO from Pt(111)," Chemical Phyics Group, Los Alamos National Laboratory, Los Alamos, NM, May 8, 1989.

Buntin, S., "Dynamics in Laser-Induced Desorption of NO from Pt(111)," New Mexico Chapter of the American Vacuum Society, Albuquerque, NM, May 11, 1989.

Buntin, S., "Quantum-State-Specific Dynamics in the Laser-Induced Desorption of NO from Pt(111)," 1989 Conference on the Dynamics of Molecular Collisions, Asilomar Conference Center, Asilomar, CA, July 20, 1989.

Camus, P., "Ultra-High Spatial Resolution Composition Analysis - Application of Atom Probe Field Ion Microscopy to Alloy Clustering and Segregation," Sixth International Conference on High Temperatures, National Institute of Standards and Technology, Gaithersburg, MD, April 3, 1989.

Cavanagh, R. R., "Laser Probes of Surface Dynamics: Distinguishing Photochemistry From Thermal Chemistry," Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, October 27, 1988.

Cavanagh, R. R., "Time Resolved Measurements of Vibrational Relaxation at Surfaces: Phonons vs. Electron-Hole Pairs," Department of Chemistry, University of Illinois, Chicago, IL, November 3, 1988.

Cavanagh, R. R., "Laser Probes of Surface Dynamics: Distinguishing Photochemistry From Thermal Chemistry," Department of Chemistry, Northwestern University, Chicago, IL, November 4, 1988.

Cavanagh, R. R., "Laser-Induced Desorption: State-Resolved Evidence for Optically Driven Surface Reactions," Molecular & Surface Dynamics Seminar, University of Pennsylvania, Philadelphia, PA, March 31, 1989.

Cavanagh, R. R., "Laser Induced Desorption of NO from Pt(111): The Role of Hot Carriers," Surface Physics Group, AT&T Bell Laboratories, Murray Hill, NJ, May 5, 1989.

Cavanagh, R. R., "Laser Probes of Transient Excited States at Surfaces," Gordon Research Conference, Andover, NH, August 9, 1989.

Cavanagh, R. R., "Laser Induced Desorption of NO from Pt(111): Evidence for Hot Carrier Driven Reactions," American Chemical Society Meeting, Miami, FL, September 14, 1989.

Egelhoff, Jr., W. F., "XPS and Auger Forward Scattering: A Structural Tool for Studying Ultrathin Films, Epitaxial Growth, Surface Segregation, and Interdiffusion," Materials Science and Technology Division, Naval Research Laboratories, Washington, D.C., May 10, 1989.

Egelhoff, Jr., W. F., "XPS Forward Scattering Studies of Epitaxial Films," Surface Canada Conference, Vancouver, B.C., Canada, May 31, 1989.

Egelhoff, Jr., W. F., "XPS Forward Scattering Studies of Epitaxial Growth Modes of Magnetic Thin Films," Office of Naval Research Workshop on Monolayer Magnetism, Berkeley Springs, WV, August 16, 1989.

Fine, J., "Interface Modification During Sputter Depth Profile Analysis," American Vacuum Society National Symposium, Atlanta, GA, October 4, 1988.

Fine, J., "Nanometer Depth Analysis of Sputter Profiled Interfaces," Eleventh International Vacuum Congress and Seventh International Conference on Solid Surfaces," Cologne, W. Germany, September 29, 1989.

Gadzuk, J. W., "Semiclassical Dynamics of Molecules at Electronically Excited Surfaces," Solid State Physics Colloquium, Cornell University, Ithaca, NY, November 8, 1988.

Gadzuk, J. W., "Real-Time Dynamics of Molecular Processes at Surfaces by Femtosecond Excitation," NIST Staff Research Seminar, National Institute of Standards and Technology, Gaithersburg, MD, February 17, 1989.

Gadzuk, J. W., "Real-Time Dynamics of Molecular Processes at Surfaces by Femtosecond Excitation," Workshop on Dynamics of Surface Reactions, Copenhagen, Denmark, May 9, 1989.

Gadzuk, J. W., "Vibrational Relaxation in Molecules Adsorbed on Metal Clusters," Surface Science Center Colloquium, University of Liverpool, Liverpool, England, May 15, 1989.

Gadzuk, J. W., "Aspects of Surface Physics Theories," Washington Academy of Science Awards Banquet, Washington, DC, May 18, 1989.

Gadzuk, J. W., "Electron Scattering Off Molecules Adsorbed on Surfaces," Aspects of Electron-Molecule Scattering and Photoionization Conference, Yale University, New Haven, CT, July 23, 1989.

Gadzuk, J. W., "Pumping and Probing: Dynamics and Spectroscopy in the Time Domain," Fourth Annual Joint Workshop on Interface Phenomena, Campobello Island, ME, August 17, 1989.

Gadzuk, J. W., Chaos in Surface Dynamics," International Summer Institute in Surface Science, University of Wisconsin-Milwaukee, Milwaukee, WI, August 24, 1989.

Gadzuk, J. W., "Excitement in Electron Scattering from Adsorbed Molecules," NIST Neutron Physics Seminar, September 28, 1989.

Jach, T., "X-ray Standing Waves, Grazing Angles, and Atomic Positions," Department of Physics, Purdue University, Lafayette, IN, November 3, 1988.

Jach, T., "X-ray Standing Waves, Grazing Angles, and Atomic Positions," Department of Physics and Chemistry, Indiana University, Bloomington, IN, November 4, 1988.

Jach, T., "The Berry Phase," Laser Physics Group, National Institute of Standards and Technology, Gaithersburg, MD, January 11, 1989.

Jach, T., "X-ray Diffraction, Glancing Angles, and Atomic Positions," Physics Deparment Colloquium, University of Virginia, Charlottesville, VA, February 17, 1989.

Jach, T., "X-ray Diffraction, Standing Waves, and Atomic Positions," Department of Physics, University of Dortmund, Dortmund, W. Germany, September 13, 1989.

Jach, T., "X-ray Diffraction, Standing Waves, and Atomic Positions," Hamburg Synchrotron Radiation Laboratory, Hamburg, W. Germany, September 15, 1989.

Jach, T., "Determining Atomic Positions by X-ray Standing Waves in New Geometries," Risø National Laboratory, Roskilde, Denmark, September 18, 1989.

Jach, T., "X-ray Standing Waves in New Geometries to Measure Atomic Positions," Department of Physics, Chalmers University, Göteborg, Sweden, September 20, 1989.

Joyce, S. A., "Determination of the Geometric and Electronic Structure of Adsorbates Using Stimulated Desorption Techniques," Chemistry and Physics Laboratory, Aerospace Corporation, Los Angeles, CA, April 12, 1989.

Joyce, S. A., "Determination of Adsorbate Structures Using Stimulated Desorption Techniques," Surface Science Department, Sandia National Laboratories, Albuquerque, NM, April 27, 1989.

Joyce, S. A., "Determination of Adsorbate Structures Using Stimulated Desorption Techniques," Surface Science Division, Hoechst-Celanese, Inc., Summit, NJ, May 23, 1989.

Joyce, S. A., "Determination of Adsorbate Structures Using Stimulated Desorption Techniques," Argonne National Laboratories, Argonne, IL, June 1, 1989.

Kurtz, R. L., "Water Adsorption on TiO_2 Surfaces," Chemically Modified Oxide Surfaces Symposium, Midland, MI, May 29, 1989.

Melmed, A. J., "FIM of High-T_c Materials," American Vacuum Society National Symposium, Atlanta, GA, October 3, 1988.

Melmed, A. J., "Field Ion Microscopy of High Transition Temperature Superconductors," Naval Surface Weapons Laboratory, Silver Spring, MD, November 16, 1988.

Melmed, A. J., "Oxygen Concentration in the Near-Surface Region of $EuBa_2Cu_3O_{7-x}$ in Vacuum," Fifth NIST Superconductivity Information Exchange Meeting, Boulder, CO, September 20, 1989.

Powell, C. J., "Electron Inelastic Mean Free Paths and Attenuation Lengths for Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy," 5th International Conference on Quantitative Surface Analysis, London, UK, November 17, 1988.

Powell, C. J., "International Efforts to Develop Reference Procedures, Reference Data, and Reference Materials for Surface Chemical Analysis," Pittsburgh Conference, Atlanta, GA, March 8, 1989.

Powell, C. J., "Electron Inelastic Mean Free Paths and Attenuation Lengths for Quantitative Surface Analyses by AES and XPS," University of Kaiserslautern, Kaiserslautern, W. Germany, May 19, 1989.

Powell, C. J., "Reference Materials for the Quantification of Surface Analyses," European Central Bureau of Nuclear Measurements, Geel, Belgium, May 25, 1989.

Powell, C. J., "Standard Reference Materials for Surface Analysis," Workshop on Standard Reference Data and Reference Materials for Surface Analysis, Cleveland, OH, May 30, 1989.

Powell, C. J., "Progress and Pitfalls in Quantitative Surface Analysis by AES and XPS," Eleventh Symposium on Applied Surface Analysis, Cleveland, OH, June 2, 1989.

Richter, L. J., "Quantum-State Specific Studies of the Dynamics of Excitation and Desorption of NO from Pt(111)," Laboratory of Surface Modification Interface Dynamics Group, Rutgers University, Piscataway, NJ, February 9, 1989.

Richter, L. J., "Quantum-State Specific Studies of the Dynamics of Excitation and Desorption from Surfaces," Department of Physics, Brown University, Providence, RI, February 22, 1989.

Robey, S. W, "Synchrotron Radiation Studies of High Temperature Superconductors," Fifth NIST Superconductivity Information Exchange Meeting, Boulder, CO, September 20, 1989.

Stiles, M. D., "Theory of Electrical Transmission Through Epitaxial Interfaces," American Physical Society Meeting, St. Louis, MO, March 20, 1989.

Stiles, M. D., "Electron Transmission Through Interfaces," IBM Research Center, Yorktown Heights, NY, April 15, 1989.

Stiles, M. D., "Distored-Wave-Born-Approximation Calculations of Inelastic Scattering," Workshop on Dynamics of Surface Reactions, Copenhagen, Denmark, May 9, 1989.

Stiles, M. D., "Electron Transmission Through Interfaces," University of Virginia, Department of Physics, Charlottesville, VA, September 21, 1989.

Stockbauer, R. L., "Studies of Electronic Interactions and Material Degradation of High Temperature Superconductors," Workshop on the Materials Science of High T_c Superconductors: Magnetic Interactions, National Institute of Standards and Technology, Gaithersburg, MD, October 20, 1988.

Stockbauer, R. L., "Photoemission Studies of Tℓ based High T_c Superconductors," Fourth NIST Superconductivity Information Exchange Meeting, National Institute of Standards and Technology, Gaithersburg, MD, December 13, 1988.

Yarmoff, J. A., "Synchrotron Radiation Studies of the Silicon-Fluorine Interaction," IBM Almaden Research Center, Almaden, CA, October 24, 1988.

Yarmoff, J. A., "Synchrotron Radiation Studies of the Silicon-Fluorine Interaction," Advanced Light Source Department, Lawrence Berkeley Laboratory, Berkeley, CA, October 25, 1988.

Yarmoff, J. A., "Synchrotron Radiation Studies of the Silicon-Fluorine Interaction," Department of Physics, University of California, Riverside, CA, October 27, 1988.

Yarmoff, J. A., "Synchrotron Radiation Studies of Silicon-Fluorine Interactions," Physical Chemistry Research Department, AT&T Bell Laboratories, Murray Hill, NJ, April 5, 1989.

Yarmoff, J. A., "Studies of Semiconductor Surfaces," University of California, Riverside, CA, June 14, 1989.

8. SURFACE SCIENCE DIVISION SEMINARS AND INTERFACE SCIENCE SEMINARS

Alkemade, P. F. A., "Production of Auger Electrons by Ions under Channeling and Random Conditions," Interface Science Western, Department of Physics, The University of Western Ontario, London, Ontario, Canada, January, 9, 1989.

Batson, P. E., "Spatially Resolved Electron Energy Loss Spectroscopy: Bonding and Electronic Structure from Sub-Nanometer Sized Areas," IBM Thomas J. Watson Research Center, Yorktown Heights, NY, Interface Science Seminar Series, April 7, 1989.

Bedzyk, M., "Long-Period X-ray Standing Waves," Cornell High Energy Synchrotron Source, Cornell University, Ithaca, NY, Interface Science Seminar Series, February 1, 1989.

Brillson, L. J., "New Techniques for Characterizing and Controlling Metal-Semiconductor Interfaces," Xerox Webster Research Center, Webster, NY, Interface Science Seminar Series, June 14, 1989.

Bristowe, P. D., "Diffraction from Grain Boundaries in Gold: Recent Observations and Computer Simulations," Massachusetts Institute of Technology, Cambridge, MA, Interface Science Seminar Series, November 16, 1988.

Cheng, Y.-T., "Fractal Geometric and Thermodynamic Aspects of Ion-Solid Interactions," Physical Chemistry Department, General Motors Research Laboratories, Warren, MI, Interface Science Seminar Series, March 17, 1989.

Dieleman, J., "Low Energy Ion and Laser Assisted Surface Reactions," Philips Research Laboratories, Eindhoven, The Netherlands, December 5, 1988.

Fontaine, A., "Time Resolved X-ray Absorption Spectroscopy: Applications to High T_c Superconductivity and Phase Transitions at High Pressure," LURE, Orsay, France, December 6, 1988.

Fuggle, J. C., "Atomic Effects and Strong Magnetic Dichroism in X-ray Absorption of Solids and Surfaces," Laboratorium voor Fysische Chemie, Katholieke Universiteit, Nijmegen, Nederland, April 10, 1989.

Gray, H. F., "Vacuum Microelectronics: Field Emission Based," Naval Research Laboratory, Washington, DC, March 29, 1989.

Gumhalter, G., Institute of Physics of the University of Zagreb, Zagreb, Yugoslavia, "Dynamic Electronic Structure of Chemisorbed CO: $2\pi^*$ Resonance Features," June 27, 1989.

Gutowski, V., "Physico-Chemical Criteria for Maximum Adhesion," CSIRO, Australia, Interface Science Seminar Series, October 7, 1988.

Harris, J., "Sticking in the Quantum Regime: H_2 on Cu(110)," Institut fur Festkorperforschung, KFA, Julich, W. Germany, October 17, 1988.

Holloway, S., "Dynamics of Gas-Surface Scattering: Quantum vs. Semi-classical vs. Classical: When and How?," Liverpool University, Surface Science Research Center, Liverpool, UK, March 7, 1989.

Ishida, H., "Quantitative Surface FT-IR Spectroscopy," Case Western Reserve University, Cleveland, OH, Interface Science Seminar Series, March 1, 1989.

Jones, R. O., "Density Functional Calculations with Simulated Annealing - The Answer to Problems in Condensed Matter and Molecular Physics?," Institut fur Festkorperforschung, der KFA, Jülich, West Germany, April 3, 1989.

Kaiser, W. J., "Ballistic-Electron-Emission Microscopy Investigation of Semiconductor Interfaces," California Institute of Technology, Pasadena, CA, Interface Science Seminar Series, May 25, 1989.

Kruse, N., "Kinetics of Surface Reactions on the Atomic Scale," Technical Hochshule, Zurich, Switzerland, October 11, 1988.

Lince, J., "Reactivity, Modification, and Electronic Structure of MoS_2(0001) Surfaces," Aerospace Corporation, El Segundo, CA, August 4, 1989.

Mancini, D., "X-Ray Lithography and Chemistry of Diazonapthoquinone-novolak Resist," University of Wisconsin-Madison, Madison, WI, March 17, 1989.

Osgood, R. M., "Photon Processing of Materials: Techniques and Basic Surface Physics," Columbia University, New York, NY, Interface Science Seminar Series, January 18, 1989.

Polak, M., "Segregation to Different Surfaces in Polycrystalline Ni-9%Al Solid Solution," Department of Materials Engineering, Ben Gurion Univesity of the Negev, Negev, Israel, August 2, 1989.

Reutt-Robey, J. E., "Microscopic CO Diffusion on a Pt(111) Surface by Time Resolved Surface Infrared Spectroscopy," Department of Chemistry, University of Maryland, College Park, MD, January 11, 1989.

Sathyamurthy, N., "Time-Dependent Quantum Mechanical Approach to Reactive Scattering," Indian Institute of Technology, Kanpur, India, October 12, 1988.

Schwarzacher, W., "Spin Polarized Neutron Reflection Measurements on Epitaxial fcc Fe/Cu(100) Sandwich Structures," Cambridge University, Cavendish Laboratories, Cambridge, England, March 16, 1989.

Semancik, S., "The Chemical and Electronic Character of Sensing Interfaces," NIST Chemical Process Metrology Division, Interface Science Seminar Series, June 8, 1989.

Vernon, M., "Molecular Beam Studies of Organometallic Photodissociation Dynamics," Columbia University, New York, NY, October 19, 1988.

Vvedensky, D. D., "Computer Stimulations of RHEED Oscillations and the Epitaxial Growth of Semiconductors," Imperial College, London, England, November 28, 1988.

Weaver, J. H., "Surfaces and Interfaces of High T_c Superconductors," Department of Chemical Engineering and Material Sciences, University of Minnesota, Minneapolis, MN, Interface Science Series, February 16, 1989.

White, R. C., "Electronic Structure and Disordered Systems - What Photoemission Can Tell Us About Metal - Polymer Interfaces," Department of Electrical Engineering and Microelectronics Sciences Laboratories, Columbia University, New York, NY, September 1, 1989.

Zare, R. N., "The H + D_2 Reaction," Stanford University, Chemistry Department, Stanford, CA, November 30, 1988.

9. CONFERENCES ORGANIZED

Applied Surface Science Sessions of the 11th International Vacuum Congress/7th International Conference on Solid Surfaces, Cologne, Federal Republic of Germany, September 25-29, 1989 (sponsored and organized by the International Union for Vacuum Science, Technique and Applications and the German Vacuum Society).

Third Topical Conference on Quantitative Surface Analysis, Salem, Massachusetts, October 20-21, 1989 (cosponsored by the Applied Surface Science Division of the American Vacuum Society, the New England Combined Chapter of the American Vacuum Society, Committee E-42 on Surface Analysis of the American Society for Testing and Materials (ASTM), and the Surface Chemical Analysis Technical Working Party of the Versailles Project on Advanced Materials and Standards (VAMAS).

10. TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Cavanagh, R. R.

Treasurer, General Committee of the Physical Electronics Conference

Local Co-Chairman, Physical Electronics Conference, Gaithersburg, MD, June, 1990

National Measurement Laboratory Representative, NIST-NRC Postdoctoral Committee

Member, Organizing Committee, 6th International Conference on Vibrations at Surfaces, Shelter Island, NY, September, 1990

Member, Executive Committee, Surface Science Division, American Vacuum Society

Member, Surface Science Division Program Committee, American Vacuum Society National Symposium, Boston, MA, October, 1989

Division Laser Safety Officer

Member, NIST Research Advisory Committee

Fine, J.

Chairman, Subcommittee E-42.09 on Standard Reference Maerials of ASTM Committee E-42 on Surface Analysis

Gadzuk, J. W.

Member, Editorial Advisory Board, "Progress in Surface Science"

Member, International Advisory Committee, 6th International Conference on Vibrations at Surfaces, Shelter Island, NY, September, 1990

Board Member, Greater Washington Solid State Physics Colloquium

Jach, J.

Division Safety Officer (from 5/89)

Powell, C. J.

Member, Executive Committee, and International Liaison, ASTM Committee E-42 on Surface Analysis

Vice-Chairman, Surface Chemical Analysis Technical Working Party, Versailles Project on Advanced Materials and Standards

Member, Long Range Planning Committee, American Vacuum Society

Chairman, Applied Surface Science Division Steering Committee, International Union of Vacuum Science, Technique, and Applications

Chairman, Applied Surface Science Program Committee, 11th Internatinal Vacuum Congress and 7th International Confeence on Solid Surfaces, Cologne, Federal Republic of Germany, September 25-29, 1989

Co-Opted Member, Subcommittee on Surface Analysis, Commission V.2 on Microchemical Techniques and Trace Analysis, International Union of Pure and Applied Chemistry

Chairman, Organizing Committee, 3rd Topical Conference on Quantitative Surface Analysis, Salem, MA, October 20-21, 1989

Member, Scientific Committee, European Conference on Applications of Surface and Interface Analysis, Antibes, France, October 23-27, 1989

Member, Editorial Board, "Applications of Surface Science"

Member, Editorial Board, "Surface and Interface Analysis"

Member, Editorial Board, "Methods of Surface Characterization"; co-editor of two volumes in series

Stockbauer, R.

Member, Office Automation Committee, American Vacuum Society

Co-Chairman, Topical Conference on High Temperature Superconducting Thin Films, American Vacuum Society National Symposium, Boston, MA, October, 1989

Consultant, Abstract Processing Computer Database, American Vacuum Society

11. PROFESSIONAL INTERACTIONS, CONSULTING AND AVISORY SERVICES

Camus, P. P.

Collaborating (with A. J. Melmed) with Dr. R. D. Shull of the NIST Metallurgy Division on composition and structural measurements on a nanometer scale of magnetic thin-film composites.

Collaborating (with A. J. Melmed) with Dr. C. K. Chiang of the NIST Ceramics Division on studies of stoichiometries and compositional inhomogeneities of high-temperature superconducting oxides.

Cavanagh, R. R.

Collaborating with Dr. D. S. King of the NIST Molecular Spectroscopy Division on state-specific diagnostics of molecular desorption processes.

Collaborating with Drs. J. C. Stephenson, E. J. Heilweil, and M. P. Casassa of the NIST Molecular Spectroscopy Division on time-resolved measurements of vibrational relaxation processes at surfaces.

Collaborating with Drs. J. J. Rush, J. M. Nicol, and T. J. Udovic of the NIST Reactor Radiation Division on quasi-elastic neutron scattering studies of adsorbates on high-surface-area materials.

Egelhoff, Jr., W. F.

Collaborating with Drs. W. Schwarzacher, W. Allison, R. F. Willis, and J. Penfold of Cambridge University, England to make neutron scattering measurements of the absolute magnetic moment of epitaxial Fe-Cu structures prepared at NIST.

Collaborating with Dr. W. Schwarzacher of Cambridge University, England and Drs. J. Lecante and D. Chandesrif of the Orsay Synchrotron, France on extended x-ray absorption fine structure measurements of epitaxial Fe-Cu structures prepared at NIST.

Collaborating with Drs. B. Heinrich, J. Cochran, and J. Dutcher of Simon Fraser University, Canada on ferromagnetic resonance measurements of the magnetocrystalline anisotropy of epitaxial Fe-Cu structures prepared at NIST.

Fine, J.

Collaborating with Dr. I. Terzic of the Boris Kidric Institute, Belgrade, Yugoslavia on electronic excitation and electron emission for ion-bombarded surfaces. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Drs. L. and N. Tanovic of the University of Sarajevo, Yugoslavia on charactgerizing surface topography changes that result from ion bombardment. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Dr. T. Nenadovic of the Boris Kidric Institute, Belgrade, Yugoslavia on the surface topography effect of both particle and laser-beam interactions with thin solid films. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Dr. J. D. Fassett of the NIST Inorganic Analytical Research Division on the use of laser multiphoton-ionization techniques to identify sputtered atoms and to determine their kinetic energies.

Collaborating with Dr. W. Kirchhoff of the Department of Energy on a data analysis procedure for sputter-depth-profile interface characterization.

Collaborating with Drs. C. Le Gressus and J. P. Duraud of the Centre d'Etudes Nucleaires, Saclay, France on the collosional excitation and electron decay of atoms at single-crystal surfaces.

Collaborating with Dr. P. Roncin of the Université Paris, CNRS/Orsay, France on the use of laser multiphon-ionization techniques to identify sputtered atoms and to determine their kinetic energies.

Collaborating with Dr. M. H. Shapiro of the California State University at Fullerton on multiple-interaction calculations of ion-induced collisional atomic excitation and ejection at single-crystal surfaces.

Collaborating with Dr. R. Freemire of the NIST Center for Computing and Applied Mathematics on generating computer movies from the results of calculations of ion-surface collisional excitations and ejection trajectories.

Collaborating with Dr. G. P. Chambers of the Naval Research Laboratory, Washington, D.C. on the compilation and evaluation of absolute sputtering yield data.

Collaborating with Dr. M. Szymonski of the Jagellonian University, Krakow, Poland on energy distributions of collisionally excited and ejected atoms at surfaces.

Collaborating with Dr. D. Lo of the Institute for Defense Analysis, Alexandria, VA on multiple interaction calculations of collisional excitation and ejection processes of atoms located on single-crystal surfaces as a probe of site geometry.

Collaborating with Dr. V. C. Kannan of the AT&T Laboratories, Allentown, PA on structure characterization of NIST SRM 2135 by transmission electron microscopy and x-ray diffraction.

Collaborating with Drs. L. Holdeman and E. Sparks of COMSAT, Germantown, MD on the fabrication and characterization of new batches of Ni/Cr thin-film structures intended for use as SRM 2135.

Gadzuk, J. W.

Collaborating with Prof. M. Sunjic of the Ruder Boskovic Institute and the University of Zagreb, Yugoslavia on theories of electron spectroscopies and dynamics of moleuclar processes at surfaces. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Dr. S. Holloway, University of Liverpool, England on theories of molecular processes at surfaces. This collaboration is assisted by a grant from the NATO Scientific Affairs Division.

Collaborating with Dr. N. Sathyamurthy, Indian Institute of Technology, Kanpur, India, and serving a monitor for a project "Chemical Dynamics and Laser Spectroscopy", under the auspices of the India-U.S. Materials Science Program funded via the provisions of PL-480.

Collaborating with Dr. C. W. Clark of the NIST Radiation Physics Division on atomic physics aspects of resonance-enhanced electron-stimulated desorption.

Consulted with Prof. B. Cooper of Cornell University on topics related to charge transfer in ion-beam scattering from surfaces.

Consulted with Prof. J. K. Nørskov of the Technical University of Denmark on problems associated with theoretical modeling of molecular processes at surfaces.

Served as an invited discussion leader at the Gordon Research Conference on Dynamics of Gas-Surface Interactions.

Jach, J.

Collaborated with Drs. M. B. Bedzyk and Q. Shen of Cornell University on grazing-angle x-ray diffraction experiments at surfaces.

Collaborated with Dr. L. B. Holdeman of COMSAT and Dr. G. Hembree of Arizona State University on reflection electron microscopy studies of the growth of thin gold films.

Collaborated with Drs. J. Geist, D. Novotny, and G. P. Carver of the NIST Semiconductor Electronics Division on the development of novel semiconductor devices for x-ray experiments.

Collaborated with Dr. R. Crandall of the Solar Energy Research Institute on the fabrication of silicon x-ray detectors.
Collaborated with Drs. D. W. Lindle, P. L. Cowan, R. E. LaVilla, and R. D. Deslattes of the NIST Quantum Metrology Division and Dr. R. C. C. Perera of Lawrence Berkeley Laboratory on analysis of atomic and molecular spectra obtained with x-ray excitations at the Brookhaven National Synchrotron Light Source.

Collaborated with Drs. J. R. Patel, F. Sette, P. H. Citrin, J. E. Rowe, and D. W. Berreman of AT&T Bell Laboratories and Dr. P. L. Cowan of the NIST Quantum Metrology Division on back-reflection x-ray standing-wave experiments.

Joyce, S. A.

Collaborating (with L. J. Whitman and J. A. Yarmoff) with Dr. F. R. McFeely of the IBM Watson Research Center on studies of semiconductor surface deposition and etching reactions.

Kurtz, R. L.

Collaborating with Prof. J. L. de Segovia and Dr. E. Roman-Garcia of the Instituto Ciencia de Materiales, CSCIC, Madrid on a study of the electronic structure and molecular adsorption of H_2O and NH_3 at low temperatures on transition-metal oxide surfaces.

Collaborating with Dr. A. Shih of the Naval Research Laboratory in photoemission and ion desorption studies of Ba and BaO on W as model systems for high-emission dispenser cathodes.

Collaborating with Dr. R. Walkup of IBM in studies of ion desorption using molecular dynamics calculations to predict surface reconstructions, stability of various defect structures, and ion-desorption trajectories.

Melmed, A. J.

Collaborating (with P. P. Camus) with Dr. C. K. Chiang of the NIST Ceramics Division on studies of stoichiometries and compositional inhomogeneities of high-temperature superconducting oxides.

Collaborating (with P. P. Camus) with Dr. R. D. Shull of the NIST Metallurgy Division on composition and structural measurements on a nanometer scale of magnetic thin-film composites.

Collaborating with Dr. H. A. Fowler of the NIST Mathematical Analysis Division on simulations of field-ion-microscopy images.

Collaborating with Drs. N. Ernst and W. A. Schmidt of the Fritz-Haber-Institute, West Berlin, FRG on studies of the electronic structure of high-T_c superconducting materials.

Collaboration with Dr. W. Drachsel of the Fritz-Haber-Institute, Berlin, FRG on the performance of a reflectron lens for increasing the mass resolution of an atom probe.

Powell, C. J.

Collaborating with Drs. J. K. N. Sharma and S. M. Shivaprasad of the Indian National Physical Laboratory, under the auspices of the U.S.-India Cooperative Program, on experimental studies of metal-semiconductor interfaces.

Collaborating with Dr. D. R. Penn of the NIST Electron Physics Group and Dr. S. Tanuma of the Nippon Mining Company, Japan on calculations of the inelastic mean free paths of low-energy electrons in solids.

Collaborating with Dr. M. P. Seah of the UK National Physical Laboratory on an analysis of the factors affecting the accuracy and precision of quantitative surface analyses of Auger-electron spectroscopy and x-ray photoelectron spectroscopy.

Collaborating with Dr. M. P. Seah of the UK National Physical Laboratory on the development of plans and programs for the Surface Chemical Analysis Technical Working Party of the Versailles Project on Advanced Materials and Standards.

Adjudicator for the Science Prize of the UK ESCA Users Group.

Robey, S. W.

Collaborating with Dr. L. H. Bennett of the NIST Magnetic Materials Group on resonant photoemission investigations of half-metallic ferromagnetic materials.

Stiles, M. D.

Collaborating with Dr. D. R. Hamann of AT&T Bell Laboratories on calculations of ballistic electron transport through interfaces.

Collaborating with Dr. D. R. Penn of the NIST Electron Physics Group and Dr. S. M. Girvin of Indiana University on studies of Coulomb blockade effects.

Whitman, L. J.

Collaborating (with S. A. Joyce and J. A. Yarmoff) with Dr. F. R. McFeely of the IBM Watson Researxch Center on studies of semiconductor surface deposition and etching reactions.

Yarmoff, J. A.

Collaborating (with S. A. Joyce and L. J. Whitman) with Dr. F. R. McFeely of the IBM Watson Research Center on studies of semiconductor surface deposition and etching reactions.

Collaborating with Dr. J. R. Lince of The Aerospace Corporation on studies of the surface chemistry of MoS_2.

MOLECULAR PHYSICS DIVISION

FISCAL YEAR 1989 TECHNICAL ACTIVITIES

INTRODUCTION

The properties of molecules and molecular systems as determined by theoretical and experimental spectroscopic methods are a major part of the interdisciplinary field of chemical physics. Originally limited to the study of molecular properties per se, molecular spectroscopy is now ubiquitous in many areas of physics, chemistry, astronomy, biology, environmental science, and various branches of engineering, all of which require data, models, and theoretical concepts to meet their respective needs.

In recent years Molecular Physics has undergone many changes and NIST has both responded and contributed to them in response to the developments of new experimental techniques and theoretical predicitions, challenges posed by basic problems at the forefront of chemical physics, and the needs of the user community. At the present time the work of the Division is conducted in three broad areas: molecular dynamics, high resolution spectroscopy, and quantum chemistry. Although seemingly disparate, the conduct of research in these three broad areas is marked by collaboration, and sharing of equipment and expertise, by the staff.

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, e.g., the Air Force Office of Scientific Research (AFOSR), the Department of Energy (DOE), the National Aeronautics and Space Administration (NASA), industry, or as long term research projects to establish data bases for newly emerging technologies and to meet the contemporary challenges implied in the mission statement of NIST, newly reformulated in the Omnibus Trade Bill of 1988.

GOAL

The goal of the Molecular Physics Division is to conduct research at the forefront of theoretical and experimental spectroscopy in order to provide NIST, other government agencies, industry, and the research community with:

- Critically evaluated reference spectroscopic data.
- State-of-the-art calibration frequency standards.
- Forefront spectroscopic results and expertise.
- Data on molecular species of importance to environmental and climatic concerns.

- Data and models on ultrafast molecular processes, intramolecular dynamics, energy transfer in dilute and condensed phase systems, and molecule-surface interactions.

- Properties and behavior of weakly bound molecular aggregates.

- Properties and behavior of atomic and molecular systems in the presence of strong laser fields, and at ultra low temperatures.

- Advanced spectroscopic measurement methods and techniques.

- Theoretical concepts and quantum theoretical methods for predicting properties and energetics of molecules, clusters, and systems of biological importance.

ORGANIZATION AND STAFFING

The Division is composed of 22 full time permanent staff members as well as post doctoral research associates, guest researchers and contractors from other institutions in the U.S. and abroad. During the past year several changes have occurred. Wm. Bruce Olson and Arthur G. Maki of the High Resolution Group have retired while Robert Heather has joined the Quantum Chemistry Group.

To carry out its research the Division is organized into three working groups: Molecular Dynamics, High Resolution Spectroscopy, and Quantum Chemistry.

GROUP REPORTS

The activities conducted during the past year by the three research groups are presented in the following three sections.

HIGH RESOLUTION SPECTROSCOPY GROUP

The work of this group covers a variety of spectroscopic topics, many of which are part of programmatic efforts. The research reports are divided into six general topics: Data Center Activities, Spectroscopic Studies of Environmental Species, Hydrogen-bonded and van der Waals Complexes, Matrix Isolation Studies and Spectroscopic Theory. A number of guest researchers or contractors participated in the work. They are identified by an asterisk affixed to their names.

A. Data Center Activities

We collect under this heading the work most closely connected with the core mission of NIST, namely, the production and dissemination of compilations of accurately measured frequencies or wavenumbers for use as secondary standards, and of critically evaluated molecular properties for use in other disciplines. The group devotes a significant portion of its effort each year to this program which serves the needs in the microwave, infrared, and ultraviolet spectral regions.

1. Microwave Spectral Tables
(F. J. Lovas, R. D. Suenram, and G. L. Rotter)

In June 1988 we submitted a manuscript entitled "Microwave Spectral Tables III. Hydrocarbons, CH to $C_{10}H_{10}$" to the J. Phys. Chem. Ref. Data for publication. The manuscript includes 135 tables of molecular constants and 91 tables of spectral frequencies. This critical review contains all of the rotational spectral lines observed and reported in the open literature for 91 hydrocarbon molecules. Progress in publishing this compilation has been slow owing to the need for substantial editing on the Bedford computer by OSRD staff and further proofing of the edited copy; however, this review will appear in the next issue of the journal. During FY 1989 we continued work on the Microwave Spectral Tables IV which treats organic species containing oxygen. Our reprint collection currently contains 171 species in this class with empirical formulas CHO through $C_7H_{12}O$. Spectral data for 55 species (262 isotopic forms) have been coded for spectral fitting and table generating programs. The first part of this review (about half of the species) is projected to be completed in the fall of 1990.

2. Rest Frequencies for Radio Astronomy
(F. J. Lovas and G. L. Rotter)

The objective of this effort is to provide astronomers with a convenient source of molecular transitions previously identified in stellar and interstellar objects, and to provide the most accurate transition frequency available, which may be a measured or calculated value. Since the 1985 revision of this publication, 18 new interstellar species have been identified and many new transitions of previously known species have been reported. We are currently updating the compilation for publication next year.

Quite often we have been called upon to assist astronomers in identifying new spectral features and occasionally asked to participate in new observational projects. Last year a project to carry out a survey of the Orion A molecular cloud in the 330 - 360 GHz frequency window was initiated by P. Jewell, NRAO, Tucson, AZ. He invited us to collaborate in this project by providing expertise in identifying and assigning new transitions in this spectral region which arise from known interstellar molecules. This project was successfully completed and resulted in the observation of about 190 transitions from 37 species and 30 transitions for which the molecular source could not be identified. These results have been published recently in Astrophys. J. Supplement.

3. Molecular Structures
(W. J. Lafferty)

In collaboration with J. H. Callomon (Univ. College, London), E. Hirota (Okazaki), and K. Kuchitsu (Univ. Tokyo), a compilation of molecular structures, reported in the literature though the end of this year is well underway. This compilation, which will be the third update--and probably the last--of this series, includes structures determined in the gas phase by IR, MW, and visible spectroscopy as well as electron diffraction techniques. The IR section of the compilation is being done here at NIST. This work will be published as one of the Landolt-Börnstein series of scientific data reports.

4. Vibrational and Electronic Energy Levels
(M. E. Jacox)

All of the data from the compilations of the vibrational and electronic energy levels of small polyatomic transient molecules and much more recent spectral data have been converted to dBase III format for distribution of a searchable disk version (named VEEL) through the Office of Standard Reference Data. More than 1000 molecules are included in VEEL. There has been a collaboration with OSRD staff on search algorithms and menu design for the finished database, which, together with the documentation, is currently in review.

A supplement to the earlier compilations of vibrational and electronic spectral data for transient molecules is in preparation. As of August 15, it contained new data for approximately 270 molecules. In late 1989 or early 1990 it will be submitted to the Journal of Physical and Chemical Reference Data. As new data are added to the transient molecule supplement, they will also be added to VEEL, in preparation for its second edition.

5. Frequency Calibration Benchmarks
(A. G. Maki)

This laboratory has been involved in a collaboration on frequency calibration measurements with J. Wells at the NIST/Boulder laboratory. New measurements on a number of bands of OCS have led to new frequency calibration data for the 490 to 3000 cm^{-1} region. Nearly all the energy levels of OCS below 3000 cm^{-1} have now been tied to the cesium frequency standard with an uncertainty of ±9 MHz (±0.0003 cm^{-1}) or better.

New heterodyne measurements were also made on N_2O to provide improved accuracy for the frequency values for the ν_2 band in the 520 to 660 cm^{-1} region as well as to improve our knowledge of the lower energy levels of this molecule.

To fill a gap between the N_2O and OCS calibration data, the frequencies of a number of transitions of the strong ν_3 band of CS_2 were measured. By combining data on both $^{12}CS_2$ and $^{13}CS_2$, which are easily seen in a low pressure sample, calibration tables were prepared for the 1460 to 1550 cm^{-1} region.

The new far-infrared heterodyne measurements made on the high-J transitions in the rotational spectrum of OCS are a major new contribution for the preparation of calibration tables. These will give greater accuracy to our evaluation of the centrifugal distortion constants in the vibrational levels below about 1900 cm^{-1}.

B. Spectroscopic Studies of Environmental Species

Many molecular species play a significant role in the chemistry of planetary atmospheres, and are of significant interest to agencies like NASA, DOD and the CMA (Chemical Manufacturer's Association). The major interest of these agencies focusses on molecular spectroscopy as a remote sensing tool for the determination of concentration profiles. Thus the emphasis of the work described here is on band analyses and the important properties of line strengths, line shapes, and collisional line broadening.

1. FTIR Studies of CO_2, ClO_2 and $(CN)_2$
(W. J. Lafferty, A. Weber, and W. B. Olson*)

This year significant effort was spent on the study of the high resolution infrared spectra of molecules of atmospheric or stratospheric interest, both obtained in this laboratory as well as in other laboratories. A laborious, long term laboratory project, studying collisional broadening in the Q-branches in the region of the ν_2 bending mode of CO_2 has been completed. This Air Force sponsored project is of practical as well as scientific interest since several of the "hot band" Q-branch lines are used for satellite temperature sounding measurements. The NIST data is now being analyzed by M. L. Hoke and S. A. Clough at AFGL, and it is proposed to include the Y collisional mixing parameters in the next edition of the Air Force Atmospheric Tables.

Work has started on the fundamental and combination bands of the ClO_2 molecule. This molecule is postulated to be involved in the stratospheric chlorine cycle, but no direct observation of it has been made as yet. The spectra were obtained by J. Burkholder and C. Howard at NOAA in Boulder, who asked our lab to analyze them. Although ClO_2 is a simple near-prolate asymmetric rotor, the spectra are complicated by the fact that the molecule is a free radical and the lines are doubled by nuclear spin splitting. Unfortunately, programs written some years ago in this laboratory using Polo approximations, which work well for the NO_2 molecule, have been found to be inadequate to treat the spectrum of ClO_2 since this molecule is a bit more asymmetric than nitrogen dioxide. In collaboration with R. Escribano at the Instituto de Estructura de la Materia in Madrid, a fitting program using direct diagonalization techniques is being written to obtain the molecular constants of this species.

A study of the cyanogen molecule, C_2N_2, one of the many molecules found on the moons of Jupiter, is nearly completed. Both the IR active fundamentals, the bending band $\nu_4{}^1$ at 225 cm^{-1} and the asymmetric stretching band near 2300 cm^{-1}, as well as a myriad of "hot" bands have been assigned. In addition a number of combination and difference bands have been studied in order to get a complete set of anharmonic constants for this molecule.

The infrared spectrum of methylene fluoride was recorded with the NIST BOMEM interferometer and analyzed by R. D'Cunha and collaborators of the Bhabha Atomic Research Centre, Bombay, India. The work on the ν_8 band is completed while new spectra of the ν_4 band were obtained at dry ice temperature to suppress the spectral congestion due to hot band transitions.

2. FTIR Studies of Nitric Acid and SO_x
(A. G. Maki)

The four low frequency fundamental bands of nitric acid (HNO_3) have been measured and analyzed for the first time. Both infrared and microwave measurements were combined to obtain values for the rovibrational constants that are needed to calculate the energy levels and transitions responsible for the infrared spectrum.

The moderately strong band at 1205 cm^{-1} was also measured and analyzed. It was shown to be due to the combination transition $\nu_8 + \nu_9$. These bands have been characterized for both line position and relative intensity.

Spectra of the two gases, SO_2 and SO_3, which are involved in the acid rain problem, have also been the subject of some studies. Many of the weaker transitions of SO_2 in the 450 to 600 cm^{-1} region have now been identified as due to the $^{34}SO_2$ species which comprises 4.2% of a normal sample. The low frequency ν_2 and ν_4 bands of SO_3 have also been studied and a complete set of constants have been determined that allow one to calculate the appearance of those bands with confidence.

3. Photoacoustic Measurement of Differential Broadening of the Λ Doublets in NO ($X^2\Pi_{1/2}$, v=2-0) by Ar
(A. S. Pine)

A differential broadening of the Λ doublets in the v=2-0 overtone band of the $^2\Pi_{1/2}$ ground electronic state of NO in an Ar buffer gas has been observed by photoacoustic spectroscopy using a tunable color-center laser. The broadening coefficients for the *f* symmetry components are larger than for the *e* symmetry components by up to ~6% for J~16.5. This differential depends on J and vanishes at low J, implicating the anisotropy of the unpaired electron Π orbital in the plane of rotation. The $^2\Pi_{3/2}$ transitions are slightly broader than the $^2\Pi_{1/2}$ as a result of spin-flipping collisional relaxation. The observed lineshapes also exhibit collisional or Dicke narrowing due to velocity-changing collisions.

4. Q-Branch Line Mixing in HCCH
(A. S. Pine)

Three Q branch profiles in the C-H stretch-bend combination region of HCCH have been measured as a function of pressure by transmission spectroscopy using a linear-scan-controlled difference-frequency laser. At low pressure, in the Doppler-limited regime, the J component spectral transitions can be accurately characterized to within about 0.0001 cm^{-1} in frequency and 0.2% in intensity. However, as the pressure is raised, up to about 1 atm, the individual lines overlap and the resulting contour cannot be fit with additive or superposable Lorentzian or Voigt component lineshapes. This is a manifestation of collisional interference or line mixing where inelastic collisions redistribute intensity among the overlapping transitions. The three Q branches, which have radically different degrees of overlap due to a small vibrational dependence to the rotational constants, can be consistently fit with a modified collisional cross relaxation matrix using a hybrid power-exponential gap rate law taking into account the symmetry of the intermolecular potential and possible extraneous relaxations to states not involved in the Q branch transitions. Models used successfully in prior studies of N_2O and CO_2 predict too much line coupling for HCCH.

C. Hydrogen-bonded and van der Waals Complexes

1. Millimeter and submillimeter wave spectrum of $(HF)_2$
(W. J. Lafferty and R. D. Suenram)

A collaboration on the spectrum of the interesting HF dimer molecule with the sub-millimeter wave spectroscopy group at Gorky in the USSR is under way. Using earlier NIST microwave and IR data and Pade approximate fitting techniques, Krupnov and coworkers tentatively assigned a line series in the 180-380 GHz region to a previously unobserved high J R-branch K=3 series. Observation of the Q- and P- branches of this subband in the millimeter wave region here at NIST verified the assignment. Both the Gorky and NIST data have been combined to obtain an improved set of spectroscopic constants. An atlas of the a- and b-type microwave and far infrared transitions is being prepared.

2. Electric-Resonance Optothermal Spectroscopy of $(H_2O)_2$
(G.T. Fraser, R.D. Suenram, L.H. Coudert*, and F.J. Lovas)

The tunneling motions in $(H_2O)_2$ and $(D_2O)_2$ have been studied by microwave spectroscopy using an electric-resonance optothermal spectrometer (EROS) recently developed at NIST. The EROS spectrometer operates by monitoring the intensity of a state-selected molecular beam of $(H_2O)_2$ as a function of microwave frequency. The molecular beam is state selected using an electric field of quadrupole symmetry. Microwave-microwave double resonance experiments are used to guide and verify spectral assignments. For $(D_2O)_2$, pulsed-nozzle Fourier transform microwave measurements have also been made.

For the protonated species, the reported measurements extend previous results on the a-type K=0-0 and 1-1 bands for the $A_2{}^{\pm}$, $B_2{}^{\pm}$, and $E^{\pm}$ rotational-tunneling states and include the first observations of the c-type K=1-0 band for the $A_2{}^{\pm}$, $B_2{}^{\pm}$ and $E^{\pm}$ states and the a-type K=0-0 band for the $A_1{}^{\pm}$ states. For the $A_1{}^{\pm}$ states an interconversion tunneling splitting of 22.6 GHz is obtained, compared to the 19.5 GHz value found previously for the K=0 $A_2\pm$ and $B_2\pm$ states.

For the deuterated species, the tunneling splitting for the K=0 $A_2\pm/B_2\pm$ states is determined to be 1083 MHz, which is slightly lower than the

1172 MHz value found previously for the $A_1^{\pm}/B_1^{\pm}$ states. These splittings are also shown to have a large K dependence, being 1077 and 992 MHz for the K=1 levels of the $A_1\pm/B_1\pm$ and $A_2^{\pm}/B_2\pm$ states, respectively. The tunneling splittings indicate that the geared type pathway dominates the tunneling process. The B+C rotational constant is relatively insensitive to tunneling state, whereas the B-C rotational constant varies by nearly a factor of two between tunneling states. This indicates that corrections for tunneling effects need to be applied before using B-C in a structural analysis.

3. Infrared Molecular Beam Optothermal Spectroscopy of Complexes (G.T. Fraser and A.S. Pine)

a. Isomerization and Vibrational Predissociation of HF-HCl and HCl-HF

Microwave and infrared spectra of HF-HCl and HCl-HF have been obtained using the EROS spectrometer. The HF-HCl microwave measurements extend to K_a=1 the previous K_a=0 results of Janda, Steed, Novick, and Klemperer, allowing the determination of the K_a dependence and asymmetry of the Cl quadrupole coupling constant. For the metastable HCl-HF isomer no previous spectroscopic measurements have been reported. Here, microwave spectra are observed for the K_a=0 and 1 states and interpreted in terms of an L-shaped hydrogen-bonded structure for the complex, with a 3.235 Å center-of-mass separation between the HF and HCl subunits. The D_J distortion constant indicates that the harmonic stretching force constant for HCl-HF is ~35 % larger than that of HF-HCl. Infrared spectra of the K_a=0-0 and 1-0 subbands of the H-F stretching band for HF-HCl and of the K_a=0-0 subband of the H-F stretch for HCl-HF are also reported. The vibrational predissociation linewidths depend on vibration, K_a state, isotopic species, and isomer excited.

b. Vibrational Predissociation in the H-F Stretching Mode of HF-DF

The high-resolution infrared spectrum of the K=1-0 subband of the H-F stretching vibrational band of the hydrogen-bonded HF-DF complex has been recorded using the EROS spectrometer. The spectrum exhibits minor perturbations and vibrational predissociation linewidths of 23±2 MHz (FWHM) for comparison to the 11±1 MHz widths found for the corresponding mode of the homonuclear HF-HF dimer. This implies that tunneling is not responsible for the predissociation of the free-H stretch of HF-HF since tunneling is quenched in the mixed isotopic species.

c. Angular-Radial Coupling Effects in Ar-HCN

Microwave and infrared spectra of Ar-HCN have been obtained by means of the EROS spectrometer. The microwave measurements extend to higher J the previous results of Leopold <u>et al</u>. and Klots <u>et al</u>., allowing the determination of higher-order centrifugal distortion constants for this quasilinear, highly non-rigid complex. A Padé approximant fit to the microwave data indicates a significant rotation-induced asymptotic increase in the zero-point center-of-mass separation between the Ar and the HCN, above that expected from pure radial distortion. This results from the large coupling between the angular and radial degrees in the intermolecular potential forcing the centrifugal alignment of the HCN. Infrared spectra are reported for the C-H stretching fundamental, ν_1, and the combination band $\nu_1+\nu_5{}^1$, where ν_5 is the van der Waals bending vibration. The band-origin difference between these two bands gives $\nu_5 = 7.8$ cm^{-1}, in rough agreement with the 10 cm^{-1} harmonic value predicted from the microwave-determined nuclear quadrupole coupling constant. The complexation-induced red shift of the C-H stretching vibration is 2.69 cm^{-1} and the vibrational predissociation linewidths, Γ, are < 10 MHz (FWHM). The vibrationally excited complex predissociates before striking the bolometer detector, implying that the predissociation lifetime, τ < 1 ms.

4. Studies of van der Waals Complexes of Reacting Molecules (J. Z. Gillies*, C. W. Gillies*, R. D. Suenram, and F. J. Lovas)

Several systems are under investigation with the pulsed-beam Fourier transform microwave spectrometer (FTMW), where the individual molecular species involved in forming the complex are very reactive towards one another under normal circumstances. The goal in these studies is to determine the structures of the reaction complexes which will help in understanding more about the mechanism of cycloaddition reactions. We have recently measured the rotational spectra and determined the structures of the ozone-ethylene and the ozone-acetylene complexes by sampling a flowing mixture of Ar/O_3 and Ar/hydrocarbon introduced into the pulsed nozzle through separate inlets near the nozzle orifice. These reactants are classical examples of the 1,3-dipolar cycloaddition reaction (Diels Alder type of reaction) in which the electrostatic positive ends of the dieneophile (ozone) react simultaneously with the diene (ethylene or acetylene) to form a five membered ring adduct. The structures of the complexes are similar to the final reaction product (1,2,3-trioxolane in the case of ethylene) with the terminal oxygen atoms directed toward the two carbon atoms. The C-O distance is ~3.3 Å in the ethylene complex compared to 1.417 Å in the compound. These studies show how the electrostatic properties of the individual compounds control the reaction pathway. It is expected that related species will be studied in the near future to further probe these reaction intermediates.

5. Van der Waals Complexes with Large Internal Tunneling Splittings (F. J. Lovas, R. D. Suenram and K. Matsumura*)

Many of the van der Waals complexes and hydrogen bonded species that we have investigated with the FTMW spectrometer are very weakly bound and exhibit large rotation-inversion tunneling splittings in their rotational spectra. Examples of complexes investigated during the past year are: argon-formaldehyde, formaldehyde dimer, argon-water, water dimer, water-ozone, water-sulfur dioxide and H_2S-CO_2. The spectra of complexes that exhibit internal motions such as this are often difficult to interpret. However, collaborations with J. Hougen, L. Coudert and G. Fraser, who have developed new mathematical modeling concepts to describe the spectra for large internal motions, have been extremely successful. In addition to defining the tunneling paths and energies, the molecular structures and electric dipole moments have been determined for the complexes listed above.

6. Fourier Transform Spectroscopy of Laser Vaporized Refractory Materials
(R. D. Suenram, F. J. Lovas and K. Matsumura*)

A technique that has been used for several years in optical spectroscopy and mass spectrometry involves the use of a pulsed high power laser, typically a Nd:YAG or eximer laser, to vaporize non-volatile materials in the exit channel of a pulsed molecular beam valve. We have adapted this technique to Fourier transform microwave spectroscopy in an effort to probe a new class of molecular species that is difficult to study by other methods. Initial tests have been promising. We have used the technique to study SiC_2 which is produced from the laser vaporization of a silicon carbide rod. The 1_{01}-0_{00} rotational transition was easily observable with a single gas pulse. The less abundant isotopic species with ^{29}Si, ^{30}Si, and ^{13}C have been observed in natural abundance.

A set of experiments has also been carried out using some refractory metal oxides as laser target materials. Rotational spectra of YO, LaO, ZrO, and HfO have been observed and the electric dipole moments measured. Two species (YO and LaO) have $^2\Sigma$ ground electronic states, and their rotational spectra are split by an interaction with the earth's magnetic field. We have constructed a set of Helmholtz coils around the Fourier-transform spectrometer to reduce the earth's magnetic field to less than 20 mG in the resonance region. With these coils installed, other paramagnetic species can now also be studied. A number of nozzle modifications are being tried which should soon improve the signal-to-noise of the laser vaporization spectrometer for the study of van der Waals complexes of refractory materials.

D. FTIR Matrix Isolation Studies
(M. E. Jacox and W. E. Thompson*)

Studies of the codeposition of a small molecule (XY) contained in a large excess of neon with a beam of neon atoms excited in a microwave discharge have continued. Spectroscopic observations on these systems using the Bomem Fourier transform system have yielded much new information on the vibrational spectra of small molecular ions and cluster ions. In each system, extensive isotopic substitution is performed to establish product identifications. The first studies, for XY = CO_2 and O_2, led to the infrared identification of CO_2^+, CO_2^-, O_4^+, and O_4^-. The results of those studies have recently been published. When XY = N_2, the Σ_u^+ stretching fundamental of N_4^+ appears at 2237.6 cm^{-1}. For the noncentrosymmetrically substituted species (e.g., $^{14}N^{14}N^{15}N^{15}N^+$), infrared activation of ν_1 (Σ^+) is observed. When XY = CO, a weak absorption of CO^+ appears a few cm^{-1} from the band center for the gas-phase vibrational fundamental. Prominent absorptions have been assigned to $(CO)_2^+$ and $(CO)_2^-$, for which vibrational data have not previously been reported. When XY = N_2O, the two stretching fundamentals of ground-state N_2O^+ appear close to the previously reported gas-phase band centers. In addition, the

1200 cm^{-1} absorption of $N{=}NO_2^-$, previously identified in this laboratory in studies of the interaction of alkali metals with N_2O isolated in an argon matrix, is present. Other product absorptions are contributed by cis-$(NO)_2$ and possibly by N_2O^- and $(NO)_2^-$. When a $Ne:CO_2:O_2$ sample is codeposited with a beam of excited neon atoms, three new infrared absorptions, which are not characteristic of experiments on either a $Ne:CO_2$ or a $Ne:O_2$ sample. All three of these absorptions are associated with CO_2 vibrations. The relative photolytic stability of the new product and the pattern of isotopic shifts are consistent with its identification as $(O_2\cdots OCO)^+$. Detailed analysis of the isotopic data is in progress. Experiments in which XY = NO have been initiated. Prominent absorptions of several different cluster ions contribute to the spectrum. Survey experiments for XY = H_2O have been extended to the OH stretching region, and a rather broad absorption near 3215 cm^{-1} has been tentatively assigned to the ν_3 fundamental of H_2O^+, for which the ν_2 absorption was previously detected in this system near 1403 cm^{-1}. During the coming year, the experiments on the NO and H_2O systems will be completed, and studies on a number of other molecules, including NO_2, C_2H_2, HCN, HCl, and the fluoromethanes, are planned.

E. Spectroscopic Theory
(J. Hougen, L. H. Coudert*, I. J. Kleiner* and W. Fawzy*)

Theoretical activity has continued to focus on the derivation, testing and application of effective rotational Hamiltonian operators for classes of molecular systems currently not discussed in the literature.

A final global fit of all known water dimer lines (173 transitions) using the formalism developed during the last three years has been successfully carried out, indicating that we now have some understanding of the four tunneling motions that occur in this complex. Attempts will now be made to apply this method to the ammonia dimer spectrum, which has been measured by Saykally's group in Berkeley. At present we know almost nothing about the tunneling motions in this complex, and even the type of bonding (hydrogen-bond or not) is still in question. In addition to these two dimers, the method has been successfully applied (by LHC) to a number of other complexes and stable molecules.

The formalism for rotational energy levels of open shell complexes, developed with W. Fawzy, has been applied successfully to the jet-cooled NO-HF infrared spectrum of Pine and Fraser. This spectrum is complicated by a large P-type doubling in the P = 1/2 state, which arises primarily from the interplay between spin-orbit interaction in the NO molecule and a Renner-Teller-like quenching of the Π orbital degeneracy of the NO molecule when the HF partner approaches.

Work has begun (with IJK) on testing the limits of applicability of various theoretical treatments for the spectra of molecules with internal rotation (methanol and acetaldehyde). Ultimately we hope to investigate vibration-rotation interactions leading to energy transfer from the high-frequency vibrations into highly excited quasicontinuum levels of the internal rotation motion, but this goal is still a long way off.

A final direction of study concerns the development of a formalism for the amino inversion motion in CH_3-NHD, the question here being how much the heavy deuterium atom "refuses to move" during the -NHD inversion tunneling. This work follows the successful descriptions of the v = 0 and $v_{torsion}$ = 1 tunneling-rotational levels in CH_3-NH_2.

MOLECULAR DYNAMICS GROUP

This group primarily performs quantum-state specific studies of molecular dynamics. A common factor in the research described below is the role of energy transfer in the spectroscopy and kinetics of molecules. Research on molecular dynamics of molecules on surfaces is done in collaboration with Surface Science Division staff (denoted by asterisk).

A. Condensed Phase Energy Transfer
(J. D. Beckerle*, M. P. Casassa, R. R. Cavanagh*, E. J. Heilweil, and J. C. Stephenson)

During the past year we continued using tunable ultrafast lasers to measure the vibrational energy relaxation times (T_1) for CO(v=1) groups bound to metal atoms.

Using a one color infrared bleaching pump/probe method, we determined T_1 for CO(v=1) chemisorbed on the surface of large (20-30 Å diameter) Pt particles. The very fast decay time (T_1 = 7 ± 1 ps) was found to be independent of temperature in the range $100 \leq T \leq 400$ K, and the same T_1 was measured for an isotopic mixture of $^{12}C^{16}O$ dilute (1:3) in $^{12}C^{18}O$. The lack of temperature dependence is consistent with a damping mechanism in which the 2090 cm^{-1} vibrational quantum decays by exciting an electron-hole (e/h) pair in the Pt, and is not consistent with decay to any available low frequency ($\nu < 500$ cm^{-1}) surface or substrate vibrational modes. Likewise, the lack of isotope dependence is consistent with relaxation by e/h pair formation, and argues, albeit inconclusively, against nearly resonant (dipole-dipole) transfer to other CO sites as the mechanism responsible for the observed bleaching decays.

Rather than continue energy transfer studies on these amorphous Pt particles, we began T_1 measurements for an ordered monolayer of CO on the surface of single crystal Pt(111). This necessitated construction of a new ultrahigh vacuum chamber especially designed for optical studies of metal surfaces using both FTIR for spectral studies (FWHM resolution ≤ 0.1 cm^{-1}) and tunable ultrafast lasers for time-resolved measurements. Our bandwidth studies of CO/Pt(111) as a function of temperature and coverage are in agreement with the most recent results from other laboratories (e.g. Bradshaw, Trenary). By the uncertainty principle, the IR absorption bandwidth (6 cm^{-1}) sets a limit $T_1 \geq 0.8$ ps for CO or Pt(111) at room temperature. We have seen transient infrared bleaching signals induced by an ultrafast infrared pump pulse for CO(v=1)/Pt(111), and we expect soon to have a time-resolved measurement of T_1 to compare to the bandwidths.

These initial experiments involve CO/Pt(111) because it is the best studied adsorbate/metal system. However, many other interesting surface species can be studied with our apparatus, such as NO and N_2; polyatomics like CH_3O (methoxy), HCO_2 (formate), CCH_3 (vinylidine), and PF_3; or CO co-absorbed with electron doners like potassium. All the preceding adsorbates form ordered adlayers on various transition metal crystal faces, and have large infrared absorptions ($\Delta R/R > 1\%$) which facilitate our infrared pump/probe experiments. We hope that future studies will determine the dependence of vibrational energy transfer rates on parameters like surface coverage, electron density, temperature, bonding site, adsorbate/substrate distance, bond dipole moment, etc.

Complementing the CO(v=1)/Pt measurements, we have studied vibrational energy transfer involving the high frequency CO(v=1) stretching modes of metal carbonyl molecules in solution. We have used a new broadband IR probe method to obtain the transient IR absorption spectrum over the entire CO stretching region, and hence to identify pathways for vibrational energy flow in these molecules.

The broadband infrared (BBIR) probing apparatus generates IR in the 2000 cm^{-1} region by taking the difference frequency in a non-linear crystal ($LiIO_3$) between a fixed frequency ps visible pulse (i.e. 532 nm) and a broadband tunable ps dye laser pulse. The BBIR probe pulse goes through the sample at a computer-controlled delay time after the pump pulse and records the transient IR spectral changes in absorption. The BBIR pulse containing transient spectral information is then upconverted in a second $LiIO_3$ crystal by sum frequency generation with the 532 nm pulse. The resultant blue (~480 nm) ps pulse is sent through a spectrograph and dispersed on a multichannel detector (i.e. an OMA III). In this way the entire IR absorption spectrum in the CO-stretch region is recorded on every laser shot with a time resolution limited by the duration of the BBIR probe pulse and spectral resolution limited by the spectrograph dispersion and detector pixel spacing.

The new BBIR studies have revealed important information about vibrational relaxation in these metal carbonyl molecules. For the molecules we have studied carefully, if one of the CO stretching modes is pumped, the vibrational excitation flows rapidly to the other high frequency CO stretch modes in the molecule. For instance, in $Rh(CO)_2(C_5H_7O_2)$ there are CO stretch modes at ν_1 = 2084 cm^{-1} and ν_2 = 2015 cm^{-1}. If ν_1 is pumped, population flow into ν_2 is evidenced by transient features at 2000 cm^{-1} ($\nu_2 \rightarrow 2\nu_2$) and 2059 cm^{-1} ($\nu_2 \rightarrow \nu_2 + \nu_1$). Absorptions at both those frequencies appear in a time short compared to the 18 ps pulses used in these experiments, suggesting that $\nu_1 \rightarrow \nu_2$ transfer occurs in a time $\leq$ 10 ps. These coupled CO stretching modes then relax together, by multiquantum transfer to lower frequency modes, on the much longer timescale which we previously reported.

During the next few months we will use BBIR pulses of much shorter duration to completely time-resolve the initial vibrational energy transfer in these molecules. Also we expect to begin IR pump/BBIR probe studies of hydrogen bonded OH stretching modes of simple alcohol dimers in solution.

This research was partially funded by AFOSR.

B. Overtone Photodissociation of HN_3
(M.P. Casassa, B.R.Foy, D.S.King, and J.C. Stephenson)

Vibrational overtone excitation of molecules enables highly state-specific studies of unimolecular decomposition. In our experiments, picosecond or high-resolution nanosecond laser pulses initiate unimolecular decomposition of hydrazoic acid, HN_3, by exciting high NH stretching overtone (ν_1) and combination levels. In the collision-free environment of a molecular beam or in a low pressure gas cell, the following reactions are observed:

$$HN_3(X\ ^1A') \longrightarrow HN(X\ ^3\Sigma^-) + N_2(X) \quad \Delta H = 15\text{kcal/mol}, \quad E_a \approx 36\text{kcal/mol},$$
$$\longrightarrow HN(a\ ^1\Delta) + N_2(X) \quad \Delta H = 51\text{kcal/mol}.$$

The NH fragments are detected by laser-induced fluorescence of the $A^3\Pi\text{-}X^3\Sigma^-$ or $c^1\Pi\text{-}a^1\Delta$ transitions using a frequency-doubled dye laser. During the past year we measured the overtone photodissociation spectra of the $5\nu_1$ and $6\nu_1$ levels at resolution sufficient to resolve widths of individual rovibrational transitions, and we performed time-resolved experiments on $5\nu_1$, $6\nu_1$ and four combination bands to determine the unimolecular decomposition rate as a function of vibrational energy and mode excited. These temporal and spectral data complement our measurements of detailed product state distributions, and together this information provides an unprecedented detailed view of unimolecular decomposition.

High-resolution overtone photodissociation spectra reveal the nature of the initially excited vibrational motion. Spectra of the $5\nu_1$ and $6\nu_1$ bands are obtained by scanning the frequency of the overtone-pump laser near 15,120 cm^{-1} and 17,670 cm^{-1}, and monitoring fluorescence excited by a probe laser tuned to a NH fragment transition ($A^3\Pi\text{-}X^3\Sigma^-$, $R_1(1)$ line near 336 nm). The spectra exhibit P,R-branch structure characteristic of parallel bands of a near-prolate top, but the (J,K=0) transitions appear as multiplets of features, and the patterns of the multiplets vary erratically with J. These sets of transitions can only arise by anharmonic (Fermi) mixing of the ($n\nu_1$,J,K=0) rovibrational levels of HN_3 with other rovibrational states of the molecule.

The $6\nu_1$ spectrum exhibits more components than $5\nu_1$, reflecting the increase in the density of nearly isoenergetic states with increasing vibrational energy. Also, the spectral extent of the Fermi-mixed components is larger for $6\nu_1$ than for $5\nu_1$, indicating an increase in the coupling matrix elements between the vibrational states. A deperturbation analysis shows the matrix elements are in the range 0.010-0.065 cm^{-1} for $5\nu_1$, and up to 0.1 cm^{-1} for $6\nu_1$. In both levels, the density of features in the spectra is comparable to the calculated total density of HN_3 vibrational states (ρ_{vib} = 7 and 13 states/cm^{-1} for $5\nu_1$ and $6\nu_4$, respectively). This suggests that the NH stretching overtones couple to any neighboring states that fall within the coupling strength of ≈0.1 cm^{-1}, regardless of the type of motion involved.

Spectra recorded with a spectral bandwidth of 0.007 cm^{-1}, obtained using a pulse-amplified single-mode dye laser, show the individual rovibrational lines in the $5\nu_1$ spectrum are Doppler broadened (160MHz FWHM in the 8K molecular beam), while the $6\nu_1$ lines show widths in excess of the Doppler width. Best-fit Voigt profiles give Lorentzian widths ranging from 150 to 270 MHz for different lines in the $6\nu_1$ spectrum. Based on comparison to the dissociation rate measured in real time, we attribute these widths to homogeneous broadening due to dissociation.

Picosecond and nanosecond lasers were used to measure product appearance rates in time-resolved experiments. Figure 1 shows data obtained for $5\nu_1$ and $6\nu_1$ and four intermediate combination bands. The modes are designated in the figure using their zero-order labels. Lifetimes decrease monotonically with energy from ≈210ns for $5\nu_1$ to ≈1ns for $6\nu_1$. There is no marked deviation from this trend, even though the initial vibrational motions are notionally quite different. For example, $5\nu_1+2\nu_4$ includes two quanta in the internal NN stretching mode (i.e., the reaction coordinate) and might be expected to dissociate more rapidly. An explanation for the lack of mode specificity in lifetimes is suggested by the mode-mixing observed in the $5\nu_1$ and $6\nu_1$ spectra: the actual motions excited are mixtures of zero-order states, and not simply the distinct motions suggested by the zero-order labels.

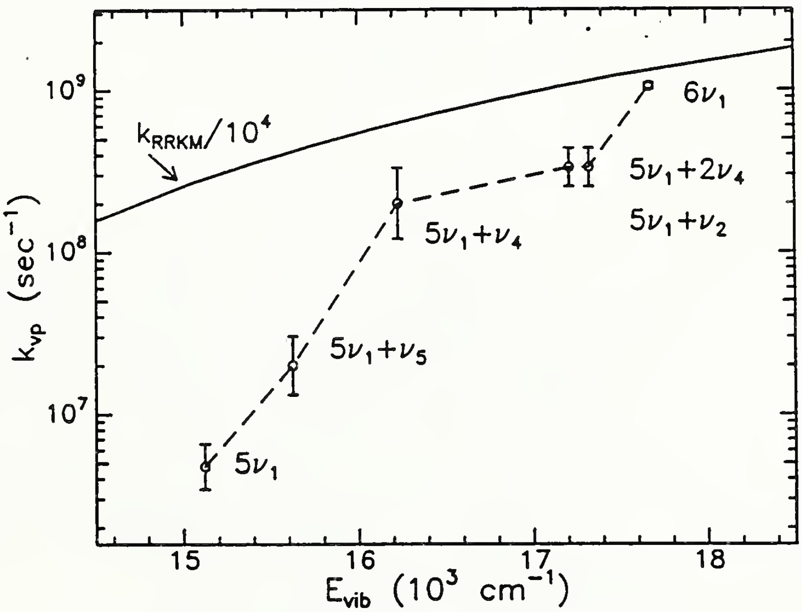

Figure 1. Unimolecular decomposition rates for overtone-excited HN_3.

Lifetimes shorter than 10 ns were measured in picosecond experiments and are actually band-averaged lifetimes, since the spectral width of picosecond pulses (limited by the uncertainty principle) subtends the multiple components in the overtone spectra. For the long-lived modes, nanosecond lasers were used, enabling measurement of lifetimes for individual Fermi resonance components of particular (J,K) levels. In these circumstances, mode-specific effects are observed, showing that lifetimes do depend upon the specific vibrational trajectory initiated. For example, lifetimes measured within the $5\nu_1$ band vary by a factor of two. Similar variation in lifetimes among the $6\nu_1$ components is deduced from the variation in the $6\nu_1$ linewidths.

Figure 1 indicates that a 200-fold increase in the vibrational predissociation rate occurs for a 17% increase in vibrational energy. Statistical theory predicts a less dramatic increase in the rate with energy and ρ_{vib}: the RRKM calculation shown in the figure gives only a factor of 4 increase at these energies. The spin-forbidden nature of the reaction at these energies is reflected in the 10^4 ratio of calculated (assuming spin-allowed) and observed rates. Ab initio calculations by M. Alexander indicate that the large increase of rate with energy arises because the activation barrier actually lies slightly above the $5\nu_1$ level, and levels near $5\nu_1$ dissociate by tunneling through the potential energy barrier.

In the future, we will measure spectra, lifetimes, and product states associated with excitations in the region of the $7\nu_1$ level, which is above the threshold for dissociation via the spin-allowed channel. Analogous experiments on molecules such as CH_3OOH, with spatially distinct groups of ν_{XH} states, and CH_2N_2 are also planned.

This work was partially funded by AFOSR.

C. Carrier-driven Surface Reactions
(S. A. Buntin*, R. R. Cavanagh*, D. S. King, and L. J. Richter*)

State-resolved diagnostics of NO desorbed from Pt(111) following laser irradiation of the surface have demonstrated that hot, photogenerated carriers can initiate selected surface reactions. Those experiments used nanosecond duration, pulsed YAG and tunable dye lasers and were performed in an ultra-high vacuum chamber. Determinations of the desorption dynamics versus incident YAG laser fluence and wavelength were used to distinguish carrier-driven processes from thermal processes. We have recently directed our exploration of laser-induced, carrier-mediated surface reactions to include the reaction/desorption of NO from Si(111). In semiconductors, as opposed to metals, both the photogenerated carriers and excited surface species are expected to have significantly longer lifetimes; therefore, the detailed dynamics of optically driven surface reactions on Si may be significantly different from those observed on Pt.

Full characterization of the energy partitioning in the desorbed NO is achieved using laser-induced fluorescence. The kinetic energy distributions of NO molecules desorbed in a specific [electronic (Ω), rotational (J), and vibrational (v)] quantum state are measured using an optically-detected time-of-flight (TOF) technique by varying the time delay between the firing of the desorption and probe lasers. Velocity-integrated state distributions are derived from the TOF spectra for a selection of states (Ω,J,v). Complete measurements are performed at various surface coverages and desorption-laser fluences and wavelengths.

A Si(111) surface saturated with NO at a temperature of 100 K (multilayer adsorption does not occur at this temperature) and irradiated by 355 nm ($E_{h\nu}$=3.5 eV) photons at fluences which induce negligible surface temperature changes ($\Delta T < 1$ K) that yields desorbed NO with very high kinetic energies. The mean kinetic energy increases from 800 to 2000 K with increasing rotational energy in the NO species being probed. These results are independent of the product vibrational state. The rotational population distributions of the desorbed NO were well described by a Boltzmann distribution, characterized by a "rotational temperature" of about 600 K. Surprisingly, almost half of the desorbed NO molecules were in vibrationally excited states. Relative populations v=0:1:2 of 1.0:0.65:0.14 were obtained. The desorption quantum yield is estimated to be 10^{-2} per absorbed photon. These dynamical results are sensitive to initial surface coverage and excitation laser wavelength, but are independent of desorption-laser fluence.

Comparison of the dynamics for carrier-mediated desorption of NO from Pt(111) versus Si(111) shows both similarities and differences. Both substrates produce desorbed NO with comparable mean kinetic energies that are dependent on rotational, but not vibrational, state, and both produce desorbed NO with significant amounts of vibrational excitation. These dynamical trends might then be taken to be signatures of carrier-mediated desorption. In the surface-harpooning model developed in collaboration with J. W. Gadzuk for the carrier-mediated desorption of NO from Pt(111), the lifetime of the high-energy ionic intermediate is seen to strongly influence both the yield and the extent of vibrational excitation. The enhanced yield and extent of vibrational excitation from Si(111) versus Pt(111) are in qualitative agreement with this expectation. Experimental work on this system will continue in order to obtain a better understanding of the microscopic details of carrier driven processes on semiconductors.

As a prototype in the exploration of molecule-surface dynamics, NO has been extensively studied, primarily because of the ease with which this species may be detected in a state-specific manner. However, the extension of results for NO to the development of general trends in surface dynamics is complicated by the fact that NO is an open shell species. Because of the extensive number of both theoretical and experimental surface science studies involving CO (closed shell ground state) we have directed our efforts toward the implementation of the hardware necessary to detect CO with rovibrational state selectivity. Laser-induced fluorescence detection requires the generation of vacuum ultraviolet radiation (VUV) in the region 140 to 155 nm. For dynamical studies of the desorption of CO from surfaces, VUV intensities must be sufficient to provide for the detection of molecular densities on the order to 10^8/cc. Our approach, given its high conversion efficiency, is to generate the necessary probe wavelengths by two-photon resonance enhanced four-wave sum frequency mixing in Mg vapor. The necessary facilities (i.e., a second dye laser, heat pipe, detectors, etc.) are now in place and being optimized. Future experiments will explore the dynamics of CO desorption initiated by thermal excitation of the substrate, by excitation of hot carriers, and by direct photoexcitation of metal carbonyl adsorbates.

This work was supported in part of the U.S. Department of Energy, Office of Basic Energy Sciences.

QUANTUM CHEMISTRY GROUP

The Quantum Chemistry Group has expanded the scattering program with the recent hire of R. Heather. This effort is enhanced by active guest researcher collaborations, strong coupling to experimental programs in slow atom spectroscopy at NIST, the University of Maryland, and in France, and by many theoretical collaborations throughout the world. The electronic structure program also maintains an active collaborative program with NIST's Center for Advanced Research in Biotechnology (CARB) and other groups to permit a range of spectroscopic and biochemical applications.

A. Scattering Theory and Molecular Spectroscopy

1. Molecular Photodissociation and Predissociation

We are actively involved in several collaborations in which a close coupling analysis of molecular photodissociation processes is necessary. These studies use standard time independent close coupling methods and offer an opportunity to apply new time dependent methods.

a. Generalized MCQDT Methods
(F. H. Mies, P. S. Julienne, and R. Dubs)

We have developed numerical methods for calculating a half collision matrix. These will prove useful in interpreting the dynamics of nonadiabatic processes in both photodissociation and full collision problems. This matrix, derived from the generalized multichannel quantum defect theory (MCQDT) of the close coupled wavefunction, is expected to have applications in developing a variety of approximations. We will make application to interpreting photodissociation experiments on K_2 and NaK.

We are also working with M. Raoult, University of Paris-Sud, to incorporate a generalized MCQDT analysis of closed channels into our close-coupled scattering codes. This allows a rigorous analysis of non-adiabatic effects and departures from the Born-Oppenheimer approximations in both predissociating and stable bound states of molecules.

b. Analysis of Molecular Predissociation
(P. S. Julienne)

In a collaboration with F. Rostas of the Observatory of Paris, we are studying predissociations and strong perturbations in the extreme ultraviolet spectrum of CO. These are due to a crossing of the $^1\Sigma^+$ states of the ns Rydberg series by the D $^1\Sigma^+$ valence state. We have constructed a model of this crossing to account for observed vibrational and rotational perturbations and predissociation widths.

The predissociation line shapes of the Schumann-Runge bands of O_2 have been and still are the object of numerous experimental studies. These line shapes are difficult to measure due to the complex triplet fine structure of these bands. In conjunction with L. Vahala of Old Dominion University close coupling and MCQDT models are being developed to interpret the role of triplet fine structure in the predissociation line shapes of the Schumann-Runge bands of O_2.

In a collaboration with H. Hotop, University of Kaiserslautern and S. Peyerimhoff, University of Bonn an ab initio model was constructed to account for the strong predissociations observed in the A $^1\Sigma^+$ state of HBr^+ in the photoelectron spectrum of HBr. The predissociation widths are comparable to the vibrational spacing, so a close coupling analysis is necessary. The model requires treating the coupling of the A state with 5 different predissociation channels through spin-orbit coupling.

c. Multiphoton Photodissociation of $H_2{}^+$
(F. H. Mies and A. Giusti*)

We have used our time-independent half collision codes to calculate the multiphoton photodissociation rate and product kinetic energy distribution of H_2^+ in an intense laser field of 10^{+13}watts/cm^2 or more. At these intensities our calculations predict above threshold dissociation (ATD), in which additional quanta of photon energy appear as evenly spaced peaks in the kinetic energy spectrum of the atomic fragments. These results are valid for laser pulse lengths that exceed the dissociation time.

d. Time Dependent Study of Molecular Photodissociation
(R. Heather and F. H. Mies)

A new project has been started to integrate the time-dependent Schroedinger equation for a photodissociating molecule subject to an intense short-time laser pulse. Excellent agreement has been obtained with the time-independent calculations in the long pulse limit. Preliminary results predict quite significant effects on the momentum distribution in the short-pulse limit which may be amendable to experimental confirmations.

2. Collisions of Ultracold Atoms

Ultracold ($T<1mK$) atom traps developed at NIST and elsewhere offer a number of new opportunities in atomic and molecular physics, including studies of fundamental physics, high precision spectroscopy, and improved time and frequency standards. It is important to understand collisions in such traps, since (1) collisions introduce heating processes which limit the density and lifetime of an atom trap and (2) ultracold collisions involve novel effects not normally encountered.

a. Threshold Behavior of Ultracold Collisions
(P. S. Julienne, F. Mies, and R. Dubs)

We have used generalized MCQDT to investigate the quantum threshold behavior of ultracold collisions. We have developed analytic and numerical treatments of various types of threshold behavior. The onset of threshold behavior depends strongly on the atomic mass and long range interaction potential. Ground state collisions in light traps will generally be in the quantum threshold regime which is not described semiclassically. We use the low temperature Penning ionization of two ^{3}S He atoms as an example of threshold behavior.

b. Spontaneous Emission in Ultracold Collisions
(P. S. Julienne)

We have studied the role of spontaneous emission in ultracold excited state collisions. This process has a dramatic effect on effective collision rates, and can not be treated by normal scattering theory. We have developed criteria for the onset of such effects as temperature is decreased from normal to ultracold. Experiments by W. Phillips' group at NIST and J. Weiner's group at the University of Maryland are investigating our predicted effects.

c. Ultracold Collisions in a Magnetic Field
(P. S. Julienne and F. H. Mies)

In a collaboration with C. Williams, Northwestern University we are developing numerical close coupling methods for treating collisions in a magnetic field, where Zeeman splittings of hyperfine sublevels can be large compared to kT. Initial applications will be to ground state H atoms, and we plan to develop codes for treating Na and Cs atoms.

B. Electronic Structure

1. Alkali Cluster Binding to Group III-V Semi-conductor Surfaces
(M. Krauss and W. J. Stevens (CARB))

The dominant binding interaction for quasi-linear clusters of Cs atoms to the (110) surface of GaAs is calculated to be van der Waals (VDW) like with only weak charge transfer from Cs to surface. Quasi-linear clusters of bound alkali atoms are calculated to have polarizabilities that increase non-linearly with the number of atoms in the cluster (see Fig. 2); since the VDW interaction is proportional to the polarizability, the binding per Cs atom increases with the length of the cluster.

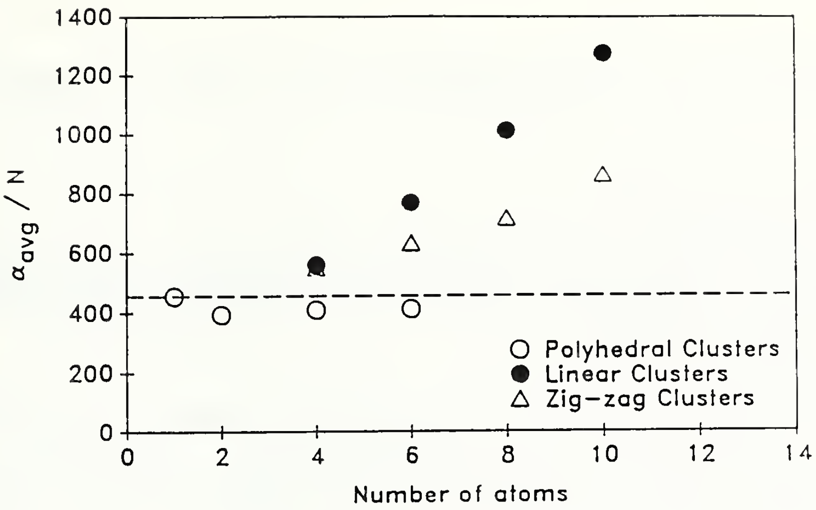

Figure 2. Computed polarizabilities of quasi-linear clusters of bound alkali atoms.

Hyperpolarizabilities of the alkali cluster are non-linear with the length of the cluster; non-linear optical transitions in the semiconductor can then be enhanced by the large alkali cluster hyperpolarizability or can induce such transitions in the alkali cluster.

Calculations planned for other alkali-semiconductor surfaces and ligand- and reaction fields will be used to simulate electronic surface field and dielectric effects.

2. Biochemical Applications
(M. Krauss, W. J. Stevens (CARB), D. Garmer (CARB), H. Basch*)

The spectroscopy and transition state behavior of the active site of the enzyme, carbonic anhydrase, is now being investigated as a function of the metal at the active site; environmental effects in the protein will be investigated with the reaction field code. The main effort in the coming year will be devoted to metalloenzyme studies now that a version of the reaction field code is completed. The need to study a variety of metals prompts us to complete construction of compact effective potentials (CEP) for elements from K to Rn.

Comparative electronic structure calculations of the P-O and V-O bonds suggest that the five-coordinate vanadate complex when bound to the active site of ribonuclease is <u>not</u> a transition state analogue because of the great disparity in the electronic structure and the binding of hydrogen to oxygen. Transition state analogue proposals in the literature will be examined to see if a study of the electronic structure would support the purely geometric considerations that are normally applied. Borate tetrahedral complexes will be considered for the protease enzymes.

Systematic studies of the vibrational frequencies of Mg, Ca, Cd, and Na cations bound to increasing numbers of water ligands show the relatively small effects on the geometry and frequencies as the number of ligands increases.

3. Spectroscopic Applications

Assignment of the electronic spectra of the PtA_4^+ (A = NH_3, PH_3) complex by ab initio calculation of the excitation energies compares well with experiment. This study shows that Co spectra in proteins may be examined for environmental effects.

Dipole moments, polarizabilities, and electronic structure were analyzed for the following systems: nucleic acid bases, heteronuclear rare gas diatomic molecules, hydrogen-bonded structures of H_2O and H_2S, HfO (data of interest to various experimental and theoretical projects in the Division and CARB).

Spectroscopic constants and energy curves were calculated to large distances for Cs_2 ground and excited states to illustrate accuracy obtainable with effective potential calculations for alkali molecules. This study evolved from the study of clusters on surfaces since the gas-phase properties are needed for comparison. The larger gas-phase clusters will be examined at low priority.

PUBLICATIONS

(a) Publications of Past Year

Beckerle, J. D., Casassa, M. P., Cavanagh, R. R., Heilweil, E. J., and Stephenson, J. C., "Time Resolved Studies of Vibrational Relaxation Dynamics of CO(v=1) on Metal Particle Surfaces," J. Chem. Phys. 90, 4619-4620 (1989).

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INVITED TALKS

Casassa, M. P., "Time and State Resolved Studies of the Overtone-Pumped Photodissociation of HN_3 ($\tilde{X}^1A'$)," 1989 Time-resolved Vibrational Spectroscopy Conference, Princeton, NJ, June 1989.

Casassa, M. P., "Time and State Resolved Studies of the Overtone-Pumped Photodissociation of HN_3 ($\tilde{X}^1A'$)," 1989 High Energy Density Materials Conference, New Orleans, LA, March 1989.

Fraser, G. T., "Vibrational Exchange upon Interconversion Tunneling in Homogenous Dimers," 198th International ACS Meeting, Miami, FL, September 1989.

Heilweil, E. J., "Population Relaxation of CO-stretching Vibrations for Carbon Monoxide on Metal Clusters," 174th Meeting of the Electrochemical Society, Symposium on "Photonics," Chicago, IL, October 1988.

Heilweil, E. J., "Picosecond Studies of Vibrational Energy Relaxation for Molecules in Solution and on Surfaces," Optical Sciences and Chemistry joint symposium, Naval Research Laboratory, Washington, D.C., November 1988.

Heilweil, E. J., "Picosecond Studies of CO(v=1) Vibrational Relaxation for Carbon Monoxide on Metal Clusters," NIST Staff Research Seminar, Research Adivsory Committee, NIST, February 1989.

Heilweil, E. J., "Picosecond Studies of CO(v=1) Vibrational Relaxation for Carbon Monoxide on Metal Clusters," Physical and Analytical Joint Seminar, University of Delaware, DE, April 1989.

Heilweil, E. J., "Picosecond Vibrational Energy Transfer Studies of Surface Absorbates," Overview Lecture, Time Resolved Vibrational Spectroscopy IV International Conference, Princeton, NJ, June 1989.

Heilweil, E. J., "Vibrational Energy Transfer Processes Studied by Ultrashort Pulsed Infrared Spectroscopy," 198th International ACS Meeting, Miami, FL, September 1989.

Hougen, J. T., "A Group Theoretical Approach to Certain Multi-Dimensional Tunneling Problems," Institute for Molecular Science, Okazaki, Japan, December 1988.

Hougen, J. T., "High-Resolution Gas-Phase Spectroscopic Studies of Tunneling Processes in Small Molecules," Rensselaer Polytechnic Institute, Chemistry Department Seminar, Troy, NY, December 1988.

Hougen, J. T., "Rotational Energy Levels and Line Intensities for Open-Shell Diatomic Molecules van der Waals Bonded to a Closed-shell Partner," All-Belgium High-Resolution Spectroscopy Mini-Meeting, Brussels, April 1989.

Jacox, M. E., "Vibrational and Electronic Spectra of Combustion Intermediates Trapped in Solid Argon," Department of Chemistry and Physics Seminar, Texas Christian University, Fort Worth, TX, October 1988.

Jacox, M. E., "Spectroscopy of Reaction Intermediates in Nitramine Decomposition and Combustion. Progress and Plans," ONR Workshop on Energetic Materials, Combustion Research Facility, Sandia National Laboratories, Livermore, CA, December 1988.

Jacox, M. E., "The Production and Spectroscopy of Molecular Ions Isolated in Solid Neon," U.S. Air Force Astronautics Laboratory, Edwards Air Force Base, CA, January 1989.

Jacox, M. E., "The Production and Spectroscopy of Small Polyatomic Molecular Ions Isolated in Solid Neon," Department of Chemistry, University of Arizona, Tucson, AZ, May 1989.

Jacox, M. E., "The Production and Spectroscopy of Small Polyatomic Molecular Ions Isolated in Solid Neon," Department of Chemistry, Arizona State University, Tempe, AZ, May 1989.

Julienne, P. S., "The Strange World of Ultracold Atomic Collisions," Physics Colloquium, University of Connecticut, Storr, CT, October 1988.

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Julienne, P. S., "The Strange World of Ultracold Atomic Collisions," Physics Colloquium, New York University, NY, November 1988.

Julienne, P. S., "Laser Modification of Ultracold Collision Processes," Conference on Quantum Electronics and Laser Science, Baltimore, MD, April 1989.

Julienne, P. S., "Theory of Ultrafast Atomic Collisions in Optical Traps," 15th International Conference on the Physics of Electron and Atomic Collisions, New York, NY, July 1989.

Julienne, P. S., "Collisions of Ultracold Trapped Atoms," 5th Interdisciplinary Laser Science Conference, Stanford University, Palo Alto, CA, August 1989.

King, D. S., "Dynamics of Highly Vibrationally Excited Molecules," XVIII Informal Photochemistry Meeting, Santa Monica, CA, January 1989.

Lovas, F. J., "Laboratory Microwave Studies of Refractory Materials: SiC_2, YO, LaO, ZrO, and HfO," Max-Plank-Institut für Radioastronomie, Bonn, Germany, September 1989.

Lovas, F. J., "Pulsed-beam Fourier Transform Microwave Spectroscopy - Studies of Weakly Bound Complexes," Eleventh Colloquium on High Resolution Molecular Spectroscopy, Giessen, Germany, September 1989.

Lovas, F. J., "Pulsed-beam Fourier Transform Microwave Spectroscopy at NIST," Institut für Physikalische Chemie, Universität Kiel, Kiel, Germany, September 1989.

Stephenson, J. C., "Laser Studies of Molecular Dynamics," Argonne National Laboratory, July 1989.

Stephenson, J. C., "State Specific Reaction Dynamics of Highly Vibrational Excited HN_3 (V,J,K)," Argonne National Laboratory, July 1989.

Stephenson, J. C., "Ultrafast Laser Studies of Vibrational Relaxation of Molecules on Surfaces," Gordon Conference on Molecular Energy Transfer, Boston, MA, July 1989.

Suenram, R. D., "Mechanistic Studies of the Ethylene Ozone Reaction," Virginia Polytechnic Institute, Department of Chemistry, Blacksburg, VA, October 1988.

Suenram, R. D., "Rotational Spectroscopy of Some Refractory Metal Oxides using Laser Vaporized Samples," Kansas State University, Department of Chemistry Seminar, Manhattan, KS, April 1989.

Suenram, R. D., "A Coupled Laser Vaporization Source-Pulsed Fabry Perot Cavity Microwave Spectrometer: Initial Tests," 198th International ACS Meeting, Miami, FL, September 1989.

MOLECULAR PHYSICS DIVISION SEMINARS

Angel, S., Department of Chemistry, University of Colorado, Boulder, CO, "Picosecond Absorption Spectroscopy of Intermolecular Electron Transfer in Solution," January 1989.

Dixit, S. N., Lawrence Livermore National Laboratory, Livermore, CA, "High Intensity Effects in Stimulated Rotational Raman Scattering," May 1989.

Dixon, R., University of Bristol, School of Chemistry, Bristol, England, "Dissociation Dynamics of NH_3 and H_2O_2," October 1988.

Dubs, R. L., Molecular Spectroscopy Division Seminar, NIST, "Circular Dichrosim in Photoelectron Angular Distributions: A New Probe of Alignment in Free and Adsorbed Molecules," January 1989.

Fawzy, W. M., Brookhaven National Laboratory, Upton, NY, "Electronic and Vibrational Spectroscopy of Open Shell Complexes," July 1989.

Glownia, J., IBM Research Division, T. J. Watson Research Center, Yorktown Heights, NY, "Femtosecond Flash Photolysis," December 1988.

Goovaerts, E., Physics Department, University of Antwerpen, Antwerpen, Belgium, "Intrinsic and Impurity Induced Dephasing of Raman-Active J=2 Rotons in Parahydrogen Crystals," August 1989.

Hansen, P. A., Department of Chemistry, University of Pennsylvania, Philadelphia, PA, "Picosecond Infrared Transient Absorption Spectroscopy," February 1989.

Heather, R., University of California at Santa Barbara, Santa Barbara, CA, "Time-dependent Theory of Photodissociation: Raman and Femtosecond Transition State Spectroscopy," December 1988.

Ho, C., Department of Chemistry, University of Pennsylvania, Philadelphia, PA, "Spectroscopy and Relaxation Dynamics of the Second Excited Singlet State of Aromatic Molecules in the Condensed Phase," January 1989.

Jones, D., University of Massachusetts at Amherst, Amherst, MA, "Theory of Associative Ionization and Laser-induced Excitation Transfer Collisions," December 1988.

Kasinski, J., Department of Chemistry, University of Rochester, Rochester, NY, "Ultrafast Dynamics of Fundamental Processes on Semiconductor Surfaces," January 1989.

Kimel'feld, Y., Institute for Spectroscopy, USSR Academy of Sciences, Troitzk, Moscow, USSR, "Molecular Interaction in Liquefied Rare Gases," December 1988.

Miller, J. C., Chemical Physics Section, Oak Ridge National Laboratory, Oak Ridge, TN, "Nanosecond and Picosecond Multiphoton Ionization of Weakly Bound Molecules," March 1989.

Mølmer, K., Ecole Normale Superieure, Paris, France, "Quantum and Semiclassical Motion of Ultracold Atoms in Laser Fields," August 1989.

Page, R., IBM Almaden Research Center, "Spectroscopy in a Sputtering Discharge: Dicopper LIF Spectra and Transition Metal IP's," May 1989.

Polyansky, O. L., USSR Academy of Sciences, Institute of Applied Physics, Gorky, USSR, "Application of One Dimensional Approximation of Effective Hamiltonian to Quasilinear Molecules and Complexes," June 1989.

Steimle, T., Arizona State University, Tempe, AZ, "High Resolution Optical Spectroscopy of Transition Metal Oxides," September 1989.

Zare, R. N., Chemistry Department, Stanford University, Stanford, CA, "The $H + D_2$ Reaction," November 1988.

Zygelman, B., Harvard, Smithsonian Center for Astrophysics, Cambridge, MA, "Radiative Emission Induced in Slow Atomic Collisions," November 1988.

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Hougen, J. T.

Member, Editorial Advisory Board, Journal of Molecular Spectroscopy.

Member, Decennial Review Committee, Journal of Chemical Physics.

Member of the subcommittee on Notations and Conventions for Molecular Spectroscopy for the "IUPAC" Commission on Molecular Structure and Spectroscopy.

Jacox, M. E.

President, NIST Chapter, Sigma Xi, 1988-1989.

Member, Editorial Board, Journal of Chemical Physics.

Member, Editorial Board, Research on Chemical Intermediates.

Lovas, F. J.

Member, International Astronomical Union Commision 14: Fundamental Spectroscopic Data.

Maki, A. G.

Member, Editorial Advisory Board, Journal of Molecular Spectroscopy.

Weber, A.

Editorial Advisory Board, Journal of Raman Spectroscopy.

Editorial Advisory Board, Journal of Physical and Chemical Reference Data.

Member, Program Committee, International Conference on Infrared and Fourier Transform Spectroscopy, Washington, 1989.

Member, International Advisory Committee, International Conference on Raman Spectroscopy, Calcutta, November 1988.

Member, Program Committee, QELS - Quantum Electronics and Laser Science Conference, Baltimore, MD, April 1989.

Member, National Organizing Committee, 12th International Conference on Raman Spectroscopy, to be held at the Univerity of South Carolina, August 1990.

Organizer and Session Chair, Lippincott Award Program, conducted at the FACSS Meeting in Chicago, IL, October 1989.

Chairman, 1990 Lippincott Award Committee (Optical Society of America, Coblentz Society, and Society for Applied Spectroscopy).

PROFESSIONAL INTERACTIONS, CONSULTING AND ADVISORY SERVICES

Casassa, M. P.

Collaborated with Dr. R. R. Cavanagh, Surface Science Division, on picosecond infrared laser studies of vibrational relaxation of adsorbed molecules.

Collaborated with Dr. W. L. Hase, Wayne State University, on classical trajectory calculations of NO dimer vibrational predissociation.

Consulted with Dr. D. L. Thompson, University of Oklahoma, on studies of the photodissociation of NO dimer and HN_3.

Fraser, G. T.

Collaborated with Dr. Wafaa Fawzy of Brookhaven National Laboratory, on NO-HF.

Collaborated with Dr. Welf Kreiner of Universität Ulm, on CO_2-laser sideband system.

Heilweil, E. J.

Collaborated with Dr. R. R. Cavanagh, Surface Science Division, on picosecond transient infrared measurements of vibrational dynamics in transition metal-carbonyl systems.

Collaborated with Dr. James Shirk, Naval Research Laboratory, on transient IR spectral hole-burning in low temperature hydrogen-bonded and SiOH systems.

Provided advice and technical expertise to Dr. Edgar S. Etz, NIST, to obtain FTIR spectra of solid dental compounds and phosphates.

Proposed study of high resolution IR spectroscopy of gaseous methanol with Drs. G. Fraser, W. Lafferty, and A. Pine, Molecular Spectroscopy Division, NIST.

Hougen, J. T.

Collaborated with Dr. W. Fawzy of Brookhaven National Laboratory and Drs. Fraser and Pine, Molecular Spectroscopy Division, NIST, on the spectrum of NO-HF.

Collaborated with Professor W. L. Meerts and Professor J. J.ter Meulen and students of Katholieke Universiteit Nijmegen, on the interpretationa of the spectra of symmetrial triazine.

Consulted with L. Yeh from Professor Y. T. Lee's group at the University of California at Berkeley, on the spectra of $H_5O_2^+$.

Jacox, M. E.

Collaborated with Dr. W. E. Thompson of the National Science Foundation, was a full-time guest researcher during the calendar year 1988 and has continued as a part-time guest researcher during 1989.

Collaborated with Dr. W. R. M. Graham, Department of Physics, Texas Christian University, Fort Worth, TX, on the spectrum of HC_3.

Collaborated with Dr. R. J. Glinski, Department of Chemistry, Tennessee Technological University, Cookeville, TN, on the spectrum of SF_2.

Collaborated with Dr. L. J. Stief, NASA Goddard Space Flight Center, Greenbelt, MD, on the photolysis of $H_2O{\bullet\bullet}O_3$.

Collaborated with Dr. K. C. Janda, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, on relaxation behavior of Cl_2 and ClF in rare-gas matrices.

Julienne, P. S.

Collaborated with Dr. L. Vahala, Old Dominion University, Norfold, VA, on photodissociation line shapes.

Collaborated with Dr. W. Phillips, NIST, on interpretation of ultracold atomic collisions.

Collaborated with Dr. F. Rostas, Observatory of Paris, on interpretation of strong perturbations in the Ryberg spectra of CO.

Collaborated with Dr. J. Weiner, University of Maryland, on theory of collisions of supercold atoms.

Collaborated with group of Dr. C. Cohen-Tannoudji, Ecole Normale Superieure, Paris, France, on Penning ionization of metastable helium atoms in light traps.

Consulted with Dr. K. Burnett, Oxford University, England, on the development of time dependent collision theory of ultracold collisions.

Consulted with Dr. P. Kleiber, University of Iowa, on interpreting atomic alignment following molecular photodissociation.

Collaborated with Dr. H. Hotop, University of Kaiserslautern, West Germany, and Dr. S. Peyerimhoff, University of Bonn, West Germany, on interpreting strong predissociations observed in photoelectron spectra of HBr^+.

King, D. S.

Collaborated with Dr. R. Bodanness, NIH, potential applications of photophysics, photochemistry, and non-linear optics in medical research.

Collaborated with Drs. Buntin, Cavanagh, Gadzuk, and Richter, NIST, on experimental and theoretical aspects of molecule-surface dynamics.

Consulted with Drs. M. Alexander, University of Maryland and P. Dagdigian, Johns Hopkins University, on experimental and theoretical aspects of molecular dynamics with particular emphasis on azide chemistry.

Consulted with Dr. D. Heller, Light Age, Inc., on the use of alexandrite for amplification of single frequency cw lasers.

Krauss, M.

Collaborated with Dr. K. J. Miller, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, NY, on reaction field analysis of binding in DNA.

Collaborated with Dr. H. Basch, Bar Ilan University, Israel, on molecular orbital calculations of biomolecules.

Collaborated with Dr. B. Gullott, University Pierre et Marie Currie, Paris, on calculations of the dipole moment functions of multimers of rare gas atoms.

Collaborated with Drs. L. Chassot, S. Lippard, Department of Chemistry, MIT, on potential functions for Pt binding.

Lovas, F. J.

Collaborates with Dr. P. R. Jewell, National Radio Astronomy Observatory and Dr. J. M. Hollis, NASA/Goddard Space Flight Center, on interstellar molecular searches.

Collaborates with Dr. K. Peterson, University of Rhode Island, on trimer complexes containing CO_2 and H_2O.

Collaborates with Drs. C. W. Gillies and J. Z. Gillies, Rensselaer Polytechnic Institute, Troy, NY, on microwave spectral studies of ozone complexes.

Collaborates with Drs. S. E. Novick and T. Blake, Wesleyan University, Middletown, CT, on structures of weakly bound complexes of CO_2 and H_2CO.

Collaborates with Drs. J. Rice, Naval Research Laboratory, Dr. S. Kukolich, University of Arizona, and W. Stahl, University of Kiel, Germany, on the rotational and structural study of CO_2-H_2S.

Collaborates with Dr. K. Matsumura, Seinan Gakuin University, Tokyo, Japan, on rotational and structural studies of complexes containing H_2O and SO_2.

Pine, A. S.

Collaborated with Dr. W. M. Fawzy of Brookhaven National Laboratory, Upon, Long Island, NY, on the anslysis of the open shell complex NO-HF.

Stephenson, J. S.

Collaborated with Professor Millard Alexander, University of Maryland, College Park, MD, on dissociation of HN_3.

Collaborated with Professor Paul Dagdigian, John Hopkins, Baltimore, MD, on dissociation of HN_3.

Suenram, R. D.

Collaborated with Professor K. I. Peterson, University of Rhode Island, on the microwave investigations of $(CO_2)_2$-H_2O and $(H_2O)_2$-CO_2 trimer species.

Collaborated with Professor S. E. Novick, Wesyleyn University, on spectroscopic studies of several van der Waals complexes.

Collaborated with Professors W. Klemperer, D. Yaron and D. Zolandz, Harvard University, and Dr. K. I. Peterson, University of Rhode Island, on the microwave investigation of the water-carbon monoxide van der Waals complex.

Collaborated with Dr. K. Matsumura of Seinan Gakuin University, Tokyo, Japan, on rotational and structural studies of complexes containing H_2O and SO_2.

Consulted with Professor M. D. Harmony, University of Kansas, concerning new microwave technology.

Consulted with Professor T. Stimele, Arizona State University, concerning new microwave technology.

Consulted with Professor R. L. Kuczkowski and Dr. C. Hillig, University of Michigan, concerning microwave improvements of their FT spectrometer.

Weber, A.

Collaborated with Dr. K. Narahari Rao, Ohio State University, Columbus, OH, on discussions of the organization of the 1987 and 1988 Columbus Symposia.

Collaborated with Drs. W. C. Harris, National Science Foundation and I. W. Levin, National Institutes of Health, on the planning for the 7th International Conference on Fourier Transform Spectroscopy, held in Washington 1989.

Collaborated with Drs. R. D'Cunha and V. B. Kartha, Bhabha Atomic Research Center, Bombay, India, on the IR spectrum of CH_2F_2.

Collaborated with Dr. V. B. Kartha, Bhabha Atomic Research Center, Bombay, India, on the IR spectra of CD_3CCH and CH_3CCD.

QUANTUM METROLOGY DIVISION

FISCAL YEAR 1989 TECHNICAL ACTIVITIES

Overview

Our programs evolve by a mixture of necessity, opportunity, chance, and choice. Where choice is an option we look to scientific issues for which improved measurement technology is needed. When this works, we gain on both levels and, assuming improved measurement technology to be of institutional interest, the institution gains as well. An overview of our current work shows a disciplinary and geographic spread which would appear to belie the suggested unifying paradigm. In point of fact there are connections not only on the technology level but also on the scientific side in several instances.

This year's report focusses on:

1. X-Ray Physics with Synchrotron Radiation
2. Neutron Physics
3. Precision X-Ray and γ-Ray Measurement
4. Miscellaneous activities.

It concludes with a brief indication of future trends.

As will be seen below, each of these areas has enjoyed reasonable progress, frustrations in appropriate measure and, in several instances, unanticipated opportunities for future work which appear exciting.

The Division's work is somewhat de-localized with activities presently at several sites overseas and in the U.S. In addition, there is a small but significant extra-terrestrial component due for 1991 launch aboard a Japanese satellite, the Solar-A Mission. In Europe we have a permanent out-station for γ-ray work at the High Flux Reactor of the Institute Laue-Langevin (ILL) in Grenoble. Until this September, the preliminary neutron lifetime exercise (joint with the University of Sussex) was also at the ILL along with an experiment (jointly with Argonne) to measure the neutron capture cross-section for ^{3}He. In West Germany, we have continued experiments at the heavy ion facility of the Gesselschaft für Schwerionenforshung (GSI) in Darmstadt. In the future we expect to play a major role in the spectroscopy program of the Experimental Storage Ring (ESR) at the GSI. In the planning stage is an experiment on anti-protonic light atoms at the Low Energy Anti-Proton Ring (LEAR) at CERN in Geneva. In the U.S., we have a permanent installation at the National Synchrotron Light Source (NSLS) in Brookhaven and the beginnings of a small effort on decelerated beams using the super-conducting linear accelerator, ATLAS, at Argonne (recent progress has rendered the acronym incorrect but the name will probably stick). None of this geographic diversity was undertaken for its own sake, rather, in each case there is a needed capability, either unavailable anywhere else in the world (e.g., ILL, GSI), or, in some cases most conveniently available at the site we have chosen (e.g., Brookhaven is the closest high performance x-ray ring). From the point of view of what is needed to do those experiments we find crucial or of maximum interest, these remote activities seem inevitable. Nonetheless they are costly and have been sustained in the face of steadily diminishing resources by dismantling in-house programs. The resulting empty-house condition cannot be maintained in the long term since all external activities evolved from internal ones and were sustained by them. Re-establishing a viable group of in-house programs has become a matter of high priority but it is evidently one for which we need to seek sources of outside support. Such support, if it can be found, will have its own demands which, as always, entails a risk of further de-stabilization.

1. X-Ray Physics with Synchrotron Radiation

The beginning of Fiscal Year 1989 closely coincided with the resumption of regular operation of the x-ray ring at the National Synchrotron Light Source following a 19 month dark period. Early in the year we were able to solve a long-standing problem that had plagued the previous operations at the Quantum Metrology Division's beamline, X-24A. The problem involved an aperture within the ring itself and required a relocation of one of the storage ring magnets. This step was taken with the direct cooperation of the NSLS Director, Dr. Michael Knotek. All observations over a year of operations indicate that the change was entirely successful in eliminating the trouble.

Although the group does not have a sophisticated experimental target chamber for conducting experiments, we have successfully produced results in a variety of fields. A great deal of mileage has been made simply by reconfiguring our rather austere experimental chamber by disassembling and reassembling various small components "tinkertoy" style to permit studies in entirely new fields. In this manner experiments have been conducted on polarization of x-ray scattering and fluorescence, resonant anisotropy of x-ray emission, x-ray standing wave studies of epitaxial films, resonant magnetic x-ray scattering and soft x-ray absorption spectroscopy.

The most active area of research concerned studies of aligned molecules. This work was selected for Competence support from the Director. We demonstrated previously that an ensemble of excited molecules is aligned by resonant excitation with polarized x-rays. Our recent studies of this effect have uncovered unexpectedly strong polarization and branching ratio changes in molecular x-ray emission due to core-to-core transitions on resonance. We have also measured a pronounced anisotropy in the emission of x-ray fluorescence from these aligned molecules which can be described in terms of the classical dipole radiative field pattern. In addition we have made detailed measurements of the resonant depolarization of elastic x-ray scattering from both atomic and molecular gases. This effect affords the opportunity to compare the atomic case, resonant elastic scattering from argon where the alignment of the initially spherical atom is entirely due to the incident polarization, to the molecular case where both the polarization and the molecular bond direction must be taken into account.

Our experience in resonant studies of fluorescence and scattering as well as in polarization analysis have led to a preliminary study of resonant magnetic x-ray scattering. Initial results from other research groups have been reported for resonant magnetic x-ray scattering at high photon energies (>3keV), but the effect is expected to be even stronger at resonances in the soft x-ray region. This energy region (<1 keV) is where the L-resonances of the important first row transition metal elements (Cr, Fe, Co, Ni etc.) are to be found. Our beamline is uniquely well suited to studies of this effect in this spectral region. The range of potential applications of this new effect is especially exciting.

Another area of ground breaking research is back-reflection x-ray standing wave studies of surface and interface structure. The back-reflection geometry has a number of significant advantages for x-ray standing wave measurements. The principal requirement of the technique is the availability of a tuneable, high energy resolution beam of incident x-rays. Again, the unique characteristics of the X-24A beamline make it the ideal facility for such studies. In FY-1989 we successfully completed a series of measurements on epitaxial layers grown on GaAs substrates.

In addition to the scientific results obtained from the above studies, we have extended the performance of our beamline by improving the focussing optics, commissioning various new diffraction elements for the monochromator and installing a variety of new detectors. In some cases this improvement in performance has involved an advance of the state-of-the-art synchrotron radiation beamline technology.

Finally, there has been progress of some significance in the development of our calculational capabilities for x-ray diffraction effects. This work has had many benefits. At the mundane, but practical, level new software permits predictions of the diffraction characteristics of arbitrary crystals at arbitrary photon energies. This software quickly found numerous applications within the Division for both synchrotron and non-synchrotron based x-ray experiments. At the more sophisticated level, the dynamical theory of x-ray diffraction has been extended to the point of applicability to a number of exotic geometries using the extended Ewald-Laue formalism and to studies of dynamical effects in imperfect crystals using the Takagi-Taupin approach. The first application of the extended Ewald-Laue theory was a study of self-filtering crystals which has already been published. The new solution to the Takagi-Taupin equation has permitted the theoretical exploration of the applicability of back-reflection x-ray standing wave technique to imperfect crystal samples.

The group underwent some expansion in FY-1989 with the addition of Dr. Steven Southworth and Dr. Rulon Mayer to the staff. In addition to this increase in manpower, much of the above work was accomplished with the aid of the many useful collaborations that the synchrotron radiation group has established. The list of institutions with which we are actively collaborating includes: the Stanford Synchrotron Radiation Laboratory, AT&T Bell Labs, Lawrence Berkeley Laboratory, the Naval Research Laboratory, the Applied Physics Department of the University of Michigan and the Tokyo Institute of Technology.

2. Neutron Physics

The last year has seen considerable progress in the overall NIST neutron program. Construction of the new Cold Neutron Research Facility (CNRF) guide hall was completed in early 1989 and the building was dedicated in the spring. The first set of neutron guides was installed in August-November 1989. Routine operation is expected in early 1990. The neutron physics group of the (QMD) has principal responsibility for two of the initial eight experimental stations. One of these stations is a full flux end position which will be primarily devoted to weak interaction physics and tests of fundamental symmetries. The other position is a monochromatic beam which will be used for neutron interferometry and for the development of advanced neutron optics. The efforts of the neutron physics group have been directed toward establishing of these stations as well as continuing an ongoing research program in neutron physics.

A major accomplishment of the last year was the completion of the initial data collection for our experiment to measure the free neutron β-decay lifetime. This experiment is a collaboration between NIST, the University of Sussex (U.K.), and the Central Bureau for Nuclear Measurements (Belgium). Within NIST this work includes personnel from the QMD's Neutron Physics Group as well as from the Center for Radiation Research (CRR) and the Center for Analytical Chemistry. This work enjoys external support from DOE, NATO, and the Science and Engineering Research Council (U.K.). The initial phase of data collection was carried out at the High Flux Reactor of the Institut Laue Langevin in Grenoble. Data from these runs are currently being analyzed. We will publish results in early 1990. The experimental apparatus has been shipped back to NIST where it is currently being reassembled on the full flux end position. It will serve as one of the initial experiments to be carried out at the guide hall.

Another fundamental neutron physics experiment was completed at ILL during this last year. This was an experiment, initiated jointly by the Neutron Physics Group and Argonne National Laboratory, to measure the radiative capture cross section for neutrons on ^{3}He. This cross section is of considerable importance in the estimation of the production rate of certain neutrinos in the solar interior. Our result has resolved an outstanding experimental discrepancy between previous determinations.

The neutron physics group is also engaged in a program to develop new methods for the absolute determination of cold and thermal neutron fluxes. This project has implications for improved absolute standards for neutron dosimetry, for the calibration of nuclear targets, and for standards in neutron depth profiling. Improved methods of neutron flux determination will also be of great significance in achieving further reduction in the uncertainty on the determination of the neutron lifetime.

Two new methods for absolute neutron flux determination were tested this year. The first was based on a calorimetric approach first suggested by collaborators at Los Alamos. The promising initial tests have led us to continue this effort with support and personnel from LANL and Harvard University. The second method is based on an α-γ coincidence method developed at NIST. This work will continue as a collaboration between QMD and CRR. We anticipate further testing of both of these approaches at the CNRF.

Extensive design work has been carried out on the monochromatic position intended for neutron interferometry. A design for the initial stage of vibration isolation has been completed and fabrication/procurement is in progress.

In the past year, we provided partial sponsorship for an International Workshop in Fundamental Neutron Physics which was held in Grenoble in March 1989.

3. Precision X-Ray and γ-Ray Measurement

Overall this program aims at a unification of the electromagnetic spectrum from the visible, near 2 eV to the γ-ray region near 4 MeV. The several motivations for the overall program include determination of fundamental constants, masses of elementary particles, tests of basic electrodynamic theory, tests of many-electron relativistic calculations, and, most recently, parameterization of strong interactions between anti-protons and the lightest nuclei. Among targeted outputs are: a new semi-empirical tabulation of the principal x-ray emissions of all stable elements, the Avogadro constant, new classes of secondary standards in the x-ray region, new values for γ-ray reference wavelengths, and a "new" fundamental constant, $N_A h/c$.

Our general procedures involve three steps: first we made an optical measurement of the lattice period of a highly perfect silicon sample, the XROI experiment; second, this calibration is distributed by a sensitive form of differential diffraction to other specimens, largely silicon and germanium using the delta-d machine. The third step involves one of several alternative angle measuring engines where Bragg-Laue relations are used to extract wavelength values from accurate (absolute) angle measurement. Two such engines are currently active. One is at the NIST facility in the Institut Laue Langevin where its main focus is in the domain of γ-ray energies above 1 MeV. The second is a vacuum two-crystal spectrometer at the Gaithersburg site whose main measurements are in the 1 to 10 keV domain. The gamma ray machine, GAMS-4, has had good successes in areas away from the main line but has encountered formidable difficulties at the highest energies and highest targeted accuracies as will be described below. The vacuum instrument, VTXI, has been for the latter part of this year engaged in an active and critical re-calibration needed for planned measurements of L-series spectra in the mid-Z domain.

In the following paragraphs, we attempt to give a flavor of the current situation in these areas beginning with the XROI experiment on which the remaining steps obviously depend. Closely associated with XROI is the lattice transfer procedure carried out on the delta-d machine. While the XROI experiment has a long and somewhat troubled history, delta-d is rather more recent and has an attractive robustness of the sort expected in well-configured differential measurement.

a) Optical measurement of a Si lattice period- the XROI experiment

Bridging the six orders of magnitude from the visible region ≤ 2 eV, to the γ-ray region--needed, for example, to determine the composite fundamental constant, $N_A h/c$,--seems to require at least one intermediate reference. Historically, there have often been many such "stepping stones" in the form of UV, soft x-ray and harder x-ray reference lines. Thus, the robustness of the optical to γ-ray connection was degraded by the multiplicity of measurements and limited additionally by the line-widths of available markers, especially in the x-ray region. In comparison with x-ray lines, certain synthetic crystals, especially silicon, have lattice periods that are much more sharply defined. Furthermore, the degrading effect of step multiplicity is largely evaded, provided one determines the lattice period directly in optical terms and uses the thus calibrated crystal for absolute diffraction spectroscopy.

Focussing on the first step only, we note that efforts were launched in several laboratories about 20 years ago, and in intervening years some programs have ceased and perhaps three new ones begun. Of these, two have produced serious results, which unfortunately (or ultimately fortunately) these were in conspicuous disagreement, at least initially. In the mid-seventies, we reported a value for the 220 repeat distance of a vacuum float-zoned specimen of Si with a claimed accuracy of 0.3 ppm. Subsequently, in about 1980 our colleagues at the Physikallsch-Technische Bundesanstalt (PTB) in Braunschweig reported a value for an, in principle, similar sample with a slightly improved level of claimed accuracy but differing from the NIST result by 1.8 ppm. In early 1986, a re-built NIST experiment fitted with several on-line diagnostics showed the origin of the discrepancy to be a relatively subtle error in interpreting available signals in the previous NIST experiment. Subsequent work has aimed to go beyond this simple resolution-of-conflict stage to achieve a definitive result at a level of accuracy consistent with the short-term reproducibility and statistical limitations, namely at a level near 0.03 ppm.

While this goal has proven unexpectedly difficult to achieve there are nonetheless indications of progress on several fronts. On the hardware side, improvements in trajectory interferometry, decoding and normalization have led to short-term reproducibility near 0.01 ppm. In spite of these elements of progress, there remain as yet unexplained patterns of residuals in plots of x-ray phase vs. optical order number whose amplitudes are large ($\approx 3\sigma$) and reproducible. At the same time, month-to-month changes are significantly larger than statistics would suggest.

Progress toward clarification and resolution of this situation has been aided significantly by the work of an external contractor with a strong background in programming, computational mathematics and statistics. Such progress has, at the same time, been limited by the fact that only one person actively engages the experimental situation with his effectiveness being limited by the need to provide administrative and technical support to the remainder of the Division. Nonetheless progress continues. We have clearly moved from a condition of an un-understood 1.8 ppm discrepancy with an estimated uncertainty of 0.3 ppm to a condition of concordance with difficulties of the order of 0.1 ppm and ultimate incertitude near 0.03 ppm.

b) Lattice intercomparisons - the delta-d experiment

The measurement of the lattice spacing of a Si crystal in terms of an optical wavelength is a formidable exercise that should not have to be repeated for every crystal used for x-ray and γ-ray wavelength measurements. One may instead measure differences between the lattice spacing of the absolutely measured crystal and other crystals used for diffraction. Lattice spacing differences are measured with an x-ray two-crystal diffractometer used in the non-dispersive mode so as to be insensitive to the wavelength spread in the x-rays. The unique features of the diffractometer are: two x-ray sources, a long (5 cm) first crystal on a precision axis equipped with an angle interferometer, a slide that automatically places crystals of known and unknown lattice spacings in the second crystal position, and two detectors. The crystals are of equal thickness (within a few microns) which causes the profiles to have reproducible fine structure with a ratio of profile width to fine structure width of ≈50. The presence of the narrow fine structure makes the measurements of the angular positions of the profiles significantly more precise.

This year we prepared a family of crystals having a thickness of 0.455 mm. (The transmitted intensity has a maximum at this thickness.) Extensive measurements of lattice spacing differences were recorded and analyzed between 1) the NIST XROI crystal, 2) a crystal sample provided by the PTB and traceable to the crystal used in the 1982 PTB absolute lattice spacing measurement, and 3) two crystals cut from a boule purchased from Supplier A. The measurements included diagnostics intended to reveal systematic measurement problems. Ag and Mo x-ray radiations were used. The first long crystal was rotated by 180 degrees. The second crystals were rotated by 180 degrees. Measurements were recorded at different positions of the second crystals. The results appear to be consistent at the 1-2 $\times 10^{-8}$ level except for one of the Supplier A crystals which shows a variation of 7×10^{-8} when the first long crystal is rotated. This variation may be due to strain introduced during cutting and polishing or to an imperfection in the crystal sample such as curved planes.

The delta-d spectrometer has recently been moved to a more stable temperature environment. During the move the spectrometer was disassembled and carefully realigned during reassembly. The first results after reassembly agree within 1×10^{-8} with the previous extensive measurements.

The lattice spacing measurements appear to be free of significant systematics associated with the mechanical and optical alignment of the spectrometer. The next series of measurements will be the comparison of the NIST XROI interferometer crystal with samples of crystals used for γ-ray diffraction at ILL. Preparation of the appropriate samples is proceeding.

c) <u>γ-ray measurements</u>

Gamma-ray measurements are made at the Institut Laue-Langevin (ILL) using a NIST precision two crystal spectrometer. Gamma-rays are diffracted by crystals whose lattice spacings have been measured on an absolute length scale and the diffraction angles are measured on an absolute angle scale. The absolute length scale for the lattice spacings is realized by comparing the crystals used for γ-ray diffraction to the NIST x-ray/optical interferometer crystal using the delta-d spectrometer. The absolute angle scale is realized by using polarization sensitive Michelson angle interferometers which are calibrated using an optical polygon. The measurements are performed at the ILL because of the unique source handling capability of this facility and the high neutron flux (5×10^{14} n/cm^2 sec).

The goals of the NIST measurement program at the ILL are:

1). Absolute wavelength measurements of intense γ-ray lines for energies up to ~5 MeV. These lines serve as standard wavelengths for curved crystal, Ge detector, and exotic x-ray measurements.
2). Measurement of the deuteron binding energy which can be combined with mass measurements to obtain a value for the neutron mass.
3). Measurement of $N_A h/c$. This combination of constants follows from measuring an energy interval in both atomic mass units and wavelengths.

During runs in 1988 we detected a 1 ppm irreproducibility in our measurements for energies in the 1 to 2 MeV range. We have extensively investigated this irreproducibility using γ-rays from the reaction $^{48}Ti(n,\gamma)\,^{49}Ti$. Some hardware changes were made including an improved thermal shield, reduction of heat loads near the spectrometer, improved servo-loops, and a different stabilized laser. The angle interferometers were carefully realigned and the frequency stability of the laser was verified. The spectrometer software was modified to permit more versatile profile scanning and to monitor crystal rotation angles using PZT voltages, autocollimator readings, and whole fringe counts in addition to the usual rotating polarizer technique. All of the methods of reading the angles are consistent, but the angular positions of γ-ray profiles are scan direction dependent, time dependent, and vary in a periodic fashion with respect to the Michelson interferometer fringe cycle. The angle interferometer on the delta-d comparator is being modified to duplicate the ILL angle interferometers so that angle interferometer diagnostics can be done at NIST. Both x-ray diffraction and a sensitive autocollimator will be available to test the angle interferometer.

One of the possible routes to $N_A h/c$ involves the measurement of the ^{15}N binding energy (10.8 MeV) available in the reaction $^{14}N(n,\gamma)$ ^{15}N. This energy interval can be obtained by measuring several γ-rays of 4-6 MeV whose sum equals 10.8 MeV in three different combinations. We attempted to measure these lines using pressure densified Si_3N_4 sources, but because of low intensity were unable to record any of the N lines. However we did record ^{29}Si lines at 3.54 and 4.93 MeV. An increase in the N content of the source is needed.

In addition to the NIST precision wavelength measurement program, the double flat crystal spectrometer has been used extensively for crystal structure factor measurements and for nuclear lifetime measurements. Whereas the precision wavelength measurements require high angular precision, these measurements require detailed profile information.

The structure factor collaboration includes NIST, ILL, the European Synchrotron Radiation Facility, and Instituto di Struttura della Materia, Roma. Using Ge crystals we have studied the energy dependence of the crystal structure factor. Profiles were recorded at 341 keV in the orders 220, 440, 660, and 10 10 0 and at 1381 keV in the orders 220 and 440. Structure factors accurate to ~0.1% were derived from the data. Accurate high energy structure factor measurements are of interest to solid state theorists because of higher order QED contributions.

The nuclear lifetime collaboration includes Physikalisches Institut, Universität Göttingen, ILL, and NIST. When a nucleus in an excited state emits a high energy γ-ray (1-5 MeV), the nucleus recoils. If a secondary γ-ray is emitted before the recoiling nucleus comes to rest, the secondary γ-ray is Doppler broadened with the amount of broadening being a measure of the lifetime of the initial state of the secondary γ-ray. Nuclear lifetimes in the range 10^{-12} to 10^{-16} seconds can be measured with this technique. Conversely, for known lifetimes the slowing down and stopping of the recoiling nucleus can be studied. The high resolution of the flat crystal spectrometer is essential for measurement of these broadened profiles.

The interest in the NIST-ILL flat crystal spectrometer remains high. During the past year approximately 75% of all nuclear spectroscopy beamtime at the ILL involved the use of the NIST flat crystal spectrometer.

d) Inner shell transition energies

The remaining in-house x-ray program focusses on transition energies with two main aims: First, almost all examples of exotic atom spectroscopy (see section 4) require nearby secondary standards. We require in this regard a large angle absolute angle measuring engine that must, among other requirements, cover the long wavelength or "vacuum" region. Second, there is persistent need for an updated tabulation of x-ray transition energies for the principal lines of all stable elements. As will be discussed in the second paragraph below, this leads naturally to requirements for certain critical measurements (beyond those already at hand) and a comprehensive theoretical effort as discussed in the third paragraph. Our main efforts have focussed on these areas principally through the work of a new staff member, Dr. T. Mooney and a long-term visiting scientist, Dr. P. Indelicato.

Immediate goals for the vacuum two crystal spectrometer include: new measurements of the xenon L-series in response to recent calculations of level shifts and broadening due to coupling of inner vacancy levels to Auger-decay continua; measurement of certain mid-Z L lines needed for clarification of apparent mis-identifications and for determination of 1s-3s and 1s-2s intervals; accurate measurement of Si $K\alpha_{1,2}$ to serve as reference markers for the Balmer series of anti-protonic helium (see section 4).

In support of these goals, Dr. Mooney undertook an overall renewal of all control software together with a comprehensive investigation of calibration procedures and a first principles re-calibration of the main encoder. He showed that the largest calibration error was periodic with an angular frequency that rendered it invisible to our customary procedures. He also showed that calibration does not survive routine maintenance (roughly semi-annual). He has therefore concentrated on developing of instrumentation, software and procedures suitable for more frequent applications perhaps in a fully automated mode. Already, Mooney has shown the effectiveness of combining a rotating optical wedge with a null-pointing autocollimator for revealing local encoder error. He has also proposed a new form of electronic autocollimator with greater precision, range, and speed. Up to now he has improved the calibration by a factor of six relative to the previously hidden errors. His present calibrations have an absolute accuracy of ±0.5 arcsec, and he sees the possibility of an additional factor of three should this be needed.

The other area of in-house x-ray work concerns the Z-dependent systematics of differences between theoretical and experimental estimates of x-ray transition energies. For sufficiently good experiments and a suitably comprehensive theoretical framework, these differences should vary slowly with atomic number, Z, and be generally understandable. In previous work, we established a sparse set of high accuracy experimental data as an initial basis. Now, through the theoretical efforts of a visitor, Dr. Paul Indelicato (Univ. Pierre et Marie Curie, Paris) we are beginning to have at hand a sufficiently robust theoretical framework. Indelicato has, in addition to other work described in Section 4 below, extended the multi-configuration Dirac-Fock (MCDF) methods of Desclaux and addressed many of its limitations. He has particularly addressed the effects of screening and finite nuclear size on the radiative corrections to the energy levels. That omission of either of these subtleties produces noticeable discord shows that considerable progress has occurred in the past few years.

These two threads taken together appear to offer an opportunity to address a practical problem of fairly broad consequences. Tabulations of x-ray transition energies (or wavelengths) are widely used in several areas that are principally but not exclusively analytical. All existing tabulations are (with trivial internal exceptions) entirely empirical. They are known to contain significant error and have noticeable lacunae even for Z<100. It is inconceivable that support could be gained for a subsequent exercise in empiricism even should there be workers so inclined. While purely theoretical estimations can clearly be generated, it is doubtful that they would be successful in the marketplace. We have therefore been led to propose a semi-empirical, all-Z tabulation which should be entirely adequate for analytical and general uses. Of course, when a marker is needed for a state-of-the-art experiment, a direct measure of that marker is unavoidable if ultimate precision is at issue. For broader purposes as requested, for example, for inclusion in the International Tables for Crystallography, and as a more adequate data base for x-ray fluorescence analysis, the semi-empirical tabulation would appear both useful and feasible. A proposal in this direction is presently under consideration by the National Standard Reference Data System (NSRDS) program at NIST.

4. Miscellaneous Activities

In this section, we gather short descriptions of a few activities not easily connected with the broader categories above and then turn to some future issues and opportunities.

a) Space-based stuff

Beginning with the satellite P78-1 and the Solar Maximum Mission, we have had a continuing involvement with spectroscopic instrumentation for orbiting platforms aimed particularly at the Sun. Following the partial failure of "Solarmax", its "on-site" repair and imminent demise, coupled with the destruction of P78-1 in an SDI target shoot, and with no other missions in the pipeline, the solar physics community has faced a sparse set of opportunities. One of these, occasioned in part by serious illness of the leading Japanese x-ray scientist, has arisen on the Japanese Solar-A mission. In a renewed collaboration with many of the P78-1 and Solarmax people, we have joined an effort aimed at improved instrumentation for studies of H-like and He-like sulfur, calcium and iron. Japanese booster capacity, telemetry bandwidth and tracking station distribution combine to return this exercise to the era before that of the multi-ton orbiters. Our contribution has been to spectrometer design, crystal choice and especially crystal fabrication and characterization. This exercise is now complete largely due to the efforts of Dr. A. Henins.

b) Theory for one- and two-electron ions

Indelicato completed a MCDF calculation of the effect of the hyperfine interaction on the lifetime of the 1s2p $^3P_0$ level in heavy helium-like ions. In this work it was shown that a measurement of this lifetime can yield precise values for the 1s2p $^3P_0$ - 1s2p $^3P_1$ fine structure separation, the value of which is dominated by contributions of the magnetic interaction at high Z (Indelicato et al., Phys. Rev. A Oct 89). An experiment has already been done in silver showing the interest of the method and giving results in good agreement with our MCDF calculation. (Marrus et al., Phys. Rev. Lett. 1989). A new project has been started, with Peter Mohr, to derive the screening correction to the self-energy from

QED. This is a major task, and some good progress has been made. Preliminary results for some of the contribution to this effect have already been obtained. The self-energy screening correction is presently the most uncertain term in atomic calculations involving inner shells.

c) Experiments on one- and two-electron ions

Some progress occurred at Argonne on two-electron calcium while a new measurement in one-electron nickel was carried out at the GSI. In both cases, our accel-strip-decel capture routine permitted high accuracy measurement of highly charged ion spectra at the cost of significant accelerator acrobatics and much beam loss. This coupling of gain and loss will continue until we enter the era of heavy ion cooler rings (see below). Most of the time at Argonne was devoted to beam development, ion source improvement and, ultimately, elimination of the Tandem van der Graaff injector in favor of linac sections optimized for low speed particles.

In the case of one-electron spectra, we had beam time for a measurement of the Lyα (2p-1s) transition in hydrogen-like Ni. As required (in our view) for any high accuracy measurement of, say, the 1s Lamb shift, the experiment was carried out using decelerated beams. The two-dimensional x-ray detector that we have developed performed satisfactorily. The x-ray spectrometer behaved as expected from Monte-Carlo simulations, enabling measurement of the x-ray energies at four different ion beam velocities. We should than be able to strongly reduce the contribution of the Doppler shift to the final error budget.

Future outlook

Suggestions of near-term future activities have appeared already in the material above; the intent here is to indicate a few particular highlights as we currently see them and to mention one or two elements not alluded to previously. Except for the possibility of external support, we expect adiabatic global resource constraint. There is, however, a reasonable probability that a highly productive utilization of the 'Competence' funding could lead to a successful rollover of these funds to the base program. Other than in these cases, new activities imply termination of old activities.

Of the many avenues for which our synchrotron radiation facility is particularly well suited, three beyond those underway or planned within the 'Competence' framework seem particularly attractive. We intend to explore the resonant magnetic scattering mentioned above to see if this scattered radiation could, in fact, be imaged, for instance by direct x-ray detection with a CCD array. Such a technique might complement electron imaging of magnetic structures which are being successfully exploited in the Radiation Physics Division. Second, we feel that the potential of normal incidence standing wave experiments for doing dynamical diffraction measurements on samples whose intrinsic imperfection would otherwise preclude such work is high indeed. We look forward to potentially interesting combinations of these controlled wavefield techniques with oriented overlayers using photon polarimetry and electron distribution spectroscopy. Third, a proposal has been submitted to the NIST Office of Nondestructuve Evaluation for the development of an evanescent x-ray microprobe. The proposal is based on earlier theoretical and experimental studies of evanescant x-rays which indicate that the effect may produce x-ray beams with sub-micron dimensions.

Within the subject area covered by the competance initiative, namely x-ray studies of oriented molecules, two new areas will be explored. First, we will begin studies of aligned molecules usign electron emission as a complement to our previous work based on x-ray emission. Second, we plan to examine the potential applications of the recently uncovered phenomena, namely polarization and anisotropy of resonantly excited x-ray emission, in the area of structural studies of large molecules. The eventual goal of this effort is to obtain structural information on molecules of biological interest without the necessity of first growing the molecules into crystals.

The Neutron Physics Group is now well established on a curve of at least moderate growth; its health and vigor are reasonably assured by the continued effective interest of the Cold Neutron Research Facility's management in the Fundamental Physics Beamline which is managed by this Division. Beyond the first experiments already taking shape on the floor of the Guide Hall, we look forward to the hopeful success of the Universities Consortium proposal presently pending at NSF. This would assure a decade long progression of end station experiments as well as the commissioning of a most advantageously founded station for combined neutron and x-ray interferometry with, for the first time anywhere, active optical interferometric control of separated function systems.

The relatively small and steadily diminishing group for precision studies of x-ray and γ-ray spectra does not expect major expansion of personnel, resources or goals. With minor exceptions, the original ambitions of this program remain as practical goals and retain their scientific interest and value. To the extent that these exercises have required advancement to the measurement art two or more orders of magnitude beyond previous limits and have placed demands on crystal perfection beyond those encountered elsewhere, the road has been a long one and is not yet fully traversed. Meanwhile, targets of opportunity have appeared from time to time, as for example determination of femtosecond nuclear lifetimes, neutrino recoil spectroscopy, the study of low energy collisions in solids, and the study of crystal structure factors at relativistic energies. More deliberate efforts are expected to continue in the study of x-ray spectra especially in the transuranic region and study of the spectra of one- and two-electron ions. The last mentioned area will head for its asymtotic form with the commissioning of the heavy ion cooler ring in Darmstadt in 1991. After an initial period of startup, this facility is expected to make available decelerated beams of fully stripped ions of all sufficiently stable species up to and including uranium. Barring possible transfer of the LEAR ring at CERN to the USSR (or perhaps even after such a transfer), we expect significant involvement in a systematic study of the fully resolved Balmer series spectra of anti-protonic H, D, T and He. This will be a limited time effort aimed at evaluating the phenomenological nucleonantinucleon potential and setting constraints on quark-quark and quark-antiquark coupling constants.

Finally, there are at least some hopes for engendering a more active in-house program at Gaithersburg. In the near-term, we are proposing to improve the technology for characterizing soft x-ray optics using hard x-rays with procedures derived from multi-axis diffractometry and diffraction topography. This is a first step in a longer-term drive toward diffraction limited optics in the x-ray region which it appears possible to approach by appropriate combination of Bragg and Fresnel diffraction in single optical elements. In the somewhat longer-term, there is hope that there will be a 200 MeV low emmittance cw electron beam facility (the Race Track Microtron) operating in a few years. This invites reconsideration of the variety of interactions by which such electrons may be encouraged to participate (coherently) in the production of x-ray beams having technically useful characteristics. A small consortium is developing that will initially aim toward testing current understanding of such processes as coherent transition radiation, channeling radiation, parametric x-ray generation and Smith-Purcell radiation. The exceptional electron emmittance anticipated makes quantitative experiments possible for the first time in the more interesting cases of coherent x-ray production, while the rather high current and cw operation permit one to think of practical applications of the resulting x-ray beams.

Invited Talks

Quantum Metrology Division (575)

Muhammad Arif

"Fundamental Neutron Physics at the National Institute of Standards and Technology Cold Neutron Facility," Institut Laue Langevin's Cold Neutron Workshop, March 9, 1989.

Paul L. Cowan

"Applications of the X-Ray Standing Wave Effect," Naval Research Laboratory Surface Division Seminar, February 2, 1989.

"X-Ray Standing Waves: Interference on a Nanometer Scale," University of Michigan Physics Department Seminar, February 8, 1989.

"Selective Excitation of X-Ray Emission Spectra," Ninth International Conference on Vacuum Ultraviolet Radiation Physics (VUV9), Honolulu, Hawaii, July 18, 1989.

"Applications of Backreflection X-Ray Standing Waves," Gordon Conference on X-Ray Physics, New London, New Hampshire, August 7-11, 1989.

Richard D. Deslattes

"High Resolution Diffraction Spectroscopy at Gamma-Ray Energies," Physics Division Seminar at Argonne National Laboratory, December 2, 1988.

"Projectile Spectroscopy in a Cooler Ring," Workshop on Highly Charged Ions: New Physics and Advanced Techniques, Lawrence Berkeley Laboratory, March 14, 1989.

"Dynamical Diffraction at Gamma-Ray Energies - Application to Nuclear Recoil Spectroscopy," Stanford Synchrotron Research Laboratory Colloquium, March 16, 1989.

"Precision X-Ray Spectroscopy," Workshop on Atomic Physics Experiments at SIS/ESR, Darmstadt, West Germany, April 28, 1989.

"Silicon Monocrystals in Metrology," Physics Colloquium at Danish Institute for Fundamental Metrology, Lyngby, Denmark, May 1, 1989.

"Balmer Series of Light Anti-Protonic Atoms," Laser Lunch Bunch, NIST, June 7, 1989.

Discussion Leader for session on "High Energy Diffraction and Scattering," Gordon Conference on "X-Ray Physics," New London, New Hampshire, August 7-11, 1989.

Maynard S. Dewey

"Fundamental Physics Using Ultra High Resolution Gamma Spectroscopy," Institut Laue Langevin's Cold Neutron Workshop, Grenoble, France, March 9, 1989.

Seminar at Saclay in Paris, March 1989.

"Determination of the Neutron Lifetime Using Cold Neutrons," Reactor Radiation Division Seminar, August 30, 1989.

Geoffrey L. Greene

Colloquium at Los Alamos, New Mexico, November 11, 1988.

Physics Department Colloquium at Swarthmore College, February 9, 1989.

"Determination of the Neutron Lifetime by Counting Trapped Protons," Institut Laue Langevin's Cold Neutron Workshop, Grenoble, France, March 9, 1989.

Chaired Session at Institut Laue Langevin's Cold Neutron Workshop, Grenoble, France, March 9, 1989.

Colloquium at Technical University Munich, Germany, May 1989.

Staff seminar at NIST (NIST Science Advisory Panel).

"Fundamental Physics with Neutrons," Reactor Radiation Division Seminar, September 8, 1989.

Dennis W. Lindle

"Photoionization Studies of Atoms and Molecules Using Synchrotron Radiation," Fourth International Symposium on Radiation Physics, Sao Paulo, Brazil, October 3, 1988.

"Near-Threshold X-Ray Fluorescence Spectroscopy Using Synchrotron Radiation," Colloquium at Laboratoro Nacional de Luz Sincrotron, Campinas, Brazil, October 11, 1988.

"X-Ray Polarized-Emission Spectroscopy," Tenth Conference on the Applications of Accelerators to Research and Industry," Denton, Texas, November 9, 1988.

"Taking X-Rays of Molecules: An Inside Look at Molecular Orbitals," Department of Chemistry Lecture at Swarthmore College, November 11, 1988.

"Polarized X-Ray Emission Spectroscopy," D.W. Lindle, P.L. Cowan, S.H. Southworth, and R.D. Deslattes, 4th International Conference on Electron Spectroscopy (ICES-4), Honolulu, Hawaii, July 10, 1989.

"Parity-Unfavored Transitions in Resonant Photoemission from Ar, Kr, and Xe: Experimental and Theoretical Results," T.A. Carlson, D.R. Mullins, C.E. Beall, B.W. Yates, J.W. Taylor, D.W. Lindle, J.W. Cooper, and F.A. Grimm, Ninth International Conference on Vacuum Ultraviolet Radiation Physics (VUV9), Honolulu, Hawaii, July 17, 1989.

"Polarized X-Ray Emission Spectroscopy of Molecules," Department of Physics lecture at University of Tennessee, September 22, 1989.

Rulon Mayer

"Auger Electron Emission Resulting from Low-Energy Positron Annihilation," Center for Atomic, Molecular and Optical Physics Colloquium, NIST, February 17, 1989.

Stephen H. Southworth

"Arpes Study of Resonant Photoionization of the $2\pi^{-1}$ Channel of NO," Ninth International Conference on Vacuum Ultraviolet Radiation Physics (VUV9), Honolulu, Hawaii, July 19, 1989.

Publications

Quantum Metrology Division (575)

H.G. Borner, J. Jolie, F. Hoyler. S. Robinson, M.S. Dewey, G. Greene, E. Kessler, and R.D. Deslattes, "Determination of Short Lifetimes with Ultra High Resolution (n,γ) Spectroscopy," Phys. Lett. B 215, 45 (1988).

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TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Quantum Metrology Division (575)

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

Paul L. Cowan - Member, Organizing Committee, First Gordon Research Conference on X-Ray Physics, 1989

Richard D. Deslattes - Member, Program Committee of the Ninth International Conference on Vacuum Ultraviolet Radiation Physics (VUV-9) 1989

Richard D. Deslattes - Member, The University of Chicago Review Committee for the Physics Division at Argonne National Laboratory

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

Richard D. Deslattes - Member, Program Committee for the International Conference on X-Ray Physics, X-89

Geoffrey L. Greene - Member, National Steering Committee for the Advanced Neutron Source (1986 -)

Geoffrey L. Greene - Member, National Academy of Sciences/National Research Council Committee on University Research Reactors (1986-1988)

Dennis W. Lindle - Member, Advanced Light Source User's Executive Committee

Dennis W. Lindle - Chair, Special Interest Group for Atomic and Molecular Science at the National Synchrotron Light Source

Dennis W. Lindle - Member, National Synchrotron Light Source User's Executive Committee

Dennis W. Lindle - Member, Editorial Board for the Journal of Research of the National Instiute of Standards and Technology

Dennis W. Lindle - Member, Washington Editorial Review Board

COLLABORATIONS

Quantum Metrology Division (575)

Paul Cowan

AT&T Bell Labs, Murray Hill

Glancing incidence x-ray diffraction studies

Collaborator	Paul Fuoss

Surface studies with x-ray standing waves

Collaborator	J.E. Rowe F. Sette J.R. Patel D.W. Berreman

EXXON Research Labs

Glancing incidence x-ray diffraction studies of surface and interface structure

Collaborator	Ken Liang

Deutsches Elektronen Synchrotron (DESY)

Glancing incidence x-ray diffraction studies

Collaborator	G. Materlik M. Clausnitzer

X-ray standing wave studies

Collaborator	G. Materlik R. Frahm B. Dev

Naval Research Laboratory

Application of x-ray standing wave effect to studies of surface adsorbates and overlayers

Collaborators	A. Shih L. Fotiadis

RISO National Laboratory, Denmark

Glancing incidence x-ray diffraction studies

Collaborator R. Fiedenhansl

Tokyo Institute of Technology

Refinement and applications of the backreflection x-ray standing wave technique

Collaborator H. Hashizuime

Max-Plank Institute fur Festkörperforschung

Glancing incidence x-ray diffraction studies

Collaborator Robert Johnson
Francois Grey

Stanford University, Stanford Synchrotron Radiation Laboratory

Novel instrumentation development for synchrotron radiation

Collaborator S. Brennan

Total reflection x-ray standing wave studies

Collaborator S. Brennan

Glancing incidence x-ray diffraction studies

Collaborator S. Brennan

Calculation of x-ray diffraction effects from perfect and imperfect crystals

Collaborator S. Brennan

Vanderbilt University, Department of Chemistry

XPS studies of multivacancy processes in gases and vapors

Collaborator S. Banna (deceased)

Paul L. Cowan, Dennis W. Lindle, and Steven H. Southworth

American University, Department of Chemistry

X-ray spectroscopy of small molecules

Collaborator Tricia A. Ferrett

Brookhaven National Synchrotron Light Source

Participating research teams (PRT) conduct research at the National Synchrotron Light Source on beam lines that were constructed in a collaborative effort.

Indiana University

Polarization of molecular x-ray fluorescence

Collaborator	Peter W. Langhoff

Lawrence Berkeley Laboratory

Applications of synthetic multi-layers in synchrotron-radiation beamlines

Collaborators	J. Kortright R.C.C. Perera

Lawrence Berkeley Laboratory

X-ray emission spectroscopy of chloro-fluoro carbons

Collaborator	R.C.C. Perera

<u>Paul L. Cowan and Rulon Mayer</u>

University of Michigan, Applied Physics Department

Studies of Resonant x-ray magnetic scattering from magnetic multilayer structures

Collaborator	R. Clarke F. Lamelas H. He

<u>R.D. Deslattes</u>

Argonne National Laboratory

Collaborator	Robert Dunford

University College, London

High resolution Bragg crystal spectrometer for the HESPP Mission (also with the Rutherford Appleton Laboratory)

Gesellschaft für Schwerionenforschung (GSI) Darmstadt, FRG

Spectra of heavy ions

Collaborator H. Beyer

U.S Navy

NIST & NRL joint project to construct, commission and operate five beamlines at the brookhaven national light Source.

Collaborators Many other researchers

R.D. Deslattes, E.G. Kessler, G.L. Greene, and M.S. Dewey

Institut Laue Langevin

Absolute gamma-ray spectroscopy at high energies

Collaborators H. Borner
S. Robinson

Geoffrey L. Greene

Sussex University & McGill University

Measurement of the neutron half life

Collaborators J. Byrne
P. Dawber

Los Alamos, Drexel University and Harvard University

Measurement of the fundamental characteristics of neutron β-decay

Collaborators J. Wilkerson
T. Bowles (LAHL)
H. Robertson
T. Chupp (Harvard)
R. Steinberg (Drexel)

Center for Radiation Research, NIST and European Center for Nuclear Measurements, Geel, Belgium

Absolute neutron dosimetry

Collaborators David Gilliam (NIST)
J. Pauwels (ECNM)

Investigations into new techniques of absolute neutron flux determination

Collaborator

University of Missouri

Neutron Interferometry

Collaborators	S. Werner H. Kaiser R. Berliner

Investigations using neutron interferometry

University of Washington, Department of Physics

Studies on nucleon-nucleon weak interactions

Collaborator	B. Heckel

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Threshold photoelectron spectroscopy of gases

Collaborators	David A. Shirley L.J. Medhurst

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Angle-resolved photoemission from atoms

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Inner-shell electron spectroscopy of atoms

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TIME AND FREQUENCY DIVISION
FISCAL YEAR 1989 TECHNICAL ACTIVITIES

I. INTRODUCTION

The principal functions of the Time and Frequency Division, located in Boulder, are: to produce and maintain the standards of time and frequency and coordinate them internationally, to provide time and frequency services for the United States, and to perform research and development on new standards and measurement methods. There is a secondary responsibility for the realization of the meter, since, by international agreement, the standard of length is now based on the frequency standard, the speed of light being a defined constant. The Division has played a major role in the measurement of the speed of light and the new realization of the meter.

Section II of this report describes current programmatic directions of the Division. Section III of the report provides a summary of some of the significant research opportunities (basic and applied) for the future. These sections are not meant to be comprehensive, but rather to convey a general sense of the program directions and research opportunities.

The remainder of this report describes the work of the Division along organizational lines as shown below.

Each of these sections begins with a short description of the general program and goals of the Group along with a list of staff and guests in the Group. In an effort to relate the Division's work to it's mission, a set of objectives have been used. The work of each group is described with these objectives as headings. Individual objectives are often supported by more than one group, and, because there is collaboration between some of the groups, some tasks are referenced in more than one place. Accomplishments and plans are listed under each objective heading.

Objectives

- o Generate NIST time scales UTC(NIST) and TA(NIST).
- o Maintain international time and frequency coordination.
- o Provide radio and satellite broadcast services.
- o Provide seminars and measurement services.
- o Develop advanced methods for time transfer.
- o Establish the second and the meter for the International System.
- o Perform research and development on new primary frequency standards.
- o Perform basic studies in areas related to future frequency standards.
- o Develop methods for precise time, frequency and length measurements.
- o Provide reference frequencies from the microwave to visible regions.
- o Measure spectral frequencies of atoms and molecules.
- o Advise industry and government agencies on time and frequency metrology.

II. PROGRAMMATIC DIRECTIONS FOR THE TIME AND FREQUENCY DIVISION

Time and Frequency Services

The broadcast services of the Division, which include WWV and WWVB in Fort Collins Colorado, WWVH on Kauai and the GOES Time Code Service, serve as important components of the Nation's technological infrastructure. Substantial care should be taken to continuously upgrade and replace equipment supporting these to insure good reliability. The staffing of these services is good and equipment is well maintained, but a few special items are at or past obsolescence and will require replacement. The new Automated Computer Time Service presents a particularly simple approach to millisecond synchronization of digital networks and the number of lines should be expanded to meet the growing use. Opportunities to tie this service into the operations of major telecommunication carriers should be pursued as they arise.

Seminars offered by the Division provide the only real tutorial introduction in the U.S. to accurate timekeeping and related metrology and these seminars should continue to be offered and upgraded. The Frequency Measurement Service, which supports accurate frequency measurement in the Nation's highest level standards laboratories, is popular and should continue operation to meet the needs of these laboratories. This service as well as the seminars are operated on a fully reimbursable basis.

The Division should continue work on the use of communication satellites for two-way time comparisons at the nanosecond level. This technique promises to be the most accurate means for time coordination and it will undoubtedly be adopted for most of the major international time comparisons in the future. The Division is a world-leader in development of this concept and has proposed a one-way broadcast service based on it. The development of this service, which promises simple network time synchronization at the 100 ns level, has already been initiated, but resources are insufficient to bring it into existence in a timely fashion.

This service could have substantial impact in telecommunications, computer networks and electrical power networks, all of which have need for improved synchronization at a level of 1 μs or better.

Time Scale and Time and Frequency Coordination

Since the time scale is the critical reference for both dissemination services and research in the Division, it must be maintained and improved to reliably meet these needs. The rebuilding of the clock measurement systems and the replacement of the time scale computer have substantially improved time scale reliability, but the Division should acquire clocks with better long-term stability to improve the long-term performance of the time scale. This improvement is needed to address imminent improvements in primary frequency standards, the accuracy of which will not be realized unless the time scale is sufficiently stable between evaluations. Planned procurement of an active hydrogen maser will provide the short-term stability needed to support research on standards based on trapped ions as well as evaluation of the new primary standard, NIST-7.

As noted in the previous section, two-way time transfer will likely play a large role in the future of international time coordination, and the Division will be properly situated to play a key role in such coordination. However, the GPS Common-View Method, also pioneered in the Division, will likely play a major time-transfer role for years to come, since it is firmly entrenched, and the acceptance of two-way time transfer will be delayed by equipment acquisition and required licensing of satellite earth terminals. We assume that the DOD program of "Selective Availability," which will produce substantial degradation of the GPS timing signals can be adequately handled in the Common-View Method. The Division is developing modified methods that should minimize the impact of this degradation, but these must yet be tested. If the accuracy of GPS time transfer is not substantially degraded, the Division should maintain a solid effort in this area. Until and unless two-way time transfer is broadly accepted, the world will probably continue to rely on GPS.

Phase Noise and Hydrogen Masers

The Division should continue development of phase-noise metrology to support rising demand for phase-noise characterization of aerospace electronic components. This effort is highly synergistic, since the characterization of clocks and oscillators is primarily a phase-noise measurement. Furthermore, the project naturally leads to improvements in phase-noise performance of system components, many of which can contribute to the Division work on frequency synthesis from the microwave to the optical region. Because the measurement of phase noise is difficult to perform accurately and substantial errors are the rule rather than the exception, the Division should consider developing a phase-noise calibration service.

The Division discontinued a program on hydrogen masers with completion of the development of a passive hydrogen maser and there are no plans to initiate new maser work. However, the Division should improve the reliability of the passive masers used in the time scale since, when they are in proper operation, they add substantially to the long-term stability of the time scale. The active hydrogen maser that is now being procured will provide needed short-term stability as noted in the previous section.

Atomic Beam Standards

The development of a new optically pumped cesium standard, NIST-7, to replace the aging NBS-6 should retain its present high priority. Not only will this standard provide improved accuracy, but it is being designed for simple, automated evaluation, a process that now takes months with NBS-6. While standards based on trapped ions promise even better accuracy, they must be viewed as in an early research phase and not likely to be ready for routine use in the near future. Furthermore, the definition of the second still rests on cesium, and that is not likely to change until long after other methods have been accepted internationally. The Division should look carefully at the recent demonstration of a fountain standard, which (using cesium atoms) could lead to a major improvement in cesium-standard accuracy. Again, this work is in a research phase and must be regarded as long term, so it is not likely to supplant NIST-7 development.

NBS-6 should be maintained and regularly evaluated well after NIST-7 is in operation. This overlap in operation will allow development of confidence in the accuracy of the new standard. Following this overlap period, NBS-6 will turned off and disassembled.

Ion Storage

The Division effort on ion storage should continue as a basic research program providing NIST with the background information needed for future generations of frequency standards. The program should continue to focus on the physics of microwave transitions and optical transitions in both single-ion and multiple-ion systems as well as the motions of ions within the traps. The commitment to this line of research is based both on real results, that is, demonstrations of ion standards, and on the enormous accuracy potentially available with particles that are nearly at rest. This potential is vividly demonstrated in the current operation of a single-ion, optical frequency standard that has a linewidth of less than 100 Hertz in the ultraviolet region. The projected systematic uncertainty of the transition in this system is less than one part in 10^{18}.

Since simple means will be needed to exactly relate the frequency of an optical standard to frequencies in the microwave region, the ion storage group should investigate their proposed synchrotron-frequency-divider concept. If the idea proves feasible, it could provide for large-integer division of optical frequencies thus simplifying locked frequency chains.

Laser Frequency Synthesis

There are several reasons why the Division should further develop a program in the area of optical frequency measurement and accurate synthesis of optical signals. The first is the emergence of a second generation of optical communication and signal-processing systems that will use coherent optical techniques. NIST will ultimately have to develop accurate optical-frequency metrology to support such systems. The second motivation for this work is the need to establish an accurate link between the microwave and optical regions in support of future frequency standards (as discussed above). The Division has put together a group in this area and expects that funding from the NIST Light Wave Initiative will allow for expansion to a level where the above problems might be attacked in a timely manner. It is clear that diode lasers will play a substantial role in this program, and the Division should develop the competence and facilities to make best use of these devices.

III. BASIC AND APPLIED RESEARCH OPPORTUNITIES

The Division has developed a number of specialized experimental capabilities that provide unique opportunities for certain basic and applied research projects. These include: (1) systems for trapping and cooling of 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 an excellent background in the statistical characterization of high-stability oscillators. Considering these strengths, we list the following examples which are appropriate areas for research in the Division. The Division clearly does not have the resources to pursue all of these.

Atomic Physics

In the area of atomic physics, Division programs are centered on strengths in ion trapping, cesium beams, low-phase-noise frequency synthesis, and accurate frequency (length) measurements.

1. Tests of Relativity Theory - Such tests include accurate measurement of the gravitational red shift and comparisons of fundamentally different oscillators with varying spatial orientation of quantization axes (Hughes-Drever type experiments).
2. Measurement of Light Shifts - Both the influence of black-body radiation and electric fields (ac-Stark shift) can be studied. The latter might possibly provide the basis for an ultraviolet power standard.
3. Study of Atomic/Nuclear Distortion by Magnetic Fields - This involves accurate measurements on ions in Penning traps to provide tests of theoretical predictions.
4. 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.

5. Study of Influence of Radiation Fields on Atoms - Here we can compare predictions of quantum and semi-classical theory and study radiation damping and frequency pulling in cavities.
6. Precision Measurements in Hydrogen - Important quantities to be obtained from accurate measurements in hydrogen include the electron-to-proton mass ratio, the Rydberg constant and the Lamb shift.
7. Search for Violation of Time-Reversal Invariance - A search in an alkali metal (e.g., cesium) for a static electric dipole moment could provide a exacting test of this important principle.
8. Precise Measurements of Mass Ratios - Laser fluorescence mass spectroscopy developed by the Division could yield measurement of such ratios as m_{e+}/m_{e-}, m_e/m_p and $m_p/m_{\bar{p}}$, as well as g-factor measurements.

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 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, areas in which the Division interacts strongly. 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 can also be precisely determined.

Optical Physics

Studies in optical physics revolve around the need to develop 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-T_c superconductors. Another approach to the problem involving synchrotron division offers the opportunity to study laser excitations of a single relativistic electron in a Penning trap.

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 interesting nonneutral plasmas. These plasmas have distribution functions that are closely related to those for neutral plasmas. Under proper laser-cooling conditions, such plasmas become strongly coupled and can enter the liquid and solid states. Important experiments to consider involve study of Bragg scattering, ion diffusion, phase transitions, Coulomb clusters, 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 that 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 that they add. Alternatively, 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 that 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 noise properties 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.

Optimal Use of Ensembles of Clocks

The NIST time scales are based on an algorithm that intelligently combines the outputs of many clocks to arrive at a smooth time scale that 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 the Millisecond Pulsar. Such comparisons could ultimately result in the detection of gravitational waves.

IV. TIME AND FREQUENCY SERVICES

The Time and Frequency Services Group provides the Division's direct support to science, industry, other government agencies and the general public. Division broadcast services, the Frequency Measurement Service, and the Time and Frequency Bulletin all fall within its responsibility. In addition to these on-going services the Group is working on two other projects: synchronization of clocks using two-way satellite time transfer, and a time broadcast service using commercial communication satellites. The Group's work is described in more detail below.

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A. J. D. Clements
D. A. Howe
J. L. Jespersen
G. Kamas
M. A. Lombardi
A. Sen Gupta (Guest Researcher)
R. E. Beehler (Broadcast Manager)

<u>WWV, WWVB, Ft. Collins</u>	<u>WWVH, Hawaii</u>
J. E. Folley (Part-time)	A. Fabro (Part-time)
M. J. Deutch	E. F. Farrow
J. M. Maxton, Chief Eng.	M. Ferguson (Part-time)
C. S. Snider	N. Hironaka, Chief Eng.
A. R. Trevarton	D. Okayama

Convenient access to NIST standards of time and frequency is accomplished for the majority of users through the radio broadcasts of stations WWV, WWVH, and WWVB and a time code broadcast by the GOES satellites. NIST also provides telephone time-of-day services (voice), a new digital telephone service designed for automated setting of computer clocks, publications of time and frequency values of other radio stations as received at NIST, portable clock comparisons and calibrations. Seminars concerning time and frequency metrology are regularly scheduled to acquaint users with techniques for characterizing oscillators and distributing frequency and time signals. Examples of important applications of time and frequency services are given below.

<u>Navigation</u>

Celestial navigators need time to determine their precise location. An error of 2 s could cause a ship to miss its destination by about 1 km. Thus, military and commercial shipping and small boat owners depend in a life and death sense on the availability of the signals from WWV and WWVH. More sophisticated electronic navigation systems such as LORAN-C and the Global Positioning System (GPS) must maintain time much more accurately. An error of only 3 μs could produce the same 1 km error for the navigator.

System Control and Synchronization

The electric power industry uses both frequency and time information in the management of generation and distribution of electric power. Frequency measurement has been fundamental to the industry for many years and is satisfied by signals from WWVB and GOES. Time is becoming increasingly important in the location and analysis of fast occurring events (faults), measurement of power flow, and the control of systems to minimize losses and avoid outages caused by exceeding stability limits.

Radio and TV stations need accurate frequency to broadcast signals at exactly their assigned frequencies. They need accurate time to set clocks so they can join the networks at the right instant. The aviation and aerospace industries need accurate time for aircraft traffic control systems and for synchronization at satellite and missile tracking stations.

The telecommunications industry needs time accurate to 1 μs or better to synchronize communication nodes spread over wide geographical areas. Divestiture by AT&T along with the growth of other major carriers poses significant difficulty for synchronous transfer of calls through the interfaces between companies. Increasing data rates in the newer digital communication systems will further complicate system synchronization.

Data Acquisition

The FAA records accurate time on its audio tapes along with the air-to-ground communications from airplanes. Having an accurate record of when particular events occur can be an important factor in determining the cause of a plane crash or equipment malfunction.

Geophysicists and seismologists studying lightning, earthquakes, weather, and other geophysical disturbances need time to synchronously and automatically obtain data from wide geographical areas and to label geophysical events. Other scientists use time for controlling the duration of physical and chemical processes, while astronomers use time for labeling astronomical events, such as lunar occultations, eclipses, and pulses.

Science and Metrology

Manufacturers need time and frequency to calibrate counters, frequency meters and test equipment. Accurate spectra of molecules including information on pressure broadening are needed to accurately determine atmospheric concentrations of important pollutants. Laser frequency measurements provide accurate calibration frequencies for spectroscopists and for radio astronomy as well as the means for realization of the meter.

OBJECTIVE: Provide radio and satellite broadcast services.

NIST offers several around-the-clock time and frequency dissemination services to the general public. In 1923, radio station WWV was established by NIST and has been operated since that time. A sister station, WWVH was established in 1948, on the Hawaiian Island of Maui, and relocated to Kauai in 1971. In 1956, WWVB began low frequency broadcasts. WWV's signal is also offered by telephone, not toll-free, by dialing (303) 499-7111. A similar service from WWVH is available by dialing (808) 335-4363 in Hawaii. Broadcasts from WWV and WWVH can be received on conventional shortwave receivers nearly anywhere in the world. Broadcast frequencies include 2.5, 5, 10, and 15 MHz for both stations and 20 MHz from WWV only. Accuracies within 1 ms can be obtained from these broadcasts if one corrects for the station's distance from the receiver. These services also provide standard frequencies, a BCD time code, astronomical time corrections, and certain public service announcements from other government agencies. The telephone service offers the capability of obtaining NIST time and audio frequency signals. The caller can receive a time signal, accurate to 30 ms or better, about the maximum delay in cross-country telephone lines. WWVB offers a direct path signal of greater accuracy than WWV or WWVH, but a special 60 kHz low frequency receiver is required. WWVB's signal includes a binary-coded system, needing special decoding equipment. The WWVB broadcast covers the North American continent. These broadcast services are coordinated with similar operations in other countries through active participation in the international CCIR organization.

NIST time and frequency signals have been relayed through the GOES geostationary satellites since 1975. The GOES broadcast covers North and South America as well as major portions of the Pacific and Atlantic including parts of Europe. More than 10 years of experience has shown that such a system provides continuous time and frequency reception with more dependable propagation characteristics than HF and LF broadcasts. The satellite position broadcast with the time permits automatic correction for variations in path delay resulting in time accuracy of 100 μs.

A new digital telephone service, the Automated Computer Time Service (ACTS), was initiated in March of 1988. This service provides for automated setting of computer and other clock systems with optional compensation (to the 1 ms level) for telephone line delays.

FY 1989 Plans and Accomplishments

Install, evaluate, and place into regular operation the new transmitters for WWV as soon as they become available from the manufacturer.

Accomplishment - Completion of this project was delayed due to default by the firm that had originally won the contract. A new request for proposals was issued resulting in a recent contract award to a well known vendor. The new delivery date is approximately March 1, 1990. All local WWV preparations for the new transmitters are complete.

Procure and install modern, custom-designed time code generator systems at WWV and WWVH. Implement requested format changes and additions after consultation with receiver manufacturers.

<u>Accomplishment</u> - Through discussions with the manufacturers, we arrived at format changes that are acceptable to everyone. The company that won the competitive contract spent substantial time developing a design for the new time code generators and then went out of business. Their assets and patents were sold to still another company, but we have not been able to get them to complete the design and fabricate the systems. Discussions are continuing and we are also exploring other alternatives.

Complete construction, testing, and evaluation of two new voice announcement approaches for other agency announcements on WWV.

<u>Accomplishment</u> - Both systems are complete. The first of these is a digitized voice system which is in regular operation and has performed reliably. No complaints about voice quality have been received. The second system, based on a WWVH design, uses standard tape recorders. It is available as a backup system.

Complete final report on the results of the user survey.

<u>Accomplishment</u> - A detailed summary of the survey results was produced for submission to an international CCIR meeting in September of 1989. A final, internal report will be prepared shortly.

Maintain reliable broadcasts from WWV, WWVH, WWVB, and the GOES satellite time code.

<u>Accomplishment</u> - All broadcast services operated within specified tolerances with down times of less than 0.1% of total broadcast time.

Conduct a series of U.S. meetings in preparation for the final meeting of the international CCIR Study Group 7. Provide NIST input to the documents of the study group as well as input on timing methods for a CCIR handbook.

<u>Accomplishment</u> - NIST provided chairmanship for the U.S. delegation. Five U.S. meetings were held in preparation for the final meeting in September, 1989 in Geneva. The seven documents submitted by the U.S. represented the largest input from any delegation and virtually all of the U.S. recommendations were accepted, although there were the usual changes on minor points. Specific NIST contributions included an extensive section for an international CCIR handbook on satellite time dissemination and a glossary of terms used in time and frequency technology.

<u>FY 1990 Plans</u>

Evaluate and install new transmitters at WWV after delivery in FY 1990.

Explore alternatives for procuring modern, more-flexible time code generators for WWV and WWVH. Initiate procurement if suitable sources and funds are available.

Test and implement appropriate modified procedures in the GOES time code system for generating more accurate satellite-position data during periods immediately following major satellite maneuvers.

Continue CCIR activities, including completion of the satellite handbook contribution in final form and representation of Study Group 7 at CCIR plenary meetings in May, 1990.

Complete final report on the recent user survey. Complete updates of the time and frequency publications relating to WWV, WWVH, WWVB, GOES, and the ACTS computer time service.

Maintain reliable operations from WWV, WWVB, WWVH, GOES and ACTS.

OBJECTIVE: Provide seminars and measurement services on a reimbursable basis.

Frequency Measurement Service

The frequency measurement service is automated, modest in cost, and provides traceability to NIST at a level of one part in 10^{12}. The service is based on common-view reception of low frequency signals from stations such as WWVB or Loran-C. This service provides the user with a data logger and a low frequency receiver that is appropriate to the particular location. A typical system contains a receiver, microcomputer, disc units and printer-plotter. The user provides a dedicated phone line and modem so that the system data can be compared with data recorded at NIST providing assurance that the users reference is accurate. To assist the user in getting the most out of this system, the Division provides training on use of the equipment.

Time and Frequency Bulletin

The Division continues distribution of it's Time and Frequency Bulletin to over 500 service users. The bulletin provides information on the performance of many useful references and notes events and service changes of interest to users. It was expanded to cover new services.

Seminars

The annual Division seminar provides industry and other agencies with information and training on the use of frequency standards. Special effort is made to have the seminar support the introduction of new services and to be of particular interest to the Nations's calibration laboratories.

FY 1989 Plans and Accomplishments

Continue operation of the Frequency Measurement Service. Modify systems to improve the match to the calibration lab needs.

Accomplishment - The number of users of this service grew by about 20% during the past year. Approximately 30 laboratory personnel from a variety of government and industrial standards laboratories were trained in the use of the NIST system. Software changes were made in order to improve ease of operation of the user systems and a new instruction manual was written and distributed.

Provide a comprehensive Time and Frequency Seminar (reimbursable) in 1989. This seminar will be held in conjunction with the Frequency Control Symposium which will be in Denver.

Accomplishment - The seminar was held in Boulder on June 5, 6 and 7, 1989 during the week following the Frequency Control Symposium in Denver. Measurement systems were demonstrated at the Boulder labs with lectures presented in a meeting room at the local seminar hotel. Of the total registration of 43, more than half were from industry. A short, unsigned survey at the end of the seminar elicited highly favorable comments and some good suggestions for future improvements in the seminar.

Additional Accomplishment - A preliminary draft of the "Time and Frequency User's Manual" was written to replace the outdated version (NBS Special Publication 559). After appropriate review this will be published and distributed.

FY 1990 Plans

Continue operation of the Frequency Measurement Service. Study options for acquisition of more-reliable and lower-cost measurement equipment for the service.

Provide a comprehensive Time and Frequency Seminar (reimbursable) in 1990.

OBJECTIVE: Develop advanced methods for time transfer.

The use of communications satellites for time transfer at all levels of performance appears to be widely accepted. In a recent annual report, the BIPM/BIH urged further development of the concepts. Much of this is due to improvements in the available technology and significant reduction in the cost of components and leased transceivers on satellites. At the higher levels of performance, work reported by Japan and unpublished tests involving NIST, USNO, and COMSAT Laboratories have demonstrated half-nanosecond time comparison precisions using two-way time exchanges through a satellite, and comparable accuracy is expected when all systematic effects are evaluated. Additional tests have indicated that 20 ps comparisons are possible using the same techniques with higher transmission power levels. NIST, USNO and the NRC in Canada have informally agreed to develop a permanent time-transfer network to serve the three laboratories. All of the necessary equipment has been acquired and preliminary tests have begun.

In addition, NIST is exploring the use of two-way time transfer as a means for tracking a communications satellite. With the addition of satellite location to a time message, this could provide a one-way (receive-only) dissemination service with time accuracy of 100 ns or better. Antennas for receive-only use would be quite small. The same satellite and signal structure could also be used to provide a reimbursable two-way service with an accuracy of 1 ns. The tracking scheme involves three earth stations as shown in the figure below. Two of the three stations are passive providing only a turn around for the signal from the satellite.

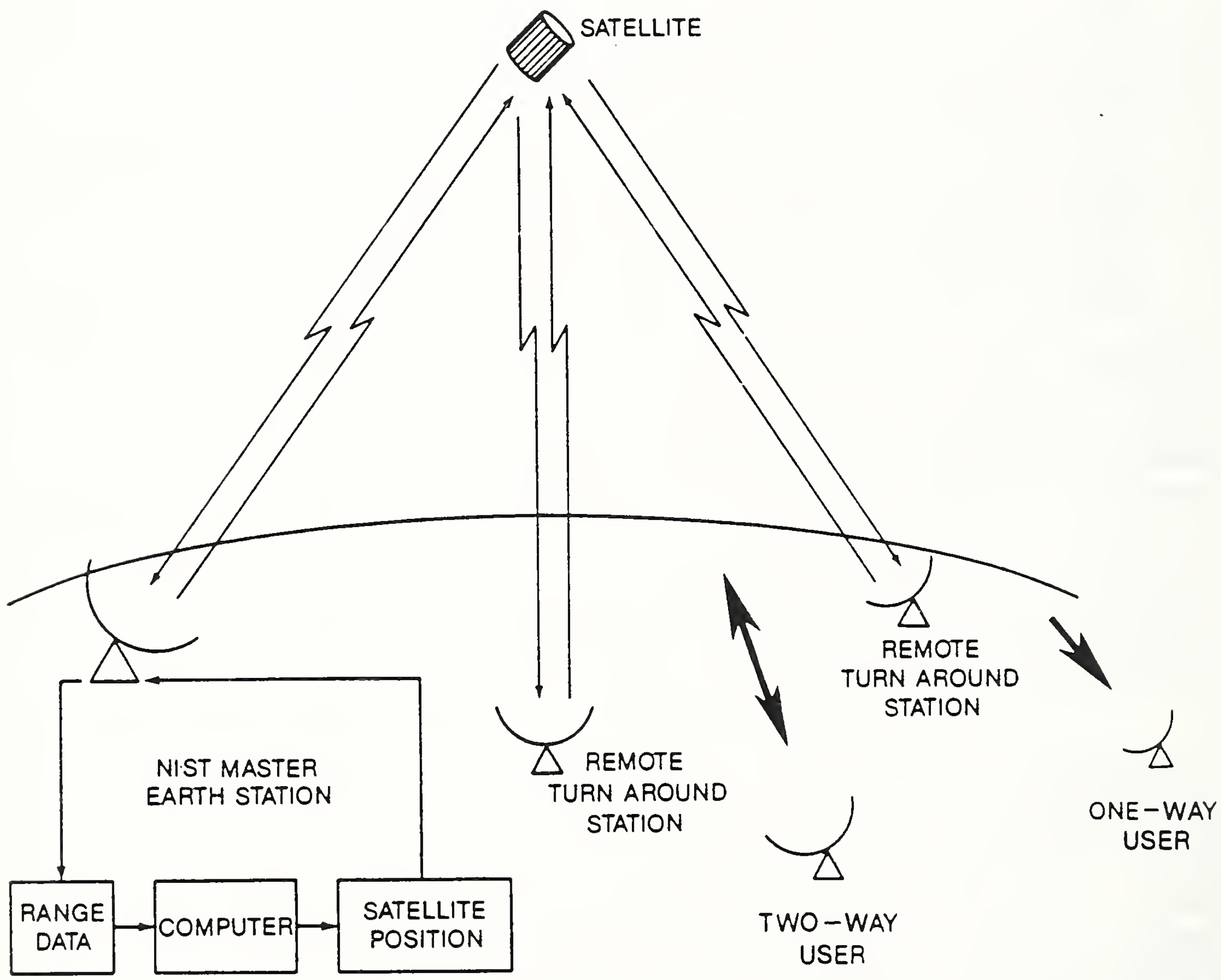

Figure 1. Principle of operation for two-way and broadcast (one-way) time services using a domestic communications satellite.

FY 1989 Plans and Accomplishments

Begin transatlantic time comparisons using the INTELSAT V(F-13) satellite at 307° East longitude.

Accomplishment - Administrative procedures for licensing earth stations in Europe have proven to be complicated and lengthy, thereby delaying European participation in the time comparisons. Recent recommendations of the CCDS concerning two-way satellite comparisons are expected to accelerate the development of a European two-way network and links with the North American network.

Calibrate the NIST and USNO earth stations using the mobile earth station. Include the National Research Council (NRC) in this calibration if they have received permission to reactivate their time transfer system.

Accomplishment - Equipment in the mobile earth station has been reconfigured with some new equipment to enhance performance. The delays in this mobile station have been calibrated against the base station in Boulder, but the USNO measurements have been delayed by long delivery delays for some key components. These measurements will be completed shortly.

Evaluate the reciprocity of the atmospheric delays in two-way time transfer at the frequency assignment of 14/12 GHz for the Fixed Satellite Service.

Accomplishment - The assumption of reciprocity for atmospheric (and ionospheric) delays was evaluated using accepted models for all terms. At the accuracy level of projected use, there appear to be no serious problems with this assumption. A paper on this topic was presented at the Frequency Control Symposium.

Continue development of the two-way time transfer system. Standardize the earth station equipment and operating software.

Accomplishment - Operational software and procedures have been substantially improved and the two-way time exchanges are now made on a routine schedule with no difficulty. The stability and accuracy of comparisons with USNO are currently being studied.

FY 1990 Plans

Continue development of the two-way, satellite-time-transfer system. Complete evaluation of the accuracy of the NIST-USNO link.

Develop a spread-spectrum modem which is suitable for both two-way time transfer and a one-way broadcast service.

Develop software for 24-hour tracking and orbit prediction of communication satellites. Using the two-way equipment, collect data to evaluate the predictions of the software.

V. TIME SCALE AND TIME AND FREQUENCY COORDINATION

This Group has the responsibility for the operation and further development of the NIST time scales and for coordination of these time scales with other timing centers and the Bureau International des Poids et Mesures (BIPM). These time scales are, of course, a key responsibility since they not only provide the basis for all services, but also serve as the stable reference against which much of the Division gauges it's research. The Group has developed a coordination scheme based on common view of the Global Positioning System (GPS) satellites which is now the *de facto* coordination approach for the world.

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OBJECTIVE: Generate NIST time scales UTC(NIST) and TA(NIST).

NIST atomic time is generated from an ensemble of approximately twelve commercial and one laboratory cesium-beam frequency standards and two laboratory hydrogen masers. The time of all the clocks is automatically measured every two hours with a precision of a few picoseconds. The UTC(NIST) and AT1 time scales are computed following each measurement cycle using a weighted-average algorithm. The small dispersion of the clocks during the interval between measurements makes it possible for NIST to provide UTC(NIST) with 1 ns accuracy at all times. Coordinating with BIPM, UTC(NIST) is steered toward and kept within 1 μs of UTC. AT1 is a metrology tool, unsteered in time or frequency, and made to be as stable and uniform as possible.

At the end of each month, the TA(NIST) time scale is computed using a Kalman algorithm. This computation is optimum in the statistical sense for clocks having both white frequency noise and random-walk frequency noise, a good model for the clocks in the NIST ensemble. The second of TA(NIST) is steered toward NIST's best estimate of the SI second based on periodic calibrations of the ensemble by the primary frequency standard, NBS-6.

FY 1989 Plans and Accomplishments

Study use of the cooled-beryllium ion standard in providing periodic calibration of the NIST time scales at the targeted accuracy of 1×10^{-14}.

<u>Accomplishment</u> - Preliminary frequency stability studies were performed on the cooled-beryllium standard, and were found to be about $\sigma_y(\tau) = 3 \times 10^{-14}$ for τ values in the range of several weeks. As noted in section VIII, the instabilities are believed to result from collisions with background gases. It is probably too early in the studies of the beryllium standard to use its output in the time scale.

Finish the installation and put into operation the newly acquired time-scale computer and supporting work stations.

<u>Accomplishment</u> - The computer and all of the work stations have been installed and tested and are in full operation. The time-scale software has been transferred and the new computer is now running the time scale in parallel with the old computer. The clock analysis software is now being converted to the new system. Switchover to the new system should occur early in FY 1990.

Develop plans for acquisition of advanced clocks for the time scale in order to improve stability and reliability.

<u>Accomplishment</u> - As noted in section VII, NBS-4 is being upgraded and should have a flicker floor of less than 10^{-14}. Two new cesium clocks have been ordered. The first, which involves cooperation on a company development of a high-performance product, will be evaluated in the time scale for long-term performance. The second, which is a regular high-performance unit, will be received in FY 1990. These two clocks should provide some long-term-stability improvement for the ensemble.

Continue with the De Marchi C-field tuning experiments to improve performance of cesium standards in the NIST time scales.

<u>Accomplishment</u> - Several clocks tuned using De Marchi's method show significant improvement in long-term performance. A member of the staff has been trained in using this tuning technique. With input from NIST, CCDS has now recommended that other international timing centers adopt this technique in order to improve the long-term performance of clocks contributing to UTC.

Prepare the proceedings for the Third International Atomic Time Scale Algorithm Symposium and continue with atomic time-scale algorithm research and development.

<u>Accomplishment</u> - The proceedings were prepared and distributed to all attendees. The seminar was considered a complete success. Time scale algorithms now play a key role in obtaining stabilities of better than 1×10^{-14} for sample times longer than a month.

<u>FY 1990 Plans</u>

Complete switchover from the old to new time scale computer.

Tune the new cesium clocks for optimum performance and integrate them into the time scale. Continue working with industry on improved cesium clocks.

Study different time scale algorithms with focus on an optimum frequency-step detection. Study alternatives to the current TA(NIST) algorithm.

Develop a real-time, servosystem to control the one-pps output of the time scale to within 100 ps of the official computer time.

OBJECTIVE: Maintain international time and frequency coordination.

A satellite-based, time-transfer system developed by the Division is now in operation. Receivers are now operating at most of the international timing centers. A computer-based, automatic-data-collection network acquires data from the receivers. This data is transferred using the common-view technique to the International Bureau of Weights and Measures (BIPM). This new system has replaced Loran-C as the principal international transfer link for the SI second and the generation of International Atomic Time Scales (TAI and UTC).

FY 1989 Plans and Accomplishments

Work with Lewandowsky of the BIPM to develop means for more efficient use of GPS common-view time and frequency transfer to take advantage of the future addition of new GPS satellites.

Accomplishment - During this collaboration, we uncovered significant errors in the positions of the antennas at North American timing centers. These errors account for several nanoseconds of time-transfer inaccuracy. In addition, in cooperation with the U.S. Geodetic Survey, we obtained more accurate ephemeris information for the GPS satellites. Guinot at BIPM and Lewandowsky (while at NIST) were able to demonstrate still further improvement in time transfer accuracy by using these more accurate ephemerides.

Cooperate with PTB and BIPM in the determination of the source of possible annual terms in the respective time scales.

Accomplishment - Data exchanges between BIPM and NIST and USNO and NIST have been used to study this problem. Various algorithms for handling the data are being tested, but it is too soon to know whether they are effective. There is speculation that humidity variations may affect the long-term performance of clocks giving rise to the annual terms. To test this hypothesis, the second of the two environmental chambers housing the NIST ensemble has been humidity controlled.

Compare the NIST time scales with other research clocks to determine relative performance. Use the comparisons as the basis for development of a global research time scale to be used in study of the Millisecond Pulsar.

Accomplishment - An extensive software package, which uses the data from all of the international timing centers, has been designed to serve as a global research time scale. It is a retrospective time scale, that is, it is run after the fact to allow removal of poorly performing clocks. This highly smoothed time scale has been tested in a preliminary fashion on several data sets.

FY 1990 Plans

Make comparisons between time data from the Millisecond Pulsar and the output of the global research time scale. Participate in an international workshop on the Millisecond Pulsar.

OBJECTIVE: Develop metrology for precise time, frequency and length measurements.

Techniques for Measurement of Frequency and Frequency Stability

The Division has been a leader in the development and dissemination of the measures of frequency stability and their practical implementation. The Division developed the *de facto* international standard for practical specification of frequency stability and played a major role in the development and test of the dual-mixer concept for measuring time, frequency, and frequency stability providing for simple, precise (picosecond) measurement of the difference between state-of-the-art frequency standards. The Division developed new understanding of the effect of phase noise on frequency multiplication, and this then stimulated considerable improvement in the phase noise of crystal oscillators and signal processing equipment. In the rf region, the lowest noise crystal oscillators, buffer amplifiers, isolation amplifiers, and frequency multipliers presently available are a direct outgrowth of prototype designs and analysis developed at NIST.

Techniques for Characterizing Noise in Clocks

Memory of the rate of the primary standard is stored in a time scale, an ensemble of commercial cesium standards. The clocks in the time scale don't have the accuracy of NBS-6, but they do have good frequency stability. The stability of a clock ensemble can be improved by increasing the number of clocks and/or by improving the stability of individual clocks. The Division has chosen to use a modest number of clocks ensuring sufficient reliability and redundancy, and then to characterize the clocks with enough care so that the algorithms that average the clocks make optimum use of the performance of individual members of the ensemble.

The algorithms that control the time scale have evolved to their current state through considerable work spanning several decades. The performance of the key algorithm for UTC(NIST) has been validated through substantial study over many years. Another major development was a Kalman (or recursive) algorithm for estimating time from the ensemble of atomic clocks. The algorithm allows for the addition or deletion of clocks and provides for automatic error detection and correction. This Kalman algorithm is now used to generate the time scale TA(NIST). During this latter study, the earlier algorithm that generates UTC(NIST) was found to be near optimum in its performance. It's stability was shown to be of the highest order as it was found to be one of the most stable references for the characterization of the stability of the Millisecond Pulsar.

FY 1989 Plans and Accomplishments

Continue support of adoption by IEEE of the frequency stability characterization standard.

Accomplishment - IEEE Standard No. 1139 on frequency stability characterization in time and frequency metrology was adopted this year. NIST staff played a major role in accomplishing this.

Continue study of the influence of environmental factors on the NIST time scales and those of other laboratories.

Accomplishment - As noted earlier in this section, humidity was found to influence the performance of ensemble clocks and we now control that parameter. The algorithm that generates UTC(NIST) in real time has been studied and modified for post analysis. Methods for approaching optimum frequency-step detection have also been studied. Imperfections noted in the TA(NIST) algorithm have yet to be studied.

Study short term performance of the NIST time scales and consider options for improvements.

Accomplishment - With the advance of two-way satellite time transfer, a more-accurate, real-time, pps output is needed. The current real-time output varies by as much as 200 ps from the calculated output. This is barely adequate to support two-way time transfer.

FY 1990 Plans

Interface environmental monitoring equipment to the new time-scale computer in order to build a data base for environmental sensitivity testing.

Improve the real-time output of UTC(NIST) to be within 100 ps of the computer-algorithm average of the ensemble.

Continue work with the IEEE TC-3 standards committee on properly dealing with environmental sensitivities of clocks and oscillators.

OBJECTIVE: Provide seminars and measurement services on a reimbursable basis.

Global Time Service

The Division offers a service, based upon a NIST designed GPS receiver, which provides for highly precise time and frequency transfer to a users site. A receiver, located at the users facility, communicates data automatically to a NIST computer which stores and processes the data, and provides an optimally filtered value for the time and frequency of the user's clock with respect to the NIST Atomic Time Scales. The user is given an account on the NIST computer through which he can access the results of the NIST analysis. Extensive tests have demonstrated time comparisons with precisions of better than 10 ns using an averaging time of

13 minutes and frequency comparisons with a precision of 1 part in 10^{14} for averaging times of four days.

Calibration of Atomic Standards

In conjunction with development of the time scale algorithms the Division has developed a time and frequency measurement system with exceptional performance. Clocks are now calibrated and characterized through comparisons with the ensemble clocks using the same measurement system that reads the ensemble clocks. This system is used as a reference for research within the Division as well as for reimbursable calibrations.

FY 1989 Plans and Accomplishments

Continue work on the CGS steering committee to minimize the impact of GPS selective availability (S/A) on the civilian uses of the system.

Accomplishment - NIST, the Naval Observatory and the Air Force Space Division sponsored a proposal to leave undegraded a subset of GPS satellites. This proposal is still being considered by DOD.

Continue work on an ionospheric calibrator in order to increase the common-view, time-transfer accuracy.

Accomplishment - Hardware and software for a prototype calibrator are 99% complete. Projected accuracy is a few nanoseconds.

Increase the capacity of the time scale measurement system to accommodate additional time scale clocks and to allow for more special calibrations.

Accomplishment - The capacity of the time scale measurement system has been doubled. This additional capacity is now being used to provide independent measurement inputs to the new and old computer systems. It will be available for expansion when the old system is shut down.

Additional Accomplishment - The contributing errors to GPS common-view time transfer with S/A have been categorized and are being systematically addressed. S/A is now being introduced in the second block of new GPS satellites. The errors of concern include satellite ephemeris, ionospheric and tropospheric delays, and multipath effects. GPS satellite clock errors cancel in the common-view approach. Major advances have been made in reducing the ionospheric errors using the ionospheric calibrator, and minor modification of the antenna design has substantially reduced multipath effects.

FY 1990 Plans

Install ionospheric calibrators at key national timing laboratories to prove the performance of the system. Work with industry to make the ionospheric calibrator commercially available.

In collaboration with the University of Colorado, use timing laboratory data to develop more accurate ephemeris information than is available through S/A. This will help overcome S/A degradation of time transfer.

Continue development and documentation of antenna modifications that suppress multipath effects.

Following switchover to the new time scale computer, configure extra measurement system to provide redundancy and additional calibration ports.

OBJECTIVE: Advise industry and government agencies on time and frequency metrology.

FY 1989 Plans and Accomplishments

Provide measurement support and advice to the Air Force Space Division and the Master Control Station for GPS on the performance of the Block 2 satellites as their launch sequence starts in January of 1989.

Accomplishment - Three new GPS satellites with S/A have now been launched. The Division has chosen to avoid the secure receivers with their high initial and maintenance costs in favor of other methods (described above). These are more tedious, but retain an openness that is more conducive to civilian use of the system.

Prepare a review paper on the AT1 algorithm and its philosophy of construction in response to rising interest on the subject.

Accomplishment - Five papers on time scale algorithms were published during FY 1990. With rising performance in ensemble clocks and primary standards, this is an important part of the Division effort to improve the overall performance of the time scales.

Study the effects of a variety of measurement conditions on time-domain data analysis as part of an effort to properly treat the problem of unequally spaced data in a time series.

Accomplishment - A NIST Technical Note that was completed this year addresses both the problem of unequally spaced data and data with dead time between measurements.

Serve as general chairman of the 1989 Frequency Control Symposium.

Accomplishment - Attendance at the Denver Symposium was substantially up from previous years. Feedback indicates that attendees were highly satisfied with the program. This is the first time that the Symposium has been held in the western U.S. We took advantage of the Symposium location to offer a fairly comprehensive tour of the NIST laboratory facilities. This was well attended and received.

FY 1990 Plans

Continue to work with the Air Force Space Division on all aspects of GPS operations, including the interface to civilian timing users.

VI. PHASE NOISE AND HYDROGEN MASERS

In past years, the primary goal of this Group has been the development of passive hydrogen masers with good medium-term to long-term stability for DOD requirements and for use in the NIST clock ensemble. The project, which was funded by the Navy, has been quite successful. Two masers are currently operating in the ensemble and they have been out-performing the commercial cesium standards by a wide margin. The maser technology has been transferred to industry through the Industrial Research Associate Program. The project has also addressed other issues of importance to the Division. These include: line-center errors in high-performance servo systems and phase noise in frequency multipliers and synthesizers.

More recently the program emphasis has shifted to measurement of phase noise where emerging technology is pushing the state of the art. The Group has made a commitment to the Department of Defense to develop and demonstrate phase-noise-measurement systems in the microwave and millimeter-wave regions of the spectrum. While the primary goal is to improve the accuracy of industrial and government measurements, this work will also result in low-noise synthesis to support development of primary standards and frequency synthesis into the optical region of the spectrum.

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OBJECTIVE: Generate NIST time scales UTC(NBS) and TA(NBS).

Active hydrogen masers have long been touted for their excellent short-term stability, but long-term stability has generally been poor. The NIST maser project has focussed on improving long-term stability in a passive maser that is simple and small. The goal was a system that would fit into a package equivalent to that of a commercial cesium standard. The results obtained have been quite good. The best of these masers provides medium-term stability equivalent to that of a cesium ensemble of about 20 high performance tubes. The fundamental design advance has been the servo locking of the physical cavity resonance to the hydrogen reference.

Experience gained with the maser development, particularly of the electronic components, has substantial relevance to other frequency standards work in the Division. This experience helps support the development of servosystems and frequency multipliers for NIST-7.

FY 1989 Plans and Accomplishments

Finish testing of the sine-wave phase modulator. If satisfactory, construct several units for use in NIST-7 and other cesium standards. If unsuccessful we will probably go to slow, square-wave frequency modulation.

Accomplishment - We have aided in the successful development and construction of the sources for the reference phase modulation. These have lower harmonic distortion than that of the current measurement system. Three phase modulators were built. Full testing has been delayed by slow delivery of additional components.

Additional Accomplishment - We have made significant advances in the understanding of the ratio of the modified Allan variance to the Allan variance as a function of measurement parameters. For some types of noise the current literature is in error. Lengthy approximations, which were difficult to use, have been replaced with a simple expression. This should encourage more people to use the modified Allan variance to reduce the effect of short-term noise on time and frequency measurements.

OBJECTIVE: Provide seminars and measurement services on a reimbursable basis.

Measurement of Phase Noise

The improved phase stability of components developed for the passive maser has enhanced the Division capability to provide special calibrations of phase noise in oscillators, amplifiers, frequency multipliers and synthesizers from 5 MHz to 700 MHz. The new DOD contract for development of phase-noise metrology through the microwave and into the millimeter-wave region will permit increased automation of these measurements. The goal is to cover the region from 5 MHz to 60 GHz for oscillators, amplifiers, multipliers, dividers and synthesizers. Emphasis will be on the development of sound measurement methodology and transfer of this methodology to industry and government labs.

FY 1989 Plans and Accomplishments

Complete documentation and automation for the systems covering 5 MHz to 1 GHz, 1 to 26 GHz, and 33 to 50 GHz.

Accomplishment - We have completed the documentation for the two original Phase Noise Measurement Systems (PNMS). Construction of the 3rd unit, started in early 89, is nearly complete. The 4th and 5th units are 80% and 50% complete, respectively.

Deliver prototype phase-noise-measurement systems to DOD sponsors for evaluation.

Accomplishment - This year we have significantly modified the original design to reduce the number of cable changes that are necessary to switch from one carrier frequency to another and to make them more rugged and less easily damaged by misuse. The first unit for MILSTAR was completed and is in use at NIST as originally planned. The second unit for CCG covering 5 MHz to 26 GHz is also complete. They are considering the addition of a 33-50 GHz front-end in FY90. Final delivery will be delayed if they want the 33-50 GHz front-end. A short training session was held in June and an additional one is scheduled for November 89.

Fabricate an additional 10.6 GHz oscillator system for frequency synthesis.
Accomplishment - The system is 95% complete. We have redesigned the oven for the oscillator to reduce the warm-up time and to make the phase-lock loop less vulnerable to power-line transients. Final assembly has been delayed by problems in procurement of the X-band oscillators. The oscillators are scheduled to be delivered by the end of September. If performance is satisfactory, assembly should be complete by November.

Investigate the statistical uncertainty of phase noise measurements as a function of the number of measurements. This will establish the uncertainties in a way similar to that used for $\sigma_y(\tau)$ and help standardize the uncertainty as reported by various laboratories and vendors.
Accomplishment - Major progress has been made on this problem. We have shown that, in contrast to results obtained in the time-domain, the statistical confidence of spectral estimates of fast-Fourier-transform spectrum analyzers is constant for a given number of measurements to within 4% for noise with spectra varying from f^{-4} to f^0. We have also developed simple experimental techniques to verify both statistical confidence and biases in any other type of spectrum analyzer. The results allow us to obtain spectral-analysis results that are accurate to better than 1 dB. This work, which has been well received by users, provides for consistent results using analyzers from different vendors.

Additional Accomplishment - Demonstrated the unfolding of spectral density measurements for a special phase-noise calibration where the reference oscillator had 10 dB more noise than the device under test. This proved the power of the new phase-noise-measurement concept and demonstrated that some oscillators have frequency stability equal to or better than 1×10^{-13}.

FY 1990 Plans

Complete and deliver three phase-noise-measurement systems for DOD.

Develop capability for converting phase-noise data into short-term measurements of time domain frequency stability.

Contingent on adequate funding, develop systems and documentation for a special phase-noise-measurement service.

OBJECTIVE: Establish the second and meter for the International System.

FY 1989 Plans and Accomplishments

Investigate phase locking of Gunn diodes. These are much noisier than klystrons but last longer and are easier to use because voltages are lower.

Accomplishment - We have successfully phase locked a Gunn diode oscillator at 45 GHz and suppressed the phase noise close to the carrier by more than 80 dB by using wideband, phase-compensated, loop filters.

Study concepts for multiplication to 4.25 THz.

Accomplishment - The new contracts to develop and deliver three phase-noise-measurment systems have forced delay of this project.

FY 1990 Plans

Study various concepts for multiplication to 4.25 THz and conduct preliminary tests on the best approach.

Investigate noise characteristics of several frequency-divider concepts that might be used in place of frequency multipliers.

OBJECTIVE: Advise industry and government agencies on time and frequency metrology.

Hydrogen Maser Technology

The passive hydrogen maser developed at NIST with partial military funding has demonstrated exceptional frequency stability from a few seconds to a few weeks. Based on 2 months of data, the stability is $\approx 3 \times 10^{-15}$ at 8 days. At a level of resolution of $\pm 3 \times 10^{-16}$/day, the drift is not observable. The time dispersion per day is a factor of 4 to 5 times better than the best available commercial cesium frequency standards. Several Industrial Research Associates have worked with NIST on this program. This cooperation is nearing an end and the first passive hydrogen maser to be constructed by our industrial partner is near operation. The Division has discontinued further development of these masers.

Quartz Crystal Resonators

Vibration sensitivity is presently one of the most severe difficulties encountered when using a frequency standard in non-laboratory environments. Although NIST no longer has a quartz crystal research program, consulting support is being provided to the U.S. Army and its industrial contractors. A new method for temperature control of clocks that was developed in the hydrogen maser project would appear to offer promise for quartz resonators.

The Time and Frequency Division in cooperation with Electromagnetic Fields Division (723) has provided support to the quartz industry in the development of standards for quartz oscillators. Two industry workshops on the subject were organized in Boulder and the result is a simple measurement procedure based on conventional impedance standards. The method provides traceability to National standards and forms the basis for solid U.S. leadership in quartz standards.

Phase noise

With the initiation of new work on measurement and control of phase noise, the Division is providing significant consultation on the subject to science, industry and other government agencies. The Division has a clear opportunity to provide the definitive basis for phase noise metrology.

FY 1989 Plans and Accomplishments

Assist government laboratories and industry in implementing the new NIST concept for high accuracy phase noise measurements.

Accomplishment - We have provided detailed information on the new NIST methods to 10 different organizations. One company is now actively pursuing development of a commercial instrument based on the NIST design. In addition, we have provided consultation to over 25 organizations on other aspects of precision measurements in this field. Two government laboratories, beyond the five that have contracted to obtain phase noise measurement systems, have provided funding to cover the consulting.

FY 1990 Plans

Continue to assist government laboratories and industry in implementing the NIST concept for high accuracy phase noise measurements.

VII. ATOMIC BEAM STANDARDS

This Group is responsible for maintenance and operation of the current primary frequency standard, NBS-6 and the older standard NBS-4 which is a key contributor to the NIST time scales. It is also responsible for the development of NIST-7, the next generation primary frequency standard, which will be based on optical state selection and detection methods. The objective is a standard that can be easily operated in a nearly continuous mode with semiautomatic assessment of systematic errors at an accuracy level of 1 part in 10^{14}. Ease of evaluation is important since NIST-7 will have to be used to calibrate the time scale at least once each month. In fact, the long-term performance of the time scale will then be heavily dependant on NIST-7. The project follows successful tests of the optical pumping concept on field-size standards pumped by diode lasers. The reliable operation of these diode lasers is a key ingredient in this development. Staff of the Laser Frequency Synthesis Group is assisting with the line narrowing and stabilization of these lasers.

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OBJECTIVE: Establish the second and meter for the International System.

Operation of the U.S. Primary Frequency Standard

Since 1968 NIST has designed and developed three new cesium standards: NBS-4, NBS-5, and NBS-6. NBS-4 has a medium-length cavity of 50 cm, and was built to test new ideas for improving the stability of cesium devices. This standard is one of the most stable cesium clocks in the world, achieving a stability of 7×10^{-15}. It should be noted here that no previous NIST cesium frequency standards directly drove a clock; instead, they were used periodically to calibrate the frequency of an ensemble of commercial cesium clocks. NBS-4, because of its excellent stability, has served as a working clock in the time-scale ensemble.

NBS-5 was built on the framework of NBS-3 and in turn served as the basis for NBS-6, completed in 1975. The refinements incorporated include greatly improved components to provide narrower resonance lines (25 Hz), the ability to reverse direction of the atomic beam (which allows errors due to asymmetries in the cavity to be diagnosed), and other features aiding analysis of performance. NBS-6 has an accuracy of 8×10^{-14}; more accurate but not quite as stable as NBS-4. NBS-6 is used to generate the U.S. standard second. It also provides input to the accuracy of international timekeeping. A clock ensemble is used to carry the second forward in real time so that it is continuously available.

FY 1989 Plans and Accomplishments

Complete work on NBS-4 and return it to service in the time scale.
Accomplishment - The servo system has been completely rebuilt and the performance-limiting problem was found in the beam tube. The tube was opened and the necessary rework has been completed. Evaluation of the performance of the standard has been initiated.

Study potential reduction of the uncertainty specification on NBS-6 and determine the advisability (limited resources) of attacking this project.
Accomplishment - The servo system for NBS-6 has been largely rebuilt and the grounding of the entire system, excluding the ion pumps and vacuum enclosure, have been redone. We believe that grounding

problems were responsible for the anomalous power shifts noted during the last evaluation. Through collaboration and discussions with several experts outside NIST, we now see that there may be a systematic error in machines (such as NBS-6) that use dual beam optics. It will be particularly useful to understand this new effect more completely and to determine just how large this shift is in NBS-6. The question of reducing the uncertainty statement for NBS-6 should probably await preliminary results from NIST-7. This will be useful only if the performance of NIST-7 falls short of expectations.

Initiate another evaluation of the systematic uncertainties in NBS-6.
Accomplishment - This evaluation has been delayed by repair work on NBS-4 (see above) and development work on NIST-7

FY 1990 Plans

With the recently gained insights on systematic errors and the rebuilding of components of NBS-6, complete evaluation of NBS-6.

OBJECTIVE: Perform research and development on new primary frequency standards.

Primary Cesium Standard Development

The known limitations to the accuracy of NBS-6 lie with the microwave cavity phase shifts, exacerbated by the velocity dispersive nature of the state selection magnets. In addition, there are unknown shifts of the cesium clock frequency associated with systematic effects that cannot be readily studied in conventional systems. Replacing the magnets in a cesium standard with optical pumping and detection using diode lasers should allow reduction of cavity-phase-shift uncertainties, and permit a better understanding of the limitations of cesium standards. A small laboratory version of the optically-pumped, cesium-atomic-beam frequency standard has been constructed and performance demonstrated at $\sigma_y(\tau) < 7 \times 10^{-12}\tau^{-\frac{1}{2}}$.

A larger test bed for the optically pumped standard has been designed and the major components have been fabricated and assembled. This test bed will serve as the basis for NIST-7. The system features a longitudinal C-field and a novel Ramsey cavity which minimizes errors caused by distributed cavity phase shift. The optical pumping concept provides the means for minimizing errors due to end-to-end cavity phase shift.

FY 1989 Plans and Accomplishments

Electronics. Complete development of and test the final prototype linear modulator. Fabricate the package for all of the electronic subassemblies. Fabricate the final servo electronics for control of the lasers.
Accomplishment - The odd-to-even synthesizer is now in good working order. The frequency-multiplier chains have undergone complete phase-noise and stability evaluation and minor modifications are now being

made. The linearity of the modulation has been the single most difficult facet of development in the electronic systems. It now appears that this is under adequate control. Final boards and packaging for all electronic components are nearing completion. These circuits will allow for preliminary studies of the standard, but we plan to begin development of an all digital, square-wave servo system which should provide much better performance and more reliability in the long-term.

Lasers. Complete final design of and fabricate the laser housings. Assemble the latest version of the optical-feedback-stabilized lasers for use in optical pumping and optical detection in the system.

Accomplishment - Housings for the diode lasers have been fabricated and the optical-feedback stabilization has been demonstrated. Further engineering of the diode-laser servosystems will be needed for long-term operation of the standard.

Beam Tube. Complete assembly of the beam tube. Initiate evaluation of the light-shift and Majorana effects.

Accomplishment - We suffered a substantial setback while baking the microwave cavity at a temperature that was well below the melting point of the solder that was specified for construction. The fabrication was done with a lower-melting-point solder and several key components had to be completely rebuilt. The system envelope has been under vacuum for many months following cleaning and assembly. There had been a problem with outgassing in the main chamber which had not been properly electrocleaned during fabrication. This chamber was sent out for additional cleaning and now appears to be in good condition.

FY 1990 Plans

Complete fabrication and modification of components for NIST-7. Reassemble complete standard.

Perform initial evaluation of NIST-7.

OBJECTIVE: Advise industry and government agencies on time and frequency metrology.

Cesium Beam Technology

Recent advances in cesium beam technology, including the optical pumping concept, could improve the performance of commercial devices. For example, this research could improve both the long-term stability and the reproducibility after turn-on of satellite based cesium clocks. These improvements involve the use of laser diodes, cesium heat pipe ovens, optical pumping, and fluorescence detection of atoms. In addition, with the assistance of a guest researcher, the Division has identified methods for improving performance of commercial standards through improved tuning methods.

Much of this work is performed under contract from other government agencies. In addition, the Division has an Industrial Research Agreement with a manufacturer of cesium clocks. This agreement permits the transfer of NIST research results to the private sector, and also brings guest scientists from industry to the NIST laboratories.

FY 1989 Plans and Accomplishments

Continue collaboration with industry and government agencies on the application of optical pumping methods to field standards.

Accomplishment - Consultation in this area continues, but commercial versions of optically pumped standards are still many years off. Development of such field standards is being stimulated by DOD contracts in the private sector.

Complete fabrication and testing of the hybrid recirculating oven.

Accomplishment - Fabrication of the oven is complete and testing has been initiated.

Test a commercial version of the recirculating oven.

Accomplishment - This project has been delayed by setbacks suffered in assembly of NIST-7.

Continue development of methods for improving the performance of commercial cesium standards. This includes direct methods for reducing Rabi-pulling effects and study of the third-order-servo system.

Accomplishment - Collaboration with De Marchi on the Rabi-pulling effect continues and the results are now well accepted by industry and international laboratories. The BIPM is organizing seminars (to be taught by De Marchi) aimed at disseminating information on this subject to the major standards labs of the world. The collaboration has had an impact on the design of standards from at least one U.S. manufacturer.

FY 1990 Plans

Complete testing of both the NIST and commercial recirculating ovens.

Evaluate the systematic error associated with dual-beam clocks and determine its importance in commercial standards.

Work with visiting professor on new concepts for high-performance rubidium cells which might prove useful as local oscillators for advanced standards.

VIII. ION STORAGE

The long-term plans for primary frequency standards for the Division involve an eventual shift to ion storage and radiative cooling. For the present, the effort of this Group is being directed toward study of the physics of the concepts. The Group has already demonstrated a Be^+ ion clock which operates at a performance level equal to that of NBS-6, the present primary standard. While the focus of the work is ion standards, the techniques are also applied to other problems of fundamental interest.

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OBJECTIVE: Perform research and development on new primary frequency standards.

Atomic Clock Based on Stored Ions

As a step towards realizing a primary frequency standard based on stored ions, the Division has developed a clock based on a ground state hyperfine transition in $^9Be^+$. The combined uncertainties of all systematic frequency shifts (such as those due to Doppler effects) have been demonstrated to be at the same level as those of the present U.S. primary time standard, NBS-6, which has an uncertainty of about one part in 10^{13}.

In these experiments, a few thousand $^9Be^+$ ions were confined in a Penning trap and laser cooled to temperatures less than 1 K. An oscillator was locked to a magnetic-field-independent hyperfine transition ($\approx$ 300 MHz) using an optical-pumping, double-resonance technique. The measured stability was somewhat better than that of a commercial cesium clock. Frequency stability and accuracy performance can be improved in the future by using an ion with a higher hyperfine frequency.

Farther in the future, it appears that the most accurate clocks will be based on optical transitions in atoms or molecules. The main reason for this conjecture is that the Q's for such transitions can be extremely high

($Q \geq 10^{15}$). With this in mind, the S→D quadrupole transition in Hg^+ has been studied. The transition was observed in a miniature rf trap on a single Hg^+ ion. The present linewidth is limited by laser frequency fluctuations which broaden the line, but this transition has a fundamental Q of about 0.5×10^{15} (radiatively limited).

Trapped Ion-Cloud Studies

Studies are made of ion dynamics and the relation of these dynamics to trap design. It appears that the principle limitation to accuracy of a frequency standard based on many ions stored in a Penning trap will be the uncertainty in the second-order-Doppler (time-dilation) frequency shift due to the rotation of the ion cloud. This rotation is a non-thermal effect and is independent of the internal temperature of the cloud. Therefore, detailed studies of ion-cloud temperature, density and rotation are being made using a two-laser, optical-optical, double-resonance technique.

A new concept for a frequency standard based on "sympathetic cooling" is being studied theoretically and experimentally. In sympathetic cooling, one ion species is cooled by Coulomb coupling with another ion species that is laser cooled. This was proposed and demonstrated (on the Mg^+ isotopes) a few years ago at NIST and has now been studied in more detail using Hg^+, Mg^+ and Be^+. The advantage is that the "clock" ions can be continuously cooled, but ac Stark shifts from the cooling radiation can be made negligibly small. This has resulted in narrow linewidths (less than 1 mHz) and reduction of errors due to the second-order Doppler shift.

FY 1989 Plans and Accomplishments

Lock the local oscillator to the $^9Be^+$ hyperfine transition and evaluate all systematic effects.

Accomplishment - *$^9Be^+$ Frequency Standard*. An oscillator has been locked to a nuclear-spin-flip hyperfine transition (≃ 303 MHz) in $^9Be^+$ ions that are stored in a Penning trap. FY89 experiments have used "sympathetic cooling" whereby laser-cooled Mg^+ ions are stored simultaneously with the Be^+ ions and the Coulomb interaction between ions cools the Be^+ ions. This has allowed the hyperfine transition to be interrogated with Ramsey times of up to 550 s giving linewidths less than 0.001 Hz. Stabilities (currently limited by the reference cesium clock) are measured to be better than $3 \times 10^{-12}\tau^{-1/2}$. Uncertainties in Doppler effects are estimated to be $< 5 \times 10^{-15}$. For comparison, the smallest uncertainty previously claimed for Doppler shifts on any atomic clock is 15×10^{-15}. Unfortunately, we have discovered a hyperfine pressure shift which is about 1000 times larger than expected. This shift is caused by H_2 (or perhaps He) and limits the accuracy of the hyperfine measurement to about 10^{-13} even though the pressure in the experiment is about 10^{-8} Pa. There are straightforward ways to get around this problem, but nothing has been tried yet.

Additional Accomplishment - *Hg^+ Optical Frequency Standard* - A stable laser has been used to probe the $5d^{10}6s\ ^2S_{1/2} \rightarrow 5d^96s^2\ ^2D_{5/2}$

transition in single $^{199}Hg^+$ ions (see figure below). Linewidths of approximately 100 Hz have been observed giving a quality factor $Q \equiv \nu_0/\Delta\nu(\text{linewidth}) \simeq 10^{13}$. This is the highest Q ever reported in atomic or molecular spectroscopy.

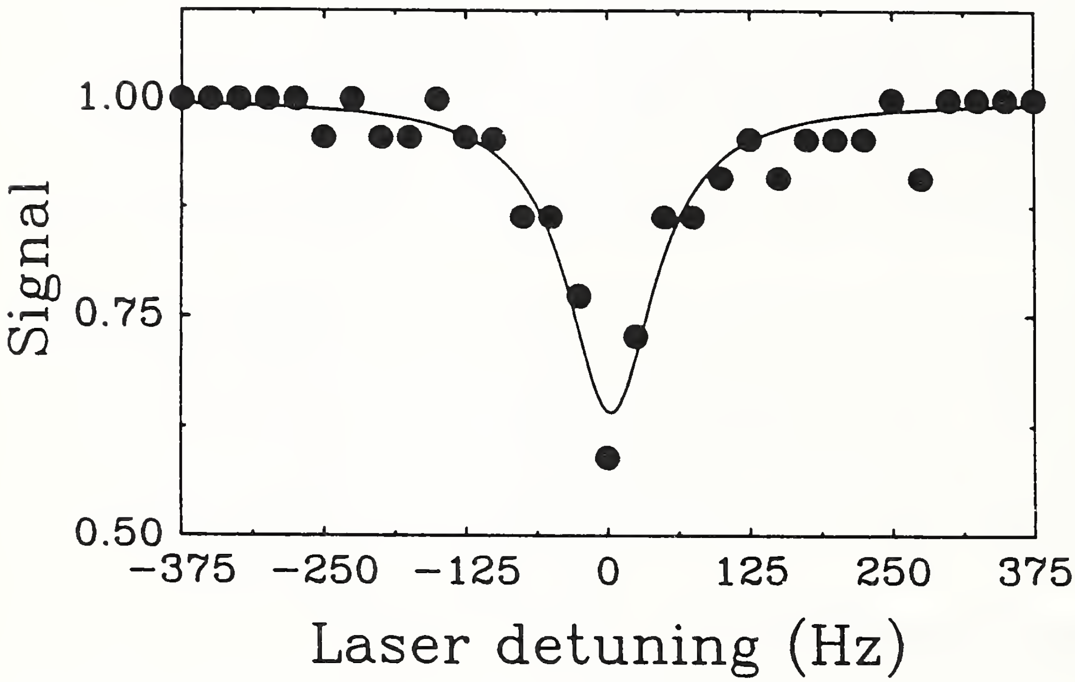

Figure 2. Absorption resonance of the $^2S_{1/2}$ (F=0, m_F=0) → $^2D_{5/2}$ (F=2, m_F=0) transition in a single laser-cooled $^{199}Hg^+$ ion in a Paul electromagnetic trap. A stabilized and frequency-doubled dye laser (563 nm) is stepped through the resonance in 25 Hz increments. The full width at half maximum is about 90 Hz.

Additional Accomplishment - *Laser Development for the* Hg^+ *Optical Frequency Standard* - Effort has been devoted to stabilizing a dye laser (563 nm) to a Fabry-Perot cavity. This laser, when doubled, is used to probe the optical transition in Hg^+. A stability/spectral width of 50 Hz was obtained for > 1 minute averaging time. This linewidth is narrower than that of any visible laser ever reported.

FY 1990 Plans

Prepare plans for measurement of pressure shifts in the $^9Be^+$ frequency standard. This will require modification of existing apparatus and therefore will have to wait until current experiments with this system are completed.

Build a linear rf trap for storage of $^{199}Hg^+$ ions and measurement of the 40.5 GHz hyperfine transition in these ions. This trap should allow storage of up to 100 $^{199}Hg^+$ ions which can be treated as independent clocks in an ensemble. Doppler shifts should be much less than 10^{-15}.

Improve laser stabilization so that the Hg^+ 281 nm clock transition can be observed with linewidths approaching 2 Hz (limited by radiative decay). The main task is to make the reference cavity, to which the laser is stabilized, as quiet as possible.

OBJECTIVE: Perform basic studies in areas related to future frequency standards.

As an outgrowth of studies on ions stored in ion traps for possible frequency standard application, several closely related basic studies have been undertaken. Two examples are given below.

Search for Spatial Anisotropy

Frequency standards, including those based on atomic or nuclear (Mossbauer) transitions, have traditionally played an important role in testing gravitational theories. One example is measurement of the gravitational red shift. In addition, the very high resolution attained in trapped ion spectroscopy enables other sensitive tests of the Einstein Equivalence Principle (EEP). As a test of the EEP the frequency of the $^9Be^+$ "clock" transition (M_J = 1/2, M_I = -3/2) → (M_J = 1/2, M_I = -1/2) has been compared to the frequency of a passive hydrogen maser to see if a correlation can be found with orientation in space. With a resolution better than 0.1 mHz, no variation was observed. These results decreased previous experimental limits by a factor of 300, but were superceded by subsequent experiments on neutral atoms (University of Washington). A projected gain of a factor of 1000 over our previous measurements should be achievable using $^{25}Mg^+$ or $^9Be^+$ in the superconducting magnet. Such measurements are a fairly straightforward extension of searches for systematic frequency shifts in an ion frequency standard.

Non-Neutral Plasmas

In the language of plasma physics, the ion clouds in a Penning or rf trap comprise a one-component, non-neutral ion plasma. In a small plasma of laser cooled $^9Be^+$ ions stored in a Penning trap, we have observed behavior that is indicative of the liquid, solid and smectic states. In this case the Coulomb coupling constant Γ was as high as 100. Calculations predict that at Γ ≃ 2, the ion pair correlation function should begin to show oscillations characteristic of a liquid, and at much larger values of Γ (Γ ≃ 170) crystallization may take place. In our experiment a second laser was used to probe the ion plasma and measure the temperature of the ions from the Doppler broadening of the optical probe transition. The ion number density was determined by measuring the ($\vec{E}\times\vec{B}$) cloud rotation frequency. Because the trap electric field and magnetic field were known, the space charge electric field was extracted from the cloud rotation frequency and used to determine the ion number density. Ion number densities of $\approx 2 \times 10^7/cm^3$ and temperatures of $\approx$ 10 mK produced values of $\Gamma \simeq 100$. Values of Γ large enough to observe a liquid-solid phase transition should be accessible in future versions of this experiment. If the theoretical cooling and density limits can be obtained, values of Γ as large as 15,000 are perhaps possible for Be^+ ions. Because experimental information on three-dimensional, strongly-coupled plasmas is almost non-existent, these experiments can provide some useful tests of the theoretical calculations. The development of a clear understanding of ion-cloud dynamics is fundamental to the estimation of systematic errors in frequency standards arising from motions of the ions.

<u>FY 1989 Plans and Accomplishments</u>

Single (Or Few) Ions. Initiate experiments on interference, radiation spectra and intensity correlations in the scattered radiation from one, two or more ions. A small trap with inner dimensions of 50 μm is under construction for these experiments.

<u>Accomplishment</u> - Optical sideband cooling experiments have been completed. The fundamental limit of cooling for any particle that is contained by some apparatus (the electrodynamic trap in our experiment) is putting the atom in the zero-point state of motion. We have achieved this (for the first time) using single Hg^+ ions and the results were published in the Physical Review Letters.

Ion Spectroscopy. (1) Redo the spatial anisotropy measurement on $^9Be^+$. (2) Compare the results of the $^9Be+$ hyperfine-splitting measurements in the superconducting magnet with those done in the conventional magnet. This comparison tests the existence of a long-range, spin-spin interaction mediated by classes of hypothetical particles such as axions.
(3) Investigate fundamental atom-cavity interactions using trapped ions.

<u>Accomplishments</u>

Test of the Linearity of Quantum Mechanics - A hyperfine transition in the ground state of $^9Be^+$ was used to test a nonlinear generalization of quantum mechanics recently formulated by Weinberg. We searched for a dependence of the frequency of coherent superposition of two hyperfine states on the populations of the states. We are able to set a limit of 4×10^{-27} on the fraction of binding energy per nucleon of the $^9Be^+$ nucleus that could be due to nonlinear corrections to quantum mechanics. This is five orders of magnitude better than the previous best estimate.

Search for Anomalous Long-Range Interactions by $^9Be+$ Nuclear Magnetic Resonance - We have searched for interactions that could arise if the $^9Be+$ nucleus has a gravitational dipole moment or has an anomalous long-range, spin-spin interaction. Such experiments are the spin-dependent counterparts of "fifth-force experiments." We believe that our measurements are at the same level or better than other tests of the existence of such interactions.

Preliminary Observations of Quantum Zeno Effect - The quantum Zeno effect is the inhibition of transitions by frequent measurements. We have observed this effect in a ground-state hyperfine transition of $^9Be^+$ ions.

Sympathetic Cooling - Sympathetic laser cooling has now been routinely used to cool $^9Be^+$ ions (sympathetically cooled by laser-cooled Mg^+ ions). This has allowed observation of linewidths as small as 0.0003 Hz, the smallest recorded in atomic or molecular spectroscopy.

Atom-Cavity Interactions - These experiments were postponed because fabrication of trap is not yet complete.

Strongly Coupled Plasmas. Experimentally investigate anisotropic diffusion in strongly coupled ion plasmas contained by a Penning trap.

Accomplishment - Liquid, smectic and solid phases of strongly coupled $^9Be+$ plasmas have been observed, but observations are still not quantitative. A plasma mode in a spheroidal sample of Be+ ions has also been observed. By using laser torque, we have reached cold, stable clouds at rotation frequencies corresponding to Brillouin flow (plasma unmagnetized in a rotating frame).

Synchrotron Divider. Assemble the newly designed synchrotron-divider apparatus and perform experimental tests of its performance.

Accomplishment - The trap construction is complete and it will be installed in vacuum in the near future.

FY 1990 Plans

Complete quantum Zeno effect measurements.

Write paper on search for anomalous long-range interactions.

Study plasma conditions at near-Brillouin-flow conditions; study plasma instabilities related to mode coupling, ie., rotation/cyclotron parametric coupling processes.

Attempt to use Raman laser cooling and temperature probing with the Be^+ ions.

Perform theoretical investigation and perhaps initiate experiments on "electronic sympathetic cooling." The idea here is to cool ions in one trap by electrically coupling them to laser cooled ions in another trap.

Initiate experiments with "small" rf traps (internal dimension $\simeq 50\ \mu m$). With extreme confinement in these small traps, we can do atom/radiation interaction studies (including atom/cavity experiments) in situations where the atom is localized to $< \lambda/2\pi$ even in the optical regime.

Install trap in vacuum system and perform initial single-electron experiments for synchrotron frequency divider.

IX. LASER FREQUENCY SYNTHESIS

This Group retains the expertise and facilities that were used in earlier measurements of the speed of light and the subsequent work that led to the redefinition of the meter in terms of the second. More recently, this frequency synthesis has proven to be extremely useful as a basis for frequency and wavelength spectroscopic standards in the infrared and far infrared. The Group is also developing the expertise needed to stabilize and line-narrow the output of tunable diode lasers. With proper development these lasers promise great simplification of systems for frequency synthesis from the microwave to optical regions, for measurement of optical frequencies, for phase-noise characterization of optical components, and for optically pumping ions/atoms in new frequency standards. The objective is to provide sources that support development of atomic frequency standards and systems for characterizing components in the next generation of optical communication systems.

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OBJECTIVE: Establish the second and the meter for the International System.

Frequency Measurements Suitable for Realizing the Definition of the Meter

In October of 1983 the General Conference of Weights and Measures approved a change in the definition of the meter, namely that: "The meter is the length of the path travelled by light in vacuum during a time interval of 1/299 792 458 of a second." With this definition the meter can be realized from the wavelength of any laser that is stabilized to a narrow atomic or molecular absorption for which the frequency is known. The wavelength λ is determined from the relation $\lambda=c/\nu$, where c is the fixed value of the speed of light and ν is the measured frequency of the laser. Thus, the realization of the meter requires measurement of the absolute frequency of spectral lines in the visible region. To this end, the Division has performed two accurate frequency measurements at 520 THz (576 nm) and 473 THz (633 nm) of hyperfine transitions in molecular iodine. Total uncertainty was 1.6 parts in 10^{10}. These frequencies, when used to realize the new meter, represent a 25-fold improvement over the krypton length standard. However, for scientific purposes, another order of magnitude in accuracy is needed. There is no active Division program in this area now, but advances in frequency synthesis and optical frequency standards could make this work important in the future.

OBJECTIVE: Provide reference frequencies from the microwave to visible regions.

Frequency References (Measured with Respect to the Cesium Standard)

The advances made by the Laser Frequency Synthesis Group in extending direct frequency measurements from the microwave to the visible portion of the spectrum are now being used to determine the frequencies of atomic and molecular transitions. These measurements are hundreds of times more accurate than the old wavelength measurements. The knowledge of the frequencies of selected species allows the spectroscopist, astronomer, or atmospheric scientist to calibrate spectrometers and receivers with appropriate atomic or molecular frequencies (or wavelengths).

The generation of reference frequencies with requisite accuracy involves accurate heterodyne frequency measurements and the reliable fitting and analysis of the spectral data. The CO_2 laser that is stabilized to CO_2 itself furnishes the main frequency grid for all of these measurements and is widely used for reference purposes.

FY 1989 Plans and Accomplishments

Measure the OCS band at 2062 cm^{-1} as standard reference frequencies.
Accomplishment - This work is now complete and publication is nearly ready for submission to the Journal of Molecular Spectroscopy.

Measure the SO_2 band at 1320 cm^{-1} as standard reference frequencies.
Accomplishment - The work on SO_2 for this band (1320 cm^{-1}) is nearly complete. Preliminary work on a publication has been initiated.

Improve the spectrometer instrumentation by adding a White cell and a Brewster angle fringe spoiler. The latter item should help to eliminate standing waves in the spectrometer.
Accomplishment - This improvement in the spectrometer has not yet been needed, so this project was postponed.

FY 1990 Plans

Measure the OCS $04^{0}0$ band at 2105 cm^{-1} to provide standard reference frequencies.

Construct a new $\Delta v = 2$ CO Laser for operation near 3000 cm^{-1}.

Use $\Delta v = 2$ CO laser to measure the OCS 01^13 band at 3057 cm^{-1} to provide standard reference frequencies.

Improve efficiency of data acquisition by converting spectrometer to computer control.

OBJECTIVE: Develop methods for precise time, frequency and length measurements.

Measurement of Frequency and Frequency Stability

Frequency metrology from the far infrared to the visible has been greatly stimulated by work in the Division. An extremely important aspect of this work was the first frequency measurement of the 3.39 μm line of CH_4 followed by the wavelength measurement of the line. The product is a value for the speed of light nearly 100 times more accurate than the previously accepted value. Coupled with frequency measurements of visible lines, this has led to replacement of the krypton lamp as the length standard and the assignment of an exact value for the speed of light. Recent work on the MIM diode has expanded the range over which frequency-difference measurements can be made in the visible by a factor of 100. This is expected to greatly simplify frequency metrology because it reduces the number of frequency reference lines needed to cover this important spectral region.

Techniques for Laser Frequency Synthesis

Frequency synthesis is achieved in a non-linear device which adds, subtracts and multiplies the frequencies of the radiations incident on it. The Division has used Schottky-barrier diodes and metal-insulator-metal (MIM) point-contact diodes as detectors, harmonic generators, and mixers of coherent radiation from the microwave to the visible region of the spectrum. The MIM diode played a major roll in the frequency synthesis chain that connected the cesium clock to the visible and hence provided a new realization of the meter.

Building on this work, the Group developed a source of tunable-far-infrared radiation that uses second-order and/or third-order mixing of CO_2 laser frequencies and microwave frequencies. This system provides complete coverage of tunable cw radiation in the entire far infrared band from 100 to 6000 GHz. This set the basis for accurate measurement of the HCl, CO, and HF spectra from 0.5 to 5.5 THz, and these simple molecules now provide for excellent calibration standards in this frequency range.

Diode Lasers as Spectrally Pure Sources for Optical Frequency Metrology

The characteristics of diode lasers are improving at an impressive rate, that is in terms of power, wavelength, and both spectral and spatial coherence properties. Not surprisingly, diode lasers have a multitude of advantages (though not always simultaneously present) including high efficiency, good power, good (solid-state) reliability, useful wavelengths, broad tunability, and reasonable spectral and spatial properties. However, the spectral and spatial properties of commercially available diode lasers are still substantially worse than those of the best gas and dye lasers. Because of the importance of spectral and spatial coherence in metrology, this area is of particular significance and interest for NIST. Recent success in this Division and JILA in narrowing the linewidth of these lasers suggests that, with further development, they might be real competitors with their conventional counterparts. With improved linewidths, the many advantages of diode lasers can be put to use in atomic/molecular physics and precise metrology. Some of the important applications include laser cooling and manipulation of atoms, high-resolution spectroscopy, and instrumentation for precise measurements. Important applications in this last category are optical frequency standards, length metrology, and characterization of advanced optical communication components and systems.

FY 1989 Plans and Accomplishments

Phase lock the 70 μm methyl alcohol line (4.5 THz) to the high-purity, X-band oscillator using a Schottky diode as the mixing element.

Accomplishment - This work has gone slower than expected because of delays in construction of the new laboratory. The 4.5 THz lasers are nearing completion.

Study concepts for stabilizing an oscillator near 1.5 μm, a region important for optical communication.

Accomplishment - Developed a simple technique for AR coating laser diodes. More sophisticated equipment with better control will be needed to perform this task within carefully specified tolerances. This capability is needed to adjust optical coupling to external components and to enhance the tunability of the lasers.

Investigate methods for stabilizing a Gunn oscillator at 80 GHz with a wideband servo system.

Accomplishment - The characteristics of the 80 GHz Gunn oscillators were not appropriate for our stabilization scheme. Thus the concepts were tested using a different Gunn oscillator at 45 GHz. Improvement in stabilization was better than 20 GHz.

Set up a new frequency measurement laboratory dedicated to research in frequency synthesis and frequency measurements in the optical region.

Accomplishment - This laboratory has been completed, but the construction (including removal of asbestos) took six months longer than expected.

FY 1990 Plans

Develop fast frequency response FIR laser (4.5 THz) for phase locking to a microwave source.

Continue work on 1 μm laser diodes including effort to better control spectral purity, mode quality, power stability, etc.

Finish laser diode work at 780 nm (Rb Standard).

Continue to look for ways (nonlinear optics) to connect 3.39 μm radiation to the visible region.

Continue study of methods for simplification of frequency synthesis between 10 and 1 μm.

Continue work on red diode lasers (650 and 670 nm) for application to spectral measurements of Li, Ca, H and I_2. These atoms and molecules are potential frequency standards in that region.

Develop diode lasers for generation of radiation useful for simplification of trapped ion frequency standards. This includes the system for generating 194 nm radiation where a 790 nm diode laser will replace one argon-ion and one dye laser as well as an all-diode-laser system at 776 nm. An additional objective is to develop a source at 1.126 μm for synthesis of the Hg^+ ion transition frequency.

X. GEOPHYSICAL MEASUREMENTS

This is a small program conducted in JILA by Time and Frequency Division staff. One of the projects involves construction and demonstration of an apparatus for measuring intermediate baselines (25 km to 50 km) with an uncertainty of 1/2 cm or less. The multiple-wavelength technique that is used is closely related to satellite navigation and timing problems which also require a complete accounting for atmospheric dispersion. A second project involves use of an array of tilt detectors to study properties of the earth's mantle and core-mantle boundary in the Yellowstone region. These tiltmeters are also installed in a seismic zone in Southern California to investigate the utility of tilt measurements for earthquake prediction. A third program involves the use of GPS signals for geodesy. This is a joint effort involving seven universities and funded by the National Science Foundation.

Staff: J. Levine, Project Leader
A. Brewer (Research Assistant - CU)
M. Holt (Research Assistant - CU)
M. McCallum (Research Assistant - CU)

OBJECTIVE: Develop methods for precise time, frequency and length measurements.

Distance Measurement Techniques

The need to accurately determine the lengths of baselines on the surface of the earth arises in many different contexts, ranging from the calibration of tracks used for rocket tests to estimation of the relative motions of large geographical regions in seismically active zones. This work is particularly timely, since the use of timing techniques for such distance measurement is expected to grow, and a key roadblock to improved resolution involves an understanding of the dispersion of the atmosphere.

Geodesy from the GPS Satellites

Signal time of flight from GPS satellites and radiometric corrections for atmospheric and ionospheric dispersion can be used to make accurate geodetic measurements. A major program, funded by NSF, involves collaboration between a number of universities to use this concept. This NIST Group has assumed responsibility for hardware and software developments involving the GPS satellites and for some aspects of the initial data reduction and analysis.

FY 1989 Plans and Accomplishments

Three-Color Geodimeter. Incorporate microwave instrumentation in the geodimeter system. Conduct full-scale tests over a known baseline and compare the results with those using GPS. Conduct measurements in Southern California on the western side of the San Andreas fault.

Accomplishment - We completed the incorporation of the microwave instrumentation and conducted several comparisons between the index of refraction deduced from the multiple-wavelength measurements and the end-point measurements of temperature and humidity obtained from the NOAA tower at Erie. These measurements were conducted over a baseline from Boulder to Erie which is about 24 km long. The results of these measurements are being prepared for publication. The tests over a known baseline and the measurements in Southern California have been postponed for lack of funds.

Tiltmeters. Install a third instrument in Southern California. Continue analysis of the output data.

Accomplishment - The borehole for the third instrument was drilled earlier this year and the instrument was installed in June. There have been several technical problems with the datalogging and recording system, but all three instruments are working and the comparison among the various instruments is partially completed. Two papers were published in the Journal of Geophysical Research (JGR) this year discussing the results in Yellowstone National Park, and two invited talks were given discussing the design of tiltmeters.

Geodesy using GPS. Cooperate in the conduct of campaigns in Turkey, South America, the Colorado Triangle and Southern California. Using CDROM disks, improve the systems for archiving GPS data.

Accomplishment - All of the campaigns were completed successfully. Approximately 2000 field tapes were recorded and the preliminary conversion to standard format tapes has been completed. The conversion to CDROM format has been postponed because of inadequate funding.

FY 1990 Plans

Three Color Geodimeter. During FY 1990, we hope to complete the accomplishments originally scheduled for 1989. Specifically, we plan to conduct measurements over known baselines and comparisons with GPS measurements both in Colorado and in Southern California.

Geophysical Tilt Measurements. We will continue our analysis of data from the instruments in Southern California. We plan a long-baseline comparison between instruments in Southern California and Yellowstone National Park to investigate long-wavelength tilt signals. We will request funds for additional instruments along the San Andreas Fault in Southern California, especially in the vicinity of the Salton Sea.

Geodesy Using GPS. Campaigns are planned in Iceland, Turkey, South America, Yellowstone and the South Pacific Islands. If promised increases in funding become available, we will begin a system for publishing our data and results using CDROM (optical disk) technology.

XI. LASER SPECTROSCOPY

This program focusses on the application of high-resolution, frequency measurements to the study of atomic and molecular spectra in the far infrared region (300 to 6000 GHz) of the spectrum. The emphasis is on the development of new and improved spectroscopic methods and on the application of these methods to the study of free radicals and other molecules that are significant in upper atmospheric and astronomical research.

staff:
- K. M. Evenson, Project Leader
- S. Beaton (Research Assistant - CU)
- R. Bernheim (Guest Researcher)
- J. M. Brown (Guest Researcher)
- C. Demuynck (Guest Researcher)
- M. Sassi (Guest Researcher)
- G. Schwaab (Guest Researcher)
- J. Towle (Guest Researcher)
- W. Urban (Guest Researcher)
- E. C. C. Vasconcellos (Guest Researcher)

OBJECTIVE: Measure spectral frequencies of atoms and molecules.

High resolution spectroscopic measurements in the far infrared have been advanced significantly through development at NIST of two measurement techniques. These permit laboratory measurements that have bearing on atmospheric and astronomical studies.

Laser Magnetic Resonance (LMR) spectroscopy has been developed into an ultrasensitive technique (i.e., several orders of magnitude more sensitive than microwave spectroscopy) for observing new atomic and molecular species and measuring reactions involving them. LMR techniques are singularly effective in measuring chemical reactions necessary to model the effects of pollutants (e.g., fluorocarbons, nitric oxide, etc.) in the atmosphere.

The new techniques of Tunable Far Infrared (TuFIR) spectroscopy promises to enhance the LMR technique by measuring frequencies of some of the same free radicals without a magnetic field. These spectroscopic measurements will have greater accuracy than the LMR measurements. The technique, an outgrowth of NIST frequency synthesis work involving MIM diodes, also allows measurement of all far-infrared-active molecules, not just the paramagnetic ones.

FY 1989 Plans and Accomplishments

Install a cooled grating prefilter in the TuFIR spectrometer.

Accomplishment - Procurement of the grating took longer than expected, but it has arrived and the system will be ready for testing in October.

Study the third-order-mixing process in MIM diodes.

Accomplishment - For tungsten-nickel diodes we have no problem obtaining I-V characteristics for second-order-mixing processes, but the third-order characteristics have been more difficult to obtain. We do not understand how these distinctly different characteristics can arise within the same diode structure. A guest researcher who has special experience in diodes arrives on October 1, 1989 for a stay of three months and we hope that this issue will be resolved during her stay.

Analyze recently obtained LMR data on NiH, FeH and CoH.

Accomplishment - Analysis of the NiH data is complete and analysis of that on FeH is nearly complete. The spectrum of CuH was also measured using TuFIR and a manuscript on the results is nearly complete. More data on CoH and CrH are being taken and analysis of that data will begin when the experimental phase of the project is completed.

Study pressure broadening and temperature dependence of the spectral lines of OH and O_2 using TuFIR.

Accomplishment - Experimental measurements of pressure broadening and temperature dependence of the spectral lines of these molecules has been completed. The data are now being analyzed. This work is especially relevant to studies of the upper atmosphere.

Search for new ions such as NH^+, NeH^+ and HeH^+ and measure more lines of H_2D^+ and D_2H^+ using TuFIR.

Accomplishment - The ground rotational-state transitions of H_3O^+, D_2H^+, and H_2D^+ have all been measured using the TuFIR system and manuscripts on this work are in preparation. In addition, high-accuracy measurements of a number of HO_2 lines have been completed.

FY 1990 Plans

Demonstrate improved performance of the TuFIR spectrometer with the cooled prefilter.

Continue study of MIM diodes in an effort to gain an understanding of the structures and mechanisms responsible for second-order and third-order mixing.

Finish LMR measurements on CoH and CrH and analysis of FeH measurements.

Search for additional metal hydrides such as CaH, MnH, and AlH.

Set up an *in situ* FIR spectrometer in an effort to directly measure OH in the upper atmosphere. This instrument will be flown in a joint project with NOAA.

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QUANTUM PHYSICS DIVISION

FISCAL YEAR 1989 TECHNICAL ACTIVITIES

OVERVIEW

Quantum Physics Division (577)

Through the Quantum Physics Division, NIST participates in the Joint Institute for Laboratory Astrophysics, a cooperative enterprise between NIST and the University of Colorado (CU). In collaboration with University faculty and visiting scientists, the Division conducts long-term, high-risk research in support of the Nation's science and technology. The Division's objectives are:

- o Developing the laser as a refined measurement tool and applying it to tests of fundamental postulates of physics such as special and general and relativity.
- o Improving the theory and instrumentation required to measure astrophysical and geophysical quantities such as the cosmic distance scale, the acceleration of the earth's gravity, and the long distances involved in determining crustal movements.
- o Researching new techniques for measuring interactions involving electrons, atoms and molecules to provide data essential in areas such as thermonuclear fusion, high power switches, advanced lighting, and laser development.
- o Developing and applying measurement techniques to advance fundamental understanding of microscopic molecular processes such as those that occur in combustion and laser-initiated chemical reactions.
- o Interacting with University faculty and visiting scientists to maintain expertise at the forefront of research in physics.
- o Transferring the results of its research and the technology developed to the Nation's industries, universities and other government agencies.
- o Exchanging ideas and skills with other scientists in NIST through visits, seminars and longer-term interchanges of personnel.

A direct outgrowth of the national space program in the early 1960s, JILA was formed in response to a report of the Space Science Board of the National Academy of Sciences. That report pointed to serious gaps in our basic understanding of the behavior of atoms and molecules in terrestrial, planetary, solar and stellar atmospheres. The unifying theme for the Institute therefore became the physics of gaseous atmospheres. Since then, however, JILA has responded to changing national needs and to the requirements of its parent organizations. Thus the Institute has become a world leader not only in atomic and molecular science and astrophysics but also in precision measurement, laser physics, chemical physics and certain areas of geophysics.

The permanent senior scientists or "Fellows of JILA," of which there are currently 25, form a governing body that sets policy, subject to review by the Director of NIST and the President of the University. A Chairman, elected every two years by the Fellows, has much the same role as the chairman of an academic department. Assisted by an executive committee, he is responsible for operating the Institute within the policies set out by the Fellows. Of the 25 Fellows, 13 are full-time faculty members in the Departments of Physics, Chemistry, or Astrophysical, Planetary and Atmospheric Sciences; 12 are NIST employees, 11 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 academic department in the other.

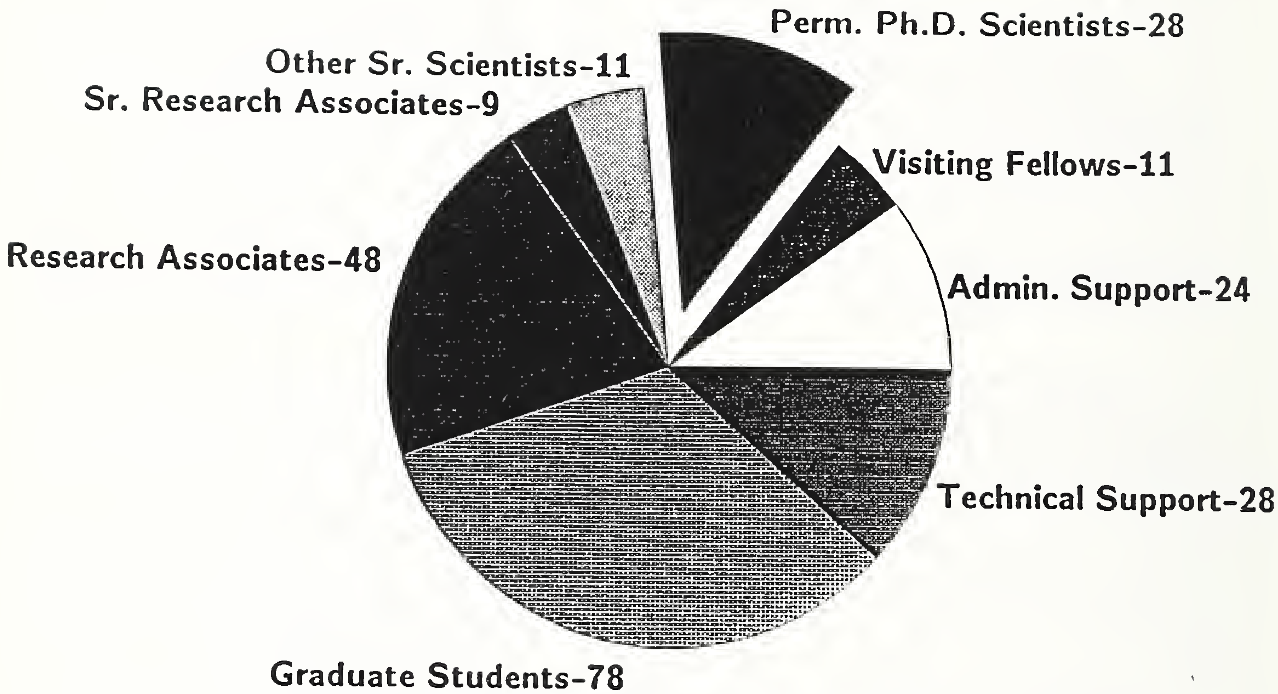
Through their adjoint faculty appointments, NIST scientists at JILA have both the opportunity and responsibility to teach courses and participate in other faculty activities. This gives them access to graduate and undergraduate students, some of whom become interested in pursuing research directed toward NIST goals. Of 78 graduate students in JILA, 40 are supervised in their research by NIST scientists; of 48 postdoctoral research associates, 29 work with NIST scientists. Some have subsequently joined NIST and now occupy positions of leadership; others are carrying the knowledge and skills acquired at NIST to the Nation's industries, universities and other government agencies. Of over 100 graduate students and research associates supervised by NIST staff at JILA during the past 9 years, 20% are now in industry, 20% in government agencies, and the remainder largely in universities.

Besides the graduate students and postdoctoral research associates, the Visiting Fellows Program is probably the single most important factor in maintaining an atmosphere of change and excitement in JILA. The Program provides partial funding for some ten internationally distinguished scientists a year to spend up to twelve months at JILA collaborating with resident scientist. Since its inception 26 years ago, the Program has become internationally renowned. More than 240 senior scientists from 29 foreign countries as well as the U.S. have participated. The number of applicants exceeds the number of positions typically by a factor of four. In accordance with the Memorandum of Understanding, applicants are chosen according to scholarly achievement, demonstrated interest in the scientific and technical objectives of JILA, and the recommendations of their peers.

For NIST and University researchers alike, perhaps the greatest attraction of JILA is the large concentration of scientific talent in atomic and molecular physics and closely related areas. Neither institution, one with a broad responsibility for measurement, the other for education, could justify such a large number of senior scientists in a single area. Together these researchers are able to collaborate, exchange ideas and attract visiting scientists in a way that would be impossible for two smaller groups operating separately.

JILA STAFFING 1988-1989

TOTAL - 237



This has been a particularly exciting year for the JILA scientists and staff:

- Stephen Leone was awarded the 1989 Herbert P. Broida Prize in Chemical Physics by the American Physical Society. The Broida Prize is awarded to an outstanding young scientist in Chemical Physics. It alternates annually between Physics and Chemistry. This year's award recognizes Leone's outstanding contributions to our understanding of the reaction dynamics of excited state, radical, and ionic species and the development of innovative probes to understand energy flow pathways in chemical reactions and to characterize energy dispositions.

- Gordon Dunn's highly successful term as Chairman of JILA came to an end on December 31. He was succeeded by Peter Conti, Professor in the Department of Astrophysical, Planetary and Atmospheric Sciences. Dunn is currently serving a one-year term as Chairman of the Division of Atomic, Molecular and Optical Physics of the American Physical Society.

- JILA is pleased to welcome a new Fellow: Chris Greene, a full Professor in the Department of Physics. Greene's principal research interests are the strong correlation effects in atoms and molecules, nonperturbative external field interactions, and alignment and orientation of photofragments.

- David Hummer received a Senior U.S. Scientist Award from the A. von Humboldt Foundation in West Germany. This award gave Hummer the opportunity to continue collaborative work at the Institute for Astronomy and Astrophysics in Munich from February through October, 1989.

- A patent was awarded to John Hall for his "Method and Apparatus for Laser Frequency Control." In addition, Hall has made a Patent Disclosure titled, "Measurement of the Refractivity of Ambient Air Using Fabry-Perot Interferometry and a Multi-Element Detector." Hall is easily the Nation's expert when it comes to precision laser technology.

- In recognition of the far-sighted and diplomatic leadership that Katharine Gebbie provided as Chief of the Quantum Physics Division, she was called to serve as Acting Director of the Center for Atomic, Molecular and Optical Physics.

- During the past year, Quantum Physics Division scientists have:

  - Achieved a practical error budget for a proposed laser gravitational-wave observatory in space (LAGOS) that will use 10^7 km separation between three small spacecraft in orbit around the L-5 point of the Earth-Sun system.

  - Defined an approach for achieving 10^{-11} cm/Hz$^{0.5}$ or lower vibration levels at 1 Hz for possible use in a medium-frequency gravitational wave detector operating at frequencies of 1 to 30 Hz.

  - Made the first measurements ever using energy loss of an absolute cross section for excitation of ions by electrons.

  - Disproved suggested deviations from Newton's $1/R^2$ law of gravity using gravity data taken on and immediately around the 300 m Erie Tower -- "Newton was saved on the plains of Colorado."

  - Measured for the first time an entire single-collision velocity changing "kernel", showing that this basis of saturated-absorption line shapes does not have the normally-assumed shape.

  - Developed a method that measures the surface reaction probability of radicals responsible for hydrogenated amorphous silicon thin-film growth in discharges.

  - Made first and detailed measurements of sub-Schawlow-Townes phase diffusion in relative phase of two-mode laser associated with "correlated spontaneous emission effect".

- Analyzed 30-month's beat frequency data of atomic frequency vs "length-physics-stabilized" lasers to yield a 300-fold improvement in Kennedy-Thorndike experiment and thus a 70-ppm determination *from experiment* of the Special Relativity Lorentz transform.

- Demonstrated for the first time that two different angular wave functions of the same electronically excited state display dramatically different alignment effects in a collisional process.

- Developed a novel, reproducible molecular beam source of translationally fast atoms and radicals by pulsed laser vaporization of continuously-deposited cryogenic films.

- Obtained the first experimental measurements demonstrating the quantitative difference between direction- and speed-changing collisions, both of which lead to the overall phenomena of velocity slowdown.

- Developed a Doppler imaging technique to infer the locations and sizes of stellar surface features with an angular resolution four orders of magnitude below the diffraction limit of the largest optical telescope on earth.

- Used high resolution IR laser spectroscopy in supersonic jets to make the first quantitative measurement of the bending potential energy surface for a hydrogen bond.

- Made the first spectroscopic detection of extremely weakly bound He-HX complexes, and from high resolution line shape analysis, measured quantum tunneling rates of He through a centrifugal dissociation barrier.

- Developed laser flash kinetic spectroscopic methods for monitoring cascade relaxation of highly rotationally excited OH radicals.

- Carried out a definitive series of calculations of electron impact vibrational excitation of H_2 that strongly support, contrary to all expectations, the beam work in seriously conflicting crossed beams and swarm measurements.

RESEARCH PROGRAMS

Quantum Physics Division (577)

ATOMIC, MOLECULAR AND OPTICAL PHYSICS

Dielectronic Ionization - G. H. Dunn

A fruitful collaboration with A. Müller and E. Salzborn continued with crossed beams measurements of electron impact ionization of Sc^{2+} and Ca^{+}: $Sc^{2+} + e \rightarrow Sc^{3+} + 2e$; $Ca^{+} + e \rightarrow Ca^{2+} + 2e$. These potassium-like structures are good theoretical proving grounds to explain the dielectronic ionization mechanisms that they have seen in these and other ions. An electron incident on the ion resonantly excites an inner-shell electron and is captured. This is followed by either sequential or simultaneous multiple autoionization: Resonant-Excitation-Double-Autoionization (REDA); Resonant-Excitation-Auto-Double-Ionization (READI); Resonant-Excitation-Triple-Autoionization (RETA); etc. Excellent high-precision data were obtained, and theorists are starting the task of the theoretical calculations of the resonant structures observed. Since these indirect ionization mechanisms appear to account for a significant amount of ionization in many ions, it is important to gain an understanding of the processes so that ionization balance and time evolution of hot plasmas can be understood and predicted.

Electron-Ion Inelastic Collisions - G. H. Dunn

The merged beams technique under development for the past few years has yielded the first data-absolute cross sections for electron-impact excitation of C^{+}. It was recognized by Dunn some years back that a new method had to be found for the experimental measurement of cross sections for electron-impact excitation of ions. The fluorescence detection techniques that had been used for all the measurements up to that time were limited to low charge ions and to optically allowed transitions, and were tedious and difficult to obtain. The needs of the fusion community, as well as those of defense, astrophysics, and high power laser development, dictated new development to understand excitation of multiply charged ions and the role of resonances, as well as indirect processes in ionization. The resulting merged-beams method, using trochoidal merger-demerger analyzers, has a detection efficiency approaching unity compared to typical fluorescence detection efficiencies of 10^{-4} or less.

The results are the first measurements of absolute cross sections for excitation of an ion using an electron energy loss technique. Both Livermore and the Jet Propulsion Laboratory have had similar development under way for several years, and Livermore has now stopped (at least temporarily) because of frustration in dealing with the excessive backgrounds present in their apparatus. Development at JPL continues, though they have not yet made any measurements, again because of excessive backgrounds. Dunn's group has also encountered severe backgrounds in the experiment, but has reduced them to operable levels by reducing background gas pressures (4×10^{-11} Torr) and by carefully modelling the beam optics. E. Wahlin, a graduate student, will write his thesis this fall on the results. The apparatus is scheduled to be moved to Oak Ridge National Laboratory for use with their Electron Cyclotron Resonance (ECR) ion source for highly charged ions.

<u>Electron-Atom and Atom-Atom Collision Processes</u> - **A. C. Gallagher**

The electric breakdown and conduction of a gas, and the radiation from the resultant plasma, are important in lasers and area lighting, in switching and power generation, and in the diagnostics of man-made and astrophysical plasmas. The radiative and electrical properties of these hot gases depend on electron-atom and atom-atom collision processes, which couple the kinetic energies of the particles into radiative transitions and vice versa. During this year, Gallagher has collaborated with postdoctoral research associates H. Werij, and graduate students D. Atkins, K. Gibble, X. Han, G. Schinn and M. Troyer to study several kinds of collision and radiative processes that occur in these hot gases. As it is neither practical nor economical to investigate all specific species and processes of current or potential interest, these investigations are designed to obtain highly detailed diagnostics of a few specific processes, thereby guiding and testing basic understanding applicable to all similar processes. Specifically, Gallagher and his colleagues are carrying out the following experiments.

An experiment to measure fully differential electron excitation of Na atoms from the 3S to 3P state has been completed, and the students involved, Han and Schinn, have graduated. This experiment uses a laser spectroscopy approach to allow measurements that are fully differential in M_ℓ, M_s, and θ. These threshold-region partial cross sections, with respect to M_ℓ and M_s and electron scattering angle θ, test theories in the critical threshold region with much more detail than had previously been feasible.

Differential inelastic atom-atom energy-transfer collisions ($A^* + B \rightarrow A^{**} + B$ or $A^* + B \rightarrow A + B^*$) are being measured in a crossed-beam apparatus. Such measurements critically test understanding of the interactions and collisions. Gallagher and M. Troyer use supersonic metal-atom beams with well-defined velocities and detect the energy transfer by laser-induced fluorescence from the final state (A^{**} or B^*). The recoil Doppler shift in the A^{**} or B^* absorption spectrum is analyzed to yield the differential cross sections with respect to scattering angle. They are currently measuring $Rb(5^2P_{3/2}) + K(4S) \rightarrow Rb(5^2P_{1/2}) + K(4S)$ or $Rb(5S) + K(4^2P_J)$.

Another experiment measures total atom-atom collision cross sections and stimulated radiation processes in Sr vapor. Here fluorescence transients following pulsed radiative excitation of Sr are being diagnosed to establish radiative and collisional pathways between excited states, leading ultimately to a highly excited and ionized vapor. As an example, $Sr^* + Sr^* \rightarrow Sr + Sr^{**}$ processes have been measured where Sr^* are 5^1P and 4^1D excited states.

Saturated absorption laser spectroscopy, laser "lamb dips" and "optical pistons" are often sensitive to a collisional velocity-changing "kernel." In spite of its ubiquitous character, the actual form of this "kernel" has not been measured or known, and various crude approximations are generally used. Using diode-laser spectroscopy on Rb, Gibble has achieved the first direct measurement of an entire kernel, and has shown that it bears little resemblance to the usually assumed forms.

<u>JILA Atomic Collision Cross Section Data Center</u> - **J. W. Gallagher**

The JILA Data Center carries on an active program to compile and evaluate data describing collisions of electrons and photons with atoms, ions, and simple molecules. Various projects entail collaboration with JILA and Data Center visitors and staff, who participated in the review and evaluation of data in their fields of expertise.

Accomplishments during the past year include progress in developing database software. An interactive program for querying the Atomic Collisions Data Base has been completed. The current version produces bibliographic indexing lines, numeric data indexing lines, or numeric data tables from query by author, citation number, process, or species. A program to add journal references to the Atomic Collisions Database has been written and tested. Work continues on documentation of software associated with the database. A user's guide to the Data Center graphing program has been completed and a manual describing the structure of the database and providing instructions for the storage and retrieval software is being prepared.

There has also been substantial progress over the past year in several scientific Data Center projects, including:

Bibliography of Electron Swarm Data. W. Lowell Morgan

This bibliography covers published data on the transport properties of electron swarms in gases and cross section information derived therefrom during the period from 1979 to mid-1989. It reflects the current emphasis in applications of swarm data to electronegative gases for use in gaseous dielectrics, to mixtures of gases for use in plasma processing and switching applications, and to dense gases where many-body effects are important.

Multiphoton Bibliography 1983-1986. S. J. Smith, J. H. Eberly and J. W. Gallagher [NBS LP-92, Supp. 5, June 1989]

This is a continuation and expansion of the collection of references describing studies of the interaction of more than one photon with individual atoms and molecules in the gas phase. Approximately 1200 references are included in the bibliography covering multiphoton ionization, excitation, and dissociation of atoms and molecules as well as new categories recognizing multiple electron processes, above threshold ionization, and collisions in intense fields.

Cross Sections and Swarm Coefficients for H^+, H_2^+, H_3^+, H, H_2, and H^- in H_2 for Energies from 0.1 eV to 10 keV. A. V. Phelps

This review has been completed and submitted to the Journal of Physical and Chemical Reference Data.

Collisional Alignment and Orientation in Atomic Outer Shells. II. Quasimolecular Excitation. N. Andersen, E. Campbell, J. W. Gallagher and I. V. Hertel

Participants in the preparation of this review, the second part in a three-part series, met at JILA in January 1989, and again in August 1989, to identify appropriate data from the articles cited in the bibliography, to plan manipulation of these data and to develop the first draft of the figures, as well as to begin writing the text.

Sub-Schawlow-Townes Laser Linewidth: "Correlated" Spontaneous Emission - J. L. Hall

The last few years have seen dramatic conceptual and experimental progress in the field of laser fluctuations, specifically in the preparation and measurement of radiation field states that display *less* fluctuation than that "inescapable" minimum set by shot-noise. Teaching and acceptance of this false limit as the fundamental limit has perhaps occurred because we have heretofore not had optical frequency sources that are phase-coherent over the time of the measurement. Therefore the elegant solution that the noise level could usefully be made phase-dependent (the light could be "squeezed") has only become appreciated in recent times. Theoretical work, confirmed by experimental work at JILA and the University of Texas by Hall and H. J. Kimble, showed that noise reduction factors of 2.5 could immediately be obtained with proper techniques. (Two other groups obtained results a little earlier, but they were limited to ≈10% effects.) This work has led to re-investigation of several other circumstances in which it may be possible to achieve noise reductions previously considered "impossible".

M. O. Scully (University of New Mexico) introduced the concept of a "correlated spontaneous emission laser" (CEL) in which a strong rf field mixes the two upper states of a two-mode laser. In his original concept, the existing phase of one of the fields might be abruptly changed by addition of an incoherent photon arising from spontaneous emission. The associated dipole moment would soon be modified to match this changed field and, because of the strong upper state coupling, the other dipole would be affected and subsequently so would the other field. Thus the relative phase diffusion of the two laser modes would be less than the "minimum possible" value, the one calculated by Schawlow & Townes based on coupling to the vacuum fields that can be said to "cause" spontaneous emission. In detail, Scully's provocative idea is incorrect -- it is a description of classical phase-locking via parametric coupling between laser modes introduced by a time-dependent perturbation of the atomic polarizability. W. Sleich (Max Planck, Garching) followed the semiclassical picture of spontaneous emission in three rotating frames, which led him to offer a geometric interpretation of the CEL effect. In one of the frames the two dipole moments are secular. If they are parallel in space and in phase, there is no way for the vacuum fields to distinguish them differentially. Thus one source of quantum fluctuation is suppressed. This three-state model predicts a 33% maximum reduction. M. P. Winters (University of Colorado) and Hall have observed relative phase diffusion reduced by 40% in their red HeNe Zeeman-split laser, and verified the predicted $\sin(\psi/2)$ dependence. (Probably the larger-sized effect is due to complexity of the actual energy level structure, compared with the simplifying assumptions used in the theory.)

This CEL effect is thus the second example where measurement sensitivity *beyond* the naive quantum limit has proved possible. This enhanced sensitivity is present only until the phase-locking effect takes over at longer times. (The CEL observation was possible only via development of a fast, elegant and precise phasemeter.) Thus the effect does not seem directly applicable to the laser gyroscope problem, but the strongest gravitational signals are expected to exist only in the pulse domain anyway. Thus this CEL effect could change the optimal strategy for gravitational wave antennas, conceivably leading one to prefer active rather than passive devices.

<u>Electron-Molecule Interactions</u> - D. W. Norcross

Collisions of electron and molecules lead to a variety effects and reaction products, e.g., rotational and vibrational excitation of the molecule, capture of the electron to form a molecular negative ion, or dissociation of the molecule into other atomic and molecular fragments. This theoretical effort is primarily developmental -- inventing and extending large-scale numerical techniques for more rigorously representing the electron-molecule interaction, and for treating ever more complicated molecules and processes -- but opportunities to produce useful data are not overlooked. Results will find application in studies of many practical and fundamental processes, e.g., laser modeling, physics of the interstellar medium, and in studies of chemical reaction dynamics.

Recent work has focused on vibrational excitation of HF and H_2, and on negative ions of these molecules and of $HC\ell$. HF and $HC\ell$ are members of the larger group of hydrogen halides and are popular subjects of studies in chemical reaction dynamics. They are also among the simplest examples of highly polar molecules, interesting for the unique properties conferred, relative to nonpolar systems, by the long-range dipole potential. Vibrational excitation of H_2 is an ideal test case for new computational techniques and is also controversial at the moment because of a substantial disagreement between two experiments, one based on crossed-beams, the other on swarm analysis.

A scattering code has been developed by Norcross and postdoctoral G. Snitchler that allows for the coupling of a manifold of lower vibrational states, while still incorporating rigorous treatments of the tricky exchange interaction and the complicated correlation and polarization forces. Calculations have been carried out for both integrated and differential cross sections for excitation of the v=1 and v=2 states in HF. They reveal for the first time a resolvable width in the v=0→1 transition at threshold, and confirm the non-isotropic angular distribution observed experimentally. Production runs for H_2 have been completed, in collaboration with the group of M. Morrison at Oklahoma, which for the 0→1 cross section agrees with the swarm measurements at only the very lowest energies and agrees with the beam measurements otherwise.

An improved package for the calculation of asymptotic solutions of scattering equations has been completed and successfully married to the molecular scattering code by Snitchler and graduate student T. Gorczyca. This has permitted the first practical and realistic calculations of the binding energies of weakly bound and diffuse molecular negative ion states, and perhaps also highly excited states of neutral molecules. The code has been successfully tested on H_2, and results for the lowest bound states of $HC\ell^-$ and HF^- have also been obtained. The goal is to finally uncover the full spectrum of the infinite number of bound states that can be trapped in the field of a polar molecule, and to provide the first systematic connection between negative ion resonances and true bound states as function of internuclear distance.

<u>Electron Impact Excitation of Atoms and Ions</u> - D. W. Norcross

Excitation by electron impact is a primary source of energy transfer and radiation emission in both fusion and astrophysical plasmas. The needs for a vast amount of data for these processes, for both modeling and diagnostic purposes, are well documented. Since theory must be relied upon to provide the bulk of the data, it must be tested against measurements for carefully selected special cases. These cases, in turn, must be designed either to test or stretch particular aspects of the theory (e.g., transitions near thresholds, between excited states, and involving resonances, relativistic effects, or state-selected projectiles or targets), or to check out particular novel experimental techniques under development (e.g., photometric calibration, recoiling- and merged-beam techniques, angular distribution measurements). Recent work at JILA has concentrated on sodium- and magnesium-like ions, and on neutral alkali-metals.

Norcross and postdoctoral J. Mitroy completed calculations on the sodium-like ion $A\ell^{++}$. The scattering code was used in a mode with all channels closed to compute binding energies for many of the low-lying bound states of $A\ell^+$, for which inclusion of polarization leads to much improved predictions of the ionization energies. This work has again demonstrated that a semiempirical approach to the treatment of core polarization effects is capable of greatly improving the quality of the calculation with relatively little extra expenditure of effort or computer time. Scattering calculations for $A\ell^{++}$ revealed a 10% effect on resonance excitation due to core-polarization.

A long-standing program to study electron scattering from several states of sodium has been extended into problems involving laser preparation of aligned states, use of polarized electrons, and coincidence measurements of ejected electrons and fluorescent radiation, with analysis as a function of angle as well as energy. All of this data can, in principle, be derived from a single set of close-coupling calculations for electron scattering from sodium. A new series of calculations and analysis of the results in terms of several new measurements, and the provision of an easily-used 'data-base' of S-matrices for those measurements yet to be contemplated, are the long term goals of this new project. The first results obtained by Norcross, graduate student H.-L. Zhu, and collaborators Mitroy, Snitchler, and B. Whitten of Colorado College, involve excitation of the 3p state as a function of the change in both spin and orbital magnetic projection quantum numbers of the target electron.

Relativistic effects are expected to be important in electron collisions with heavier alkalis. As a first step in attacking cesium, the Dirac formalism has been used by Norcross and Zhu to calculate Stark scalar and tensor polarizabilities for cesium excited states. These quantities are, incidentally, important in analyzing results of very high precision measurements of parity-violating transitions.

CHEMICAL PHYSICS

Ultra-Low Temperature Ion-Molecule Reactions - G. H. Dunn

The cooled Penning ion trap was used during the year to obtain final rate coefficient measurements on very low energy charge transfer collisions between He^+ and H_2. Both radiative and dissociative charge transfer were observed and measured. Dissociative charge transfer takes place as the colliding particles negotiate two separate barriers, the last of which is overcome by quantum mechanical tunneling. The physics of the process is interesting, and now presents a challenge to theorists. The process is of high significance in astrophysics, since H_2 is the most abundant molecule in the cosmos. The low rates measured would indicate that He^+ will be destroyed primarily by charge transfer collisions with CO even though it is much less abundant than H_2. A new detection technique involving Fourier transform ion Z-resonance spectroscopy was developed for the trap, and measurements were made of the rate coefficients and rate coefficient ratios for the processes (1) $^3He^+ + {}^4He \rightarrow {}^3He + {}^4He^+$, and (2) $^4He^+ + {}^3He \rightarrow {}^4He + {}^3He^+$. This is an extremely basic charge transfer process with an energy difference due to the reduced mass of only 0.001 eV, with process (1) being endoergic. The measurements have been compared with results we obtained using the simple theory of Rapp and Francis, but better comparisons await more sophisticated theory. Nevertheless, comparisons with the simple theory give reasonable agreement.

Silane Neutral Chemistry - A. C. Gallagher

The quality and utility of hydrogenated amorphous silicon (a-Si:H) thin film photovoltaics has increased every year since their initial production in 1976. Efficiencies of 10% are now routinely achieved, compared with crystal silicon cell efficiencies that are now about 20%. Because a-Si:H can be deposited inexpensively from a discharge as a thin layer on large areas, it is a leading contender for solar power generating systems as well as large-area photoconductors. It is also being developed in many companies for display and reading. In spite of this impressive progress, major improvements in deposition rate, large-area reliability, stability, and efficiency are still needed.

Since 1979, Gallagher and his group have been studying the discharge and surface processes that lead to the film production, in order to assist this progress with improved understanding of the microscopic processes. Working this year with J. Doyle and D. Doughty, Gallagher has developed methods to measure surface reaction probabilities and the spatial distribution of depositing radicals. These have been used to establish radical behavior in the discharges, thereby testing and advancing models for the gas and surface chemistry. Stable gas products of for a variety of Si- and Ge-containing gas discharges have also been measured and diagnosed for critical aspects of the plasma chemistry. These are the basis of the thesis and graduation of J. Doyle.

Photofragmentation Dynamics - S. R. Leone

Photodissociation processes of molecules are providing some of the most detailed results of state-resolved chemical dynamics in recent years. These photofragment processes are particularly important because they are similar to the latter half of a collision, which in principle could represent a chemical transformation. While many groups have explored the use of laser-induced fluorescence to probe the states of diatomic fragments, few laboratories have considered the possibilities of detecting infrared emission, which can ultimately be extended to more complex polyatomic fragments.

R. Fletcher, E. Woodbridge (University of Colorado) and Leone have been using a new apparatus to study photodissociation dynamics by time-resolved Fourier transform infrared (FTIR) emission spectroscopy. The method was recently shown in this laboratory to give highly precise results for the rotationally resolved product states of several photodissociation processes. Three systems have recently been studied in detail. These include the CCH radical produced on dissociation of HCCH, the CO and CH_3 fragments from the three body dissociation of CH_3COCH_3, and the HF product from $CH_2CFC\ell$. Exciting new directions for study include a first investigation of a rotationally-resolved, single collision energy transfer event, $Br^*(^2P_{1/2}) + HF(v=0) \rightarrow Br(^2P_{3/2}) + HF(v=1,J)$ and a radical-radical reaction $C\ell + C_2H_5 \rightarrow HC\ell(v) + C_2H_4$. These recent explorations demonstrate the power of the time-resolved FTIR method to study collision events with rotational and vibrational detail.

Ion-Molecule Dynamics - S. R. Leone

Several exciting breakthroughs have again been achieved this year to increase the powerful repertoire of methods to study ion dynamics.

A single mode dye laser technique is being used to study ion velocity distributions in a well-characterized electric drift field region, work carried out by S. Penn (NRC Postdoctoral Fellow), H. Beijers, V. Bierbaum, M. Bastian, and Leone. The Ba^+ ion is drifted in He or Ar buffer gases in a flowing afterglow apparatus, and the velocity distributions are recorded by scanning the single mode dye laser and detecting laser-induced fluorescence. The qualitatively new results to come out of these studies are measurements of the "moments" of the velocity distribution. The first moment is directly related to the average drift velocity and hence the mobility. The second moment gives qualitatively the temperature or width of the ion distribution in either a direction parallel or perpendicular to the drift field. A totally new measurement in the last few months has been to obtain for the first time the third moment, or skewness of the distribution, as a function of electric drift field. This third moment should be a sensitive indicator of the attractive part of the potential, and, soon, Monte Carlo simulations will be performed to determine just how sensitive the skewness parameter is to the form of the potential.

We have also been able to obtain new measurements on the alignment of the trifluorobenzene cation caused by drift collisions in He, using polarized laser fluorescence. In addition, new measurements show that the drift velocity of CO^+ in He is independent of rotational state. These results open up a tremendous number of new possibilities to study ion velocity distributions optically under well-characterized conditions and to compare the measurements to theory and provide refinements to the theoretical analyses.

In a new series of experiments, P. Miller (NRC postdoctoral), S. Rogers, B. Brehm (JILA Visiting Fellow), and Leone have developed a new apparatus to produce and study doubly-charged molecular cations. By electron impact, a large number of interesting ions have been formed, such as CO^{++}, NO^{++}, $C\ell^{++}$, NF^{++}, $CH_2C\ell^{++}$, and others. Several of the ions have not been reported before. Work is in progress to begin laser studies of the predissociation and tunneling effects of these ions, which are trapped in a metastable potential formed by the crossing of the dissociative Coulomb potential ($A^+ + B^+$) curve with the bound doubly-charged ion + neutral curve ($A^{++} + B$).

Energy Transfer - S. R. Leone

Energy transfer processes are important in a wide variety of environments, including laser 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, R. Robinson, L. Kovalenko and Leone have measured the first alignment effects of a Ca D state, which is optically prepared in either one of two different wave functions. Using two lasers with parallel polarizations, the wave function $Y_{2,0}$ is formed. Using perpendicular polarizations, a superposition wave function of $Y_{2,\pm 1}$ is prepared. These two wave functions show dramatically different alignment effects for the transfer from the $Ca(4p^2\ ^1D_2)$ state to the near resonant $Ca(3d4p\ ^1F_3)$ state upon collision with a rare gas atom. The exact form of the alignment signals is fully understood by an analysis of the rotation properties of the wave function. In addition, we have been able to extract the individual contributions to the cross section as a function of rare gas.

In this important field of alignment dynamics, there has been considerable controversy concerning whether the effects can be related to the physical pictures of an aligned orbital. Recently, G. Schatz (JILA Visiting Fellow), Kovalenko, and Leone provided a full quantum mechanical calculation and an analysis of the wave functions to prove that the physical pictures are indeed correct. The error that had been made by previous workers, which caused the controversy, was shown to be due to an

inappropriate choice of basis set to carry out the analysis. Using the appropriate basis, the simple physical pictures give a result that preserves the physical intuition.

<u>Surface Dynamics</u> - S. R. Leone

D. Oostra, R. Smilgys and Leone are pursuing a program in surface scattering dynamics and the growth of semiconductors. This project involves the use of lasers as tools for determining the participation of individual states of the gas phase species in the epitaxial kinetics and dynamics of surface semiconductor growth. The first work involves the growth of GaAs and InAs semiconductors on silicon single crystals. Measurements have been made using laser-induced fluorescence detection of Ga and In atoms and As_2 dimers as they scatter and desorb from a Si(100) crystal to determine the binding energies of the atoms on the silicon surface.

In recent work, we have been able to show the influence that a prelayer of As has on the binding dynamics of In. The indium forms three dimensional islands predominantly on top of the layer of As on Si(100). This is a difficulty for proper epitaxial growth of the InAs material, because two-dimensional layer-by-layer growth is not favored very early in the epitaxy. We have also obtained detailed measurements on the As_2 dimer species, in desorption, and for sticking coefficients. Now we have optical laser diagnostics for a wide variety of III-V semiconductor species, and the possibilities are present to develop in situ diagnostics for molecular beam epitaxy.

State-Resolved Dynamics via Infrared Laser Absorption Spectroscopy - **D. J. Nesbitt**

Nesbitt is pursuing four areas of research into molecular structure and dynamics using ultra high sensitivity infrared absorption techniques: 1) spectroscopy of weakly bound clusters in a supersonic molecular beam by direct absorption of a tunable difference frequency laser; 2) gas-solid interactions by monitoring the nascent quantum state distributions of sublimation of simple molecular solids into a vacuum; 3) intramolecular energy distribution in jet cooled hydrocarbon molecules; and 4) laser flash photolysis studies of transient radicals via time resolved laser absorption.

C. Lovejoy and Nesbitt have already obtained high quality spectra of several van der Waals and hydrogen bonded molecules. Study of these prototypic, weakly bound species provides new information on the nature of bonding, collisional energy transfer in the gas phase, and the extremely important issue of the time scale for intramolecular vibrational relaxation. Their novel technique uses time resolved, direct infrared absorption of a high resolution tunable difference frequency laser in a slit supersonic expansion. The slit expansion device provides a two-order-of-magnitude enhancement in absorption path length, but still allows the extreme cooling, lack of spectral congestion and propensity for cluster formation characteristic of a supersonic jet. In addition, much like a stream of water through a slit aperture, hydrodynamic effects in the slit expansion geometry serve to collimate the velocities along the plane of the expansion. This results in dramatically reduced Doppler widths in an unskimmed molecular beam.

Using these techniques, Lovejoy and Nesbitt have obtained the first infrared spectra of a variety of complexes, including ArHF, HFN_2, $HFCO_2$, $(HF)_2$, HFN_2O, HFH_2, $(CO_2)_2$. Many different vibrational states in each complex have been elucidated, which permits study of intermolecular potentials and coordinates far from the equilibrium geometry. Some key observations resulting from these studies are: 1) depending sensitively on the nature of the vibration, internally excited complexes can be extremely metastable even with up to 40 times the energy to dissociate; 2) in loosely bound complexes, large amplitude quantum motion leads to extensive vibrational averaging of observable quantities (such as molecular rotational constant) and hence a very high dependence on particular rovibrational quantum state; 3) isomers in molecular complexes can exist and exhibit two different, stable structures with completely different and assignable spectra; 4) particularly in H_2 containing systems, tunneling effects from weak multiple minima in the potential can be observed and analyzed by virtue of spectral doublings resolvable in our apparatus. These studies are raising new and challenging theoretical questions about the nature of full 3-dimensional solutions of the multibody Schroedinger equation in molecular systems near the dissociation limit.

A. McIlroy and Nesbitt are exploiting the novel properties of slit jet expansion to study the dynamics of vibrationally excited, but ultra cold, hydrocarbons. A given vibration in a molecule, if excited, can eventually relax into a linear combination of many other vibrational modes via intramolecular relaxation pathways. Spectroscopically, the fingerprint of this intramolecular relaxation is line broadening or excess fine structure in the spectrum, which is completely obscured at room temperature. Studies in the cooled jet environment, however, elegantly avoid this difficulty and permit a detailed spectroscopic investigation of intramolecular dynamics in a collision-free regime. In terminal acetylenes such as propyne, butyne and pentyne, they have studied the relaxation of C ≡ C-H stretch excited states and observe a systematic increase in the amount of state mixing as a function of vibrational state density. Excitation of alipstatic CH stretches, on the other hand, exhibits a much more extensive mixing with framework modes, and hence indicates a more rapid vibrational relaxation. Analysis of the spectral patterns yields quantitative predictions for specific time dependence in the excited states.

A. Schiffman and Nesbitt are in the process of building a new experiment to study transient radicals by time and frequency resolved absorption spectra. A pulsed excimer laser will be used to cleave photolytically appropriate molecular precursors in a fast gas flow to generate highly reactive radical species. By use of a tunable IR laser probe collinear with the photolysis beam, weak transient absorbance signals from the radicals can be detected, signal averaged and analyzed for the desired kinetics. Efforts have been directed towards OH in order to characterize the infrared integrated absorption strengths of this atmospherically important radical. This experiment has just recently become fully operational. Schiffman and Nesbitt have observed OH in v=0,-9, and via a novel analysis of the rotational state dependent intensities, they have determined an explicit dipole moment function for OH from 0.7 Å - 1.7 Å. Results are in remarkably good agreement with recent theoretical calculations, but in grave disagreement with previous experiments.

A rapidly evolving experiment is run by M. Schuder (University of Colorado) and Nelson for diode laser probing of molecular species in supersonic jets. The diode laser permits extension of our earlier efforts to a much wider region of the IR spectrum. The first efforts have been toward $DC\ell$ complexes to correct extensive hydrogen halide information obtained from the difference frequency experiment. They have already observed and analyzed spectra of $ArDC\ell$, $NeDC\ell$ and $(DC\ell)_2$ complexes, the last of which represent the first spectroscopic detection ever of such species. Of particular interest has been the study of tunneling splittings in $(DC\ell)_2$ caused by rapid interconversion between the two equivalent configurations. The systematic shifts in these splittings with $^{35}C\ell$, $^{37}C\ell$ substitution reveals considerable insight into the nature of the tunneling phenomena.

A new experiment is under construction by E. Kruus (Postdoctoral Fellow, National Sciences and Engineering Rearch Council (NSERC)) to investigate state-to-state energy transfer in crossed molecular beams using a combination of IR and UV laser probes. The basic strategy is to use supersonic cooling to achieve nearly single rotational state (J=0) initial populations in order to probe rotational excitation upon collision. The IR studies will start on the simplest systems, e.g., Ar + HF. Of key interest is whether the final state distributions can be determined from empirical potential surfaces developed from high resolution IR spectroscopy of the corresponding ArHF complex obtained in our laboratories. The UV based studies will start with scattering of NO by rare gases, as an introduction to more detailed studies of HX-NO scattering. Again, the goal will be to connect IR studies of the complex with the full collision process.

ASTROPHYSICAL MEASUREMENTS

Radiation Transport Theory and Applications - D. G. Hummer

This program addresses the basic physics of the transport of radiant energy through matter, works to develop powerful new techniques for radiative transfer calculations, and seeks to test and exploit them in advanced models of stellar atmospheres.

J. Puls and Hummer, working in Munich, are investigating Hummer's suggestion that the radiation force arising from the interaction of the diffuse radiation field in the optically-thick stellar winds of Wolf-Rayet stars with the sources of line and continuum opacity is sufficient to drive these winds without recourse to other mechanisms. Hummer is also working with his postdoctoral associates, W. Schmutz and J. Hillier, to calculate the total radiation force from their complete W-R models, which derive the atmospheric structure by fitting the observed lines and continuua. The radial dependence of the force obtained in this way, when used with the equation of motion for the gas, should yield the velocity law, which can then be used for further models in an iterative procedure.

Advances in the fundamental theory, codes and models also continue. The stellar atmosphere code written by I. Hubeny (JILA Visiting Fellow) is sufficiently general and powerful to permit the inclusion of elements such as C, N, O, and Si, in addition to the usually included H and He, to the extent that all of the bound-free and selected free-free transitions can be included. Hummer has outlined a program with Hubeny to carry out these calculations. The necessary atomic data (mainly from the Opacity Project) are starting to be assembled and incorporated into Hummer's code. The treatment of He is much more accurate than all existing work. This project is still in a early stage.

G. Rybicki (CFA) and Hummer have developed a powerful new method for radiative transfer calculations that provides the basis for a new generation of stellar atmosphere codes that can treat non-LTE line-blanketing essentially exactly. It appears to surpass all existing methods for *multi-level* problems. The basic idea is to replace the non-local operator that gives the mean intensity from the source function, by a local operator that can be solved trivially, and then correct for the difference iteratively. This approximate lambda operator technique is being applied by Hummer and postdoc W. Schmutz to construct model stellar atmospheres with full non-LTE line blanketing. This work will require an enormous amount of atomic data, which is now available from the Opacity Project. The analysis and general planning of the code are under way, but have been delayed by some conceptual problems which have just been resolved.

Recently, Hummer and Rybicki investigated the formation of very strong resonance lines in high-speed flows using a generalization of the Sobolev method, in which scattering with partial redistribution could be treated. In addition to obtaining numerical solutions of the equation, they found a Fokker-Planck approximation to the equations, which could be solved analytically for much of the frequency region of interest. This work is of considerable interest in modern astrophysics, as strong resonance lines are found to control the ionization balance of important ions in stellar winds.

<u>Spectral Line Formation and Primary Atmospheric Parameters</u> - **D. G. Hummer**

Advances in the atmospheric models permit development of new and more precise measurement techniques for the physical parameters of radiating gases from analysis of the emitted radiation. Recent work has concentrated on applications to hot-stars, O-star supergiants and nebulae in order to address fundamental questions concerning conditions in the early universe, and stellar evolution and decay.

For the past several years, Hummer has devoted a significant part of his time to the determination of precise values of the primary atmospheric parameters of hot stars (with D. Abbott, B. Bohannan and S. Voels). The goal is to exploit the new generation of astronomical detectors to obtain very high signal-to-noise line profiles, which are then analyzed using photospheric models incorporating all physical processes thought to be of possible relevance. The purpose of this work is to provide sufficiently accurate constraints on the theory of stellar evolution that the effect of the physical uncertainties (i.e., convective overshooting, mass-loss, and opacities) in that theory can be evaluated and ultimately removed. The errors in current determinations are much too large for this purpose.

This ongoing project is a collaborative effort with the University of Munich, with the goal of determining accurate stellar parameters for at least 30 stars in each of our Galaxy and the Large and Small Magellanic Clouds. The goal is to accurately determine the evolutionary state and chemical composition of the hot stars in the Magellanic Clouds, galaxies with low abundances of helium and heavier elements. This project has carried out extensive observations from both ground-based observatories and the IUE spacecraft. A proposal from this group for 16 hours of observing time on the Hubble Space Telescope has been accepted in full. Hummer has been primarily involved in the modeling of the atmospheres of these objects and the analysis of their optical spectra.

Hummer, working with A. Gabler in Munich, has also undertaken a major modeling effort of the lines of neutral helium in O-star supergiants using the unified model atmosphere code developed in Munich, which treats the photosphere and stellar wind regions in a consistent and unified way. This research was undertaken in order to investigate the extended atmospheres of these objects, which manifest themselves in the unusual strength of the lines in question. This project requires the extension of the line broadening theory developed by Barnard, Cooper and Smith for the 4471 Å line of He I to other transitions in this atom, which is being carried out in collaboration with L. Anderson (University of Toledo).

The cosmic abundance of helium sets a strong constraint on the conditions in the very early universe, and is best determined from the collisional-radiative recombination spectrum of helium in nebulae. For this purpose, the theoretical line strengths are necessary. Hummer and P. Storey (University College London) have been working for two years on an accurate determination of the theoretical recombination line strengths for helium. The main problem here is with the atomic data, for although excellent radiative data are now available from the Opacity Project, the collisional rate coefficients are not available for most transitions of interest. This work should be completed during Storey's tenure as a JILA Visiting Fellow.

The previous work on this project involving the collisional-radiative spectrum of hydrogenic carbon, nitrogen, and oxygen, has recently been published. The previous work on H and He^+, along with work on carbon ions carried out in 1982, has been used by L. F. Smith and Hummer to determine the He and C abundances in a number of Wolf-Rayet stars, using spectra taken by Smith for this purpose.

<u>Stellar Opacities and the Equation of State</u> - **D. G. Hummer**

The Opacity Project, which has the goal of calculating *ab initio* the mean opacities for stellar envelopes using the latest developments in computational atomic physics (developed largely by the groups of M. J. Seaton, JILA non-resident Fellow, and P. G. Burke), was conceived by Hummer, who now serves as its co-director. Since the project--which involves about 20 workers in the U.S., Great Britain, Germany, France and Venezuela--got under way in 1984, photoionization cross sections and radiative transition rates for all levels with $n \leq 10$ and $\ell \leq 2$ have been calculated for all astrophysically significant ions in the iso-electronic sequences based on the elements of the first two rows of the periodic tables. Work on the relevant ions of the third-row elements, including iron, is well along and should be finished early in 1990, according to estimates made at the July, 1989, meeting of the Project in Belfast. Enormous advances have been made in the computation of line broadening parameters for both hydrogenic and non-hydrogenic species. Two entirely independent codes are presently being tested in order to ensure that no coding or conceptual errors are present. Significant differences from selected opacities from Los Alamos have been found.

Hummer's contributions have included a new equation of state, which has been uniquely successful in predicting the frequencies of the global solar oscillations. He has also contributed codes for the exact evaluation of the hydrogenic photoionization cross sections and oscillator strengths, as well as for the free-free Gaunt factor, which is conveniently represented as a two-dimensional Chebyshev expansion.

<u>Survey of the Microwave Emission from Active Binary Systems</u> - J. L. Linsky

Linsky, S. Drake and T. Simon (University of Hawaii) have completed and published a large survey of the microwave emission (primarily at 6 cm) from active binary systems of the RS CVn class using the Very Large Array (VLA), the world's largest radio astronomy telescope array. This major observing program is important because it provides insight into the physical processes occurring in plasmas where tangled magnetic fields reconnect to create electric fields that accelerate electrons to relativistic energies and heat the plasma. Since these hot plasmas radiate at radio wavelengths and in the X-ray region by different physical processes, the study of active binary stars provides an ideal cosmic laboratory to study the physics of plasma processes in great detail. An important result of this survey of more than 120 objects is the unexpected correlation of the thermal X-ray emission from the hot coronae of these systems with the microwave emission, which has always been explained as gyrosynchrotron emission from relativistic electrons. Linsky has provided a novel interpretation of this gyrosynchrotron emission from the same thermal electrons that emit the hot component of the observed X-ray flux.

<u>Analysis of Spectral Lines from Stellar Chromospheres</u> - J. L. Linsky

Linsky and J. Neff (Goddard Space Flight Center) are continuing to apply the Doppler imaging technique to determine the size, location, and physical properties of discrete active regions in stellar chromospheres. The Doppler imaging technique is based on the idea that for a rapidly-rotating star each location on the stellar surface will contribute to the observed spectral line profile with emission at its Doppler-shifted wavelength. Thus observations of line profiles at many different rotational phases may be inverted to obtain an image of the star in which the sizes, locations and brightness contrasts of individual bright patches (called active regions) may be inferred. For typical systems this technique can resolve structures four orders of magnitude smaller than the diffraction limit of the largest optical telescope on earth. During the past year Linsky and Neff have applied the technique to infer the location of a major flare on the system V711 Tauri, and have developed a model to explain the ultraviolet spectra and nonthermal radion emission during the flare. They derived a downflow velocity of 90 km/s from the ultraviolet spectra and showed that the kinetic energy in the downflow is comparable to the total energy radiated in the flare. A major result of this program is that they can now infer for the first time the true surface brightness of distinct bright patches on the surfaces of these stars in spectral lines. This allows them to derive accurate model atmospheres for the patches and the heating rates necessary to explain these model atmospheres. Since the heating needed to explain these bright patches is presumably magnetic in character, they can understand for the first time the rate of magnetic heating and deduce the physical processes responsible.

P. Judge, a Postdoctoral Research Associate working with Linsky, has examined the formation of chromospheric emission lines using detailed radiative transfer calculations (including both coherent scattering, Doppler frequency redistribution and collisional redistribution) and escape probability techniques. He has compared these detailed calculations with approximate cooling-integral calculations that estimate the frequency-integrated line fluxes. In a recent paper he has determined for which classes of stars the cooling rates in important spectral lines may be accurately estimated using the effectively thin approximation, the complete frequency redistribution approximation, and those for which detailed partial frequency redistribution calculations are needed.

<u>Ultraviolet Explorer Satellites, Existing and Proposed</u> - J. L. Linsky

Linsky has chaired a nearly completed two-year study to determine the optimal strategy for reprocessing the complete archives of the International Ultraviolet Explorer (IUE) satellite. The IUE data set contains some 80,000 ultraviolet spectra of stars, planets, galaxies, and the gas lying in the line of sight between the stars. The main objectives of the study are to determine how to reprocess these data in a uniform way that will enhance the data-to-noise in the spectra so as to increase the scientific accomplishments of the mission.

Linsky has also been an important member of an international team of astrophysicists who have just completed a one-year Phase A study of the proposed Lyman Far Ultraviolet Spectroscopic Explorer satellite for NASA. He was responsible for defining the scientific program for this satellite and also participated in the technical discussions. The proposed Lyman satellite will obtain high-resolution spectra in the 90-125 nm spectral region and moderate-resolution spectra in the 10-90 nm spectral region of stars, planets, galaxies, quasars, and interstellar gas. The technical innovations of the proposed instrument include a 70 cm glancing incidence telescope, a Rowland spectrograph with a novel aspheric grating, and a two-dimensional multi-anode microchannel array detector.

<u>The Physics of Shock Heating in Stellar Atmospheres</u> - J. L. Linsky

Two postdoctoral Research Associates working for Linsky are studying how acoustic shock waves heat the atmospheres of stars. D. Luttermoser, in collaboration with G. Bowen and L. Willson (both at Iowa State University), is computing the emergent spectrum from strong shock waves in a class of variable stars called Mira variables. This is a fascinating problem because the radiative transfer and hydrodynamic calculations are coupled in that the shock waves heat the atmosphere locally, radiation cools the shocks, and the shocks produce velocity discontinuities that permit the plasma to more easily radiate in spectral lines. This type of fully self-consistent radiative-hydro calculation has never been successfully applied to these stars.

M. Cuntz and Luttermoser are studying the properties of shock waves in the atmospheres of cool giant stars. The innovative aspect of their program is that they include a range of wave periods. This includes for the first time an important physical process -- shorter period waves can overtake longer period waves to produce supershocks that heat the atmosphere locally to temperatures of 50,000 K or hotter. This phenomenon probably explains a long standing problem in astrophysics -- why many cool giant stars have spectra that contain spectral lines that require high temperature plasmas. One particular problem is the formation of the neutral hydrogen 1083 nm line whose lower state is 19.8 eV above the ground state. They find that this line can be easily excited by the supershocks that naturally occur when a stochastic distribution of wave periods is included in their hydrodynamic calculations.

GEOPHYSICAL MEASUREMENTS

<u>Slant Path Atmospheric Refraction Calibrator (SPARC)</u> - P. L. Bender

S. J. Walter (University of Colorado) and Bender are working with NASA funding to develop a microwave-optical system to improve the accuracy of the correction to microwave distance measurements due to atmospheric water vapor. Since optical distance measurements are affected much less by water vapor, the difference between microwave and optical measurements from an aircraft at about 6,000 meters altitude to the ground will determine the microwave distance correction. A 35.25 GHz microwave carrier from a Gunn diode oscillator and a roughly 830 nm optical carrier from a laser diode are modulated at 1.5 GHz in the transmitter. The modulation signals are then compared in phase in the receiver. The accuracy goal for the calibrator is 2 to 5 mm. It will be used in joint measurements with water vapor radiometers and radiosondes to determine improved line shape and strength information for the 22 GHz atmospheric water vapor line.

Ground tests of SPARC have been carried out over 0.14 km and 12 km ground paths. The stability of the instrument is good despite strong scintillation of the optical signal. Comparisons of the results with end point meteorological measurements have been made. Construction of two image motion compensators for use in the airborne measurements is now complete. One image motion compensator will direct the signal from the 1.5 GHz modulated laser diode in the aircraft toward the receiver on the ground, despite rapid and irregular tilts of the aircraft. The other compensator will automatically direct the light received from the aircraft onto the avalanche photo-diode detector. Improved electronics for the image motion compensator are now being built. Bender expects that aircraft tests of SPARC will be made in the next year at the NASA Wallops Flight Facility in Virginia.

Geophysical Measurements Related to the Suggested Fifth Force - J. E. Faller

The major work during the past year was conceiving, planning, and implementing the Erie Tower test of Newton's inverse square law of gravity. This was seen as an extremely important and timely target of opportunity. The test used the available instrumentation to its measurement limits. Faller orchestrated the efforts of field teams from the Defense Mapping Agency and Geodynamics (Santa Barbara, California), used guest workers C. C. C. Speake from BIPM and J. Maakinen of the Finnish Geodetic Institute, and his entire graduate student pool plus one former graduate student (Ph.D) now working in the Classics Department of the University of Colorado (on the history of science). In essence, all available resources were used to carry out this fundamental experiment, the result of which may be stated as "Newton has been saved on the plains of Colorado."

The Erie tower, located 20 km east of Boulder, was used to repeat the AFGL "North Carolina Tower Experiment", which appeared to indicate the presence of both a 5th and a 6th force, and the recent "Greenland Hole-in-the-Ice Experiment" which, it is stated, yielded evidence of a 6th force. Because of their convenient access to the 300 m tower, T. Niebauer, Speake, M. McHugh, P. Keyser and Faller have been able to acquire good up-and-down-the-tower gravity data using a number of Lacoste & Romberg relative gravimeters. They also acquired the extremely dense data set necessary to carry out the $1/R^2$ "upward continuation" of the measured surface gravity. Using this tower-upward continuation approach, the Faller group has successfully carried out the most precise test that has been done to date.

Two other target-of-opportunity experiments have been carried out or are still being worked on -- all designed to test experimentally some aspect of the fifth-force suggestion that first appeared in the January 6, 1986, issue of Physical Review Letters. Fischback *et al.* suggested, based on an analysis of a number of data-types, the possibility of a new short-range component to gravity. This suggested new component of gravity was dubbed the "fifth force."

Earlier, Niebauer (University of Colorado), M. McHugh and Faller used the dropping chamber from the JILA absolute gravimeter, together with first the Finnish and later the Defense Mapping Agency/National GS dropping chambers, to carry out a Galilean test of the Fifth Force hypothesis using U_{238} and Cu as the free-falling dropped masses. They measured no differential acceleration down to 5 parts in 10^{10}, thereby establishing better experimental limits on any material-dependent fifth force over the range $0.2\text{-}10^4$ kms.

Presently, Faller and McHugh are working on a fluid-float Eötvös experiment using Cu and Pb as the test masses to test the material-dependent fifth force hypothesis over the short 1-10 meter range. This target of opportunity experiment has resulted in the temporary suspension of their gravity gradiometer float studies.

<u>Deriving the Lorentz Transforms from Experiment: A New Laser-Based Kennedy-Thorndike Experiment</u> - J. L. Hall

Most of the most sensitive and precise laser measurement applications depend on the laser's coherence and frequency stability: Improvement of these characteristics has therefore been a long-running research activity of Hall and D. Hils (University of Colorado). Two different time domains are interesting to consider. At short times, the laser linewidth is a significant concept. One could consider the coherence time of the laser ($= 1/2\pi\delta\nu$) to be the time at which a best-fitting sinewave is no longer able to represent the laser's optical phase within 1 radian accuracy. Evidently an experimental approach to this arena will require two superbly stabilized sources. We have made extensive measurements on the difference frequency record between two such totally-independent lasers locked onto two separate high-finesse Fabry-Perot cavities. These resonators are massive (≈10 kg) bars of low expansion material, Zerodur and ULE respectively, drilled axially for the light beam, with optically-contacted "gyro-quality" mirrors. Each hangs in high vacuum inside of multiple shells of temperature-controlled walls. They are located on a floating optical table located inside our "Quiet House." Intervals of phase coherence of 50-200 sec are inferred, terminated by abrupt frequency jumps of ≈100 Hz that may be associated with residual mechanical micro-activity in the optical contacts (100 Hz translates into 0.6 milli-Angstroms motion of the effective reflection plane, averaged over the laser mode). Improved vibration isolation -- probably *active* -- will be necessary for the next advances.

Records of the heterodyne beat between one or both of these cavity-stabilized laser and an atomic-physics-stabilized (I_2) laser have been made sporadically over nearly three years. Temperature data is also available. One interesting output is the smoothly-decreasing drift rate, down to about 1 Hz/sec at present for Zerodur and 0.11 Hz/sec for ULE. The physical interest of these measurements, however, stems mainly from the fact that the two optical oscillators are controlled by different physics and therefore may transform differently. We may consider the earth's rotation as a modulation process, alternately adding and subtracting the earth's surface velocity with the observed motion of the earth and solar system relative to the frame in which the black-body radiation is isotropic, a reasonable candidate for a "preferred frame." (Our motion of about 300 km/s is in the direction of the Virgo super-cluster of galaxies, as deduced from the 1:1000 dipole anisotropy in the cosmic blackbody radiation temperature.) This sidereal modulation of V^2 thus gives us the opportunity to set a new and dramatically-improved limit on some parameters (α-β+1) in the parameterized test theory for non-accelerated relativistic systems, as developed by Mansouri and Sexl. (These parameters represent the second-order terms in transforming time and longitudinal length respectively.) Our experiment is thus equivalent conceptually to the Kennedy-Thorndike experiment of 1932 (K-T) in which they compared a wavelength controlled by energy-level-physics (the 546.1 nm line from an Hg lamp) with the length defined by the difference in length of two arms of a Michelson interferometer built on a slab of fused silica. The analysis of Turneaure *et al.* (1983) indicates that length contains an additional factor of the (fine-structure constant)^3 relative to the atomic clock so that general relativistic invariance tests also become interesting.

The short summary of our experiment is that residual environmental perturbations limit our sensitivity to about 100 Hz for a putative sidereal signal of the K-T type. This corresponds to a measurement of $(\alpha-\beta+1)$ at the 70 ppm level, about 300-fold better than Kennedy and Thorndike. Taken with the determination of $(\alpha+1/2)$ from the Mossbauer rotor experiment (0.1 ppm) and $(\delta-\beta+1/2)$ from the JILA Michelson-Morley experiment of 1979 (5×10^{-9}), the significance of the change in K-T from 2% to 70 ppm can be appreciated. Thus the Lorentz transform can now be based on experimental measurement at the 70 ppm level. A version of this experiment for the space shuttle might get another factor of 100.

Laser Gravitational-Wave Observatory in Space - P. L. Bender and J. E. Faller

There have been substantial improvements in the last year 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 10^7 km arm lengths. Test masses freely floating inside three separate spacecraft in orbit around the L-5 point of the Earth-Sun system will support the end mirrors and the equivalent of a beamsplitter for the interferometer. The gravitational wave frequencies of interest are from 10^{-5} to 1 Hz.

As discussed in previous reports, studies of expected gravitational wave signals due to binary star systems have been carried out by D. Hils, R. F. Webbink (former JILA Visiting Fellow) and Bender. To summarize, it appears that the power spectral density of signals due to different types of binary star systems will be above the instrumental sensitivity for frequencies from roughly 10^{-5} to 10^{-2} Hz. Since about 10^8 binaries in our galaxy contribute to the signals, it will not be possible to resolve individual sources unless they are unusually close by. Exceptions are double neutron star binaries, close white dwarf binaries, and black hole-neutron star binaries with frequencies above about 10^{-3} Hz, for which the number in the galaxy per cycle/yr resolution bin is less than 1. The reality of the gravitational wave signals can be checked by observing the change in signal strength as the plane of the galaxy goes through one of the nulls in the antenna pattern, which correspond to the plane bisecting the two baselines and the perpendicular plane. Information on the location of resolvable sources can be obtained in the same way. Gravitational wave pulses due to the possible collapse of supermassive stars to form black holes near the time of galaxy formation will also be sought.

Recent work on the conceptual design for the LAGOS antenna, in collaboration with R. T. Stebbins (University of Colorado), has concentrated in three areas. One is the determination of the type of propulsion system needed to buck out the solar radiation pressure and other forces on each spacecraft in order to keep it centered on the test mass; the second is the thermal design of the spacecraft; and the third is the development of 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 1×10^{-13} cm/sec^2/Hz$^{0.5}$ for the sum of the accelerations of the test masses in the frequency range 2×10^{-5} to 1×10^{-3} Hz, and 4×10^{-9} cm/Hz$^{0.5}$ for the sum of the measurement errors for the difference in arm lengths at frequencies of 10^{-3} to 1 Hz.

The LAGOS project now appears ready to go into a technology development phase. This would include in particular work on the following: the disturbance reduction system for the test masses; the thermal design for the spacecraft; the thruster and fuel storage system for counteracting the solar radiation pressure and solar wind forces on the spacecraft; and a 1 watt space-qualified laser with high stability, reliability and efficiency. NASA is now supporting a small amount of work under its Advanced Development Program on possible future gravitational physics and astronomy missions. Plans are being made for more intensive technology development work over the next five years in areas relevant to possible future new types of astrophysics and gravitational physics missions. Work on LAGOS is a candidate for inclusion in this program.

<u>1-30 Hz Isolation Systems for Ground-based Gravitational Wave Antennas</u> - **P. L. Bender and J. E. Faller**

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. An isolation factor of 10^{-5} 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 at 1 Hz in interferometric detectors such as the proposed 4 km Cal Tech and MIT laser interferometric gravitational observatories (LIGO's).

Bender and Faller are interested in demonstrating, with Stebbins and D. B. Newell (University of Colorado), that a two- or three-stage isolation system can be designed that will provide the necessary isolation without introducing too much thermal noise. The required noise level is not well known, but is in the range of 10^{-11} to 10^{-12} cm/Hz$^{0.5}$ at 1 Hz. 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. They plan to use the type of flexure-mounted torsion pendulum developed by C. C. Speake (BIPM) for sensing the tilt and rotation of each stage, and conventional pendulums for sensing a combination of horizontal displacement and tilt. An improved version of the superspring will be used as the vertical displacement sensor. Interferometric readout is planned for all of the sensors. The overall goal is to achieve a noise level of

$1 \times 10^{-11}(1\ Hz/f)^2\ cm/Hz^{0.5}$ from 1 to 10 Hz for the last stage. The thermal noise in pendulums would then be measured directly, using the last stage as the support point for two matched pendulums with long damping times.

A successful demonstration of the desired seismic isolation level and of low pendulum noise would provide a strong experimental basis for the design of low frequency gravitational wave antennas operating from 1 to 30 Hz, which could be located in the same vacuum systems as the main LIGO antennas. To this end, we are establishing a cooperative agreement with the LIGO group in order to ensure that the seismic isolation work is focused on goals that will be useful in the LIGO program. However, it is expected that the results will also be useful in connection with other gravitational wave antennas such as those being planned by a joint German-British group and by an Italian-French group.

<u>High Accuracy Atomic Mass Measurements</u> - **G. H. Dunn**

A project to develop a technique for the measurement of atomic masses, initially to parts in 10^{10}, but eventually with a goal of parts in 10^{12} has been undertaken by Dunn and graduate student S. Jefferts. These measurements will have a role in the determination of the neutrino mass, the determination of Avogadro's number, the physics of nuclear and chemical isomers, and the masses of superpositions of states.

The method involves measuring the cyclotron resonance frequency of single ions in a Penning ion trap. The trap has now been assembled in a high field (7 T) magnet of excellent stability and uniformity using for the trap itself an alloy especially developed by Dunn's group to have zero magnetic susceptibility at 4 K, the usual operating temperature of the trap. Ions have been trapped. It remains to reduce the ion cloud size to single ions and to accurately measure the cyclotron resonance. Of course, systematic effects will have to be traced down, evaluated, and corrected for. Papers were published during the year on magnetic susceptibilities of common apparatus materials and on the special amplifier developed for the single ion detection. This work will continue during the coming year, when Dunn expects (hopes) that first mass measurements will be obtained.

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1988-1989 VISITING FELLOWS

Quantum Physics Division (577)

Visiting Fellow	Home Institution	Area of Work
Burkhard Brehm	Institut fur Atom- und Molekulphysik Universitat of Hannover Hannover, West Germany	Photoionization and photofragmentation of molecules and angular distributions of photo-electrons.
John Briggs	Fakultaet fuer Physik Universitaet Freiburg Freiburg, West Germany	Theory of highly excited states of two-electron atoms.
Fang Li Zhi	Beijing Astronomical Observatory Chinese Academy of Sciences Beijing, P.R.C.	Theoretical astrophysics and cosmology.
Gary Ferland	Astronomy Department Ohio State University Columbus, OH	Photoionization models of quasars and emission line models.
Ian Howarth	Department of Physics & Astronomy University College London London, United Kingdom	Observational studies of stellar winds, interstellar media, x-ray and interacting binary star systems.
Stephen Lundeen	Department of Physics University of Notre Dame Notre Dame, IN	High resolution studies of atomic and molecular Rydburg states.
Alfred Maquet	Laboratoire de Chimie Physique Universite Pierre et Marie Curie Paris, France	Theoretical studies of collisions under the influence of radiation.
Takashi Sato	Department of Electrical Engineering Niigata University Niigata City, Japan	Laser stabilization and laser-induced particulate formation.

1988-1989 VISITING FELLOWS (cont.)

Visiting Fellow	Home Institution	Area of Work
George Schatz	Department of Chemistry Northwestern University Evanston, IL	Theoretical work on atomic and molecular collision processes and unimolecular decomposition.
Reinhard Schinke	Max-Planck-Institut fur Stromungsforschung Gottingen, West Germany	Theoretical dynamics of photodissociation of polyatomic molecules, molecular collisions.
John P. Simons	Department of Chemistry University of Utah Salt Lake City, UT	Electronic structure of negative molecular ions; dynamical behavior of anions.
Constantine E. Theodosiou	Department of Physics & Astronomy The University of Toledo Toledo, OH	Theory of interference between atomic processes and, in particular, of autoionization and radiative decay.

1989-1990 VISITING FELLOWS

Quantum Physics Division (577)

Visiting Fellow	Home Institution	Area of Work
M.N.R. Ashfold	Department of Theoretical Chemistry University of Bristol Bristol, United Kingdom	Experimental spectroscopy & photofragmentation dynamics of small molecular species.
Carl E. Heiles	Astronomy Department University of California Berkeley, CA	The magnetic properties of the interstellar medium.
Sun Kwok	Department of Physics University of Calgary Calgary, Alberta, Canada	Late stages of stellar evolution.
Edwin L. Lewis	Department of Physics The University Newcastle upon Tyne United Kingdom.	Experimental laser spectroscopy and theory of atomic collision processes.
Joseph W. Nibler	Department of Chemistry Oregon State University Corvallis, OR	Experimental and theoretical aspects of coherent Raman spectroscopy.
Hugh G. Robinson	Department of Physics Duke University Durham, NC	Laser and microwave resonance physics, optically-pumped frequency standards.
Peter R. Saulson	Massachusetts Institute of Technology Cambridge, MA	Observational cosmology and gravitational wave astronomy.
Surendra P. Singh	Department of Physics University of Arkansas Fayetteville, AR	Lasers and study of classical and quantum noise phenomena in laser and nonlinear optical processes.
A.C.H. Smith	Department of Physics & Astronomy University College London, London, United Kingdom	Theoretical electron scattering studies.

1989-1990 VISITING FELLOWS (cont.)

Visiting Fellow	Home Institution	Area of Work
A. D. Stauffer	Physics Department York University North York, Ontario, Canada	Atomic & molecular physics; the calculation of electron & positron scattering from atoms.
Peter Storey	Department of Physics & Astronomy University College London London, United Kingdom	Ab initio calculations of rates for atomic processes as they apply to astrophysical plasmas.

1989-1990 DISTINGUISHED VISITORS

Quantum Physics Division (577)

Distinguished Visitors	Home Institution	Area of Work
Roger Chevalier	Department of Astronomy Leander McCormick Observatory of the University of Virginia Charlottesville, VA	Supernovae, theory of interstellar and intergalactic media.
George W. Flynn	Columbia Radiation Lab Columbia University New York, NY	Molecular energy transfer and laser probing of collision dynamics.
Andre Maeder	Observatoire de Geneve Sauverny Switzerland	Stellar evolution, mass loss & mixing.
David E. Pritchard	Massachusetts Institute of Technology Research Laboratory of Electronics Cambridge, MA	Laser-Atom interactions, coding &. trapping of atoms, optical deflection of atoms.
Rainer Weiss	Massachusetts Institute of Technology Department of Physics Cambridge, MA	Gravitational wave research--Infrared Astronomy.

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P. L. Bender	Wei Tou Ni National Tsing Hua University Hsinchu, Taiwan Peoples Republic of China
P. S. Conti	Tomasz Chelbowski Warsaw University Observatory Warsaw, Poland
	Ed Fitzpatrick Princeton University Princeton, NJ
	H.J.G.L.M. Lamers Space Research Laboratory Utrecht, The Netherlands
	Ana Torres-Dodgen MIRA Monterey, CA
	Allan Willis University College London London, United Kingdom
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	Keith Burnett Oxford University United Kingdom
	Liwen Pan NIST Gaithersburg, MD University of Maryland

Cooper (cont.)	Kazik Rzazewski University of Warsaw Warsaw, Poland
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	R. A. Phaneuf Physics Division Oak Ridge National Laboratory Oak Ridge, TN
	L. P. Presnyakov USSR
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	Brana Jelenkovic Institute of Physics Belgrade, Yugoslavia
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CONFERENCES SPONSORED

Quantum Physics Division (577)

The Twelfth International Conference on General Relativity and Gravitation, University of Colorado, Boulder, Colorado, July 3-8, 1989. P. L. Bender and J. E. Faller were on the Scientific Committee.

The First Boulder-Munich Workshop on Hot Stars, University of Colorado, August 6-11, 1989. D. G. Hummer was on the Scientific Organizing Committee.

SEMINARS AND COLLOQUIA

Quantum Physics Division (577)

JILA Colloquia

Lothar Frommhold (University of Texas, Austin) - Supermolecular Spectra: Principles and Astrophysical Interest, October 4, 1988.

Steve Lundeen (JILA Visiting Fellow, University of Notre Dame) - Spectroscopy of High L Rydberg States of H_2: A Sensitivae New Probe of the H_2 Molecular Ion, October 11, 1988.

John C. Raymond (Center for Astrophysics, Harvard) - Diagnosing the Line Spectra of Interstellar Shocks, October 18, 1988.

James L. Kinsey (Rice University) - Spectroscopic Studies of Photodissociation Dynamics, October 25, 1988.

Ray Weiss (JILA Distinguished Visiting Scientist, Massachusetts Institute of Technology) - The Cosmic Background Radiation: Recent Results and Prospects for New Measurements, November 8, 1988.

James L. Valentini (University of California at Irvine) - State-to-State Dynamics: Do We Really Need All That Data?, November 15, 1988.

Dave M. Rank (Lick Observatory) - Recent Infrared Observations of Supernova 1987a With the Kuiper Astrophysical Observatory, November 29, 1988.

Dave MacPherson (Montana State University) - Soliton Generation and Decay in Stimulated Raman Scattering, December 12, 1988.

Dave E. Pritchard (JILA Distinguished Visiting Scientist, Massachusetts Institute of Technology) - Diffracting Atoms With Light and Matter Grating, January 31, 1989.

John Briggs (JILA Visiting Fellow, University of Friberg) - Old Symmetries for New; A Molecular Description of Resonant Atomic States, February 7, 1989.

Ewine van Dishoek (Caltech) - Translucent Molecular Clouds, February 14, 1989.

Roger Chevalier (JILA Distinguished Visiting Scientist, University of Virginia) - The Future Evolution of Supernova 1987a, February 21, 1989.

Jack Simons (JILA Visiting Fellow, University of Utah) - Are There Ever Any Breakthroughs in Molecular Quantum Chemistry? Yes!, February 28, 1989.

Abe Szoke (Lawrence Livermore National Laboratory) - Multiphoton, Multielectron Ionization, March 7, 1989.

Herschel Rabitz (Princeton University) - Making Molecules Dance: Optimal Control of Molecular Motion, March 14, 1989.

Lou Allamandola (NASA - Ames) Cometary and Interstellar Ices and A Sprinkling of PAHs, March 21, 1989.

Reinhard Schinke (JILA Visiting Fellow, Max Planck Institute) - Spectroscopical and Collisional Aspects of Molecular Photodissociation, April 4, 1989.

George Flynn (JILA Distinguished Visiting Scientist, Columbia University) - Ultrahigh Resolution IR Laser Studies of High Energy Collision Dynamics, April 11, 1989.

Kenneth Janda (University of Pittsburgh) - Vibrational Predissociation of Rare Gas- Halogen Clusters, April 25, 1989.

Joint JILA/Astrophysics, Planetary and Astronomical Sciences Colloquia

James Liebert (Steward Observatory) - White Dwarfs and the Age of the Galactic Disk, October 3, 1988.

Webster Cash (APAS/CASA) - Far Ultraviolet Rocket Observations of Supernova 1987a, October 10, 1988.

Tod Clancy (LASP) - Global Climatology of the 58 - 90 Kilometer Atmospheric Temperature, October 17, 1988.

John C. Raymond (CfA) - Diagnosing the Line Spectra of Interstellar Shocks, October 18, 1988.

Jim Green (Berkeley) - Detection of the He I Edge in the Interstellar Medium, October 24, 1988.

Eli Dwek (GSFC) - Infrared Emission From Supernova Remnants Observed by the Infrared Astronomical Satellite, November 7, 1988.

Joseph Nuth (GSFC) - Chemical Dynamics and Circumstellar Grain Formation, November 11, 1988.

John Carey (APAS) - Plasma Chaos, November 28, 1988.

Peter Quinn (StScI) - Dark Matter and the Hubble Sequence, December 5, 1988.

Peter Conti (APAS/JILA) - Numbers and Distributions of Wolf-Rayet Stars in the Local Group of Galaxies, December 12, 1988.

Jan Stenflo (Zurich/HAO) - The Sun's Magnetic Personality, January 23, 1989.

Doub Richstone (Michigan) - Black Holes in Nearby Galaxies, January 30, 1989.

Marc Davis (University of California, Berkeley - Dark Matter, February 6, 1989.

Tim de Zeeuw (Institute of Advanced Studies) - The Shapes of Elliptical Galaxies, February 13, 1989.

Dominique Staute (Arizona Planetary Science Institute) - Planetismal Accretion, February 20, 1989.

Nick Kaiser (CITA) - Galaxy Formation, February 27, 1989.

Mark Meier (Director, INSTAR) - Global Change: What's Happening and Why?, March 6, 1989.

Phil S. Marcus (University of California, Berkeley) - The Red Spot of Jupiter, March 13, 1989.

Rick Edelson (CASA) - Continuum Emission From Active Galaxies, March 20, 1989.

Joe Taylor (Princeton University) - Pulsars, April 5, 1989.

David Stevenson (Caltech) - On the Formation of Jupiter, April 10, 1989.

Jack Baldwin (Ohio State) - The Latest Fashions in Quasar Petticoats, April 17, 1989.

John Faulkner (Lick Observatory) - WIMPS in Stars, April 24, 1989.

Special JILA Seminars

Robert Shelby (IBM, San Jose) - Quantum Noise Reduction Via Quantum Nondemolition, October 7, 1988.

Stephen R. Friberg (NTT Basic Research Labs, Tokyo) - Towards a Quantum Technology: Starting Basic Research at Japan's NTT Electronic Communications Research Laboratories, November 10, 1988.

Yurii Demkov (Leningrad State University, USSR) - Perestroyka and Glasnost: A View From Inside, February 22, 1989.

Bernhard Bluemich (Max Planck Institute) - Nonlinear Incoherent Spectroscopy, March 29, 1989.

Leonid P. Grishchuk (Sternberg Astronomical Institute, Moscow State University) - Possibility of Detecting Squeezed State Relic Gravitons From the Big Bang (?), July 12, 1989.

Hartmut Hotop (University of Kaiserslautern) - Recent Progress in Studies of Penning Ionization, July 24, 1989.

Maureen McCarthy (Hebrew University, Jerusalem, Israel) - Theoretical Studies of the Photodissociation Dynamics of Molecules on Solid Surfaces, July 25, 1989.

Cool Stars Seminars

Jeffrey Linsky (JILA) - What Is Happening on AXAF and LYMAN, October 12, 1988.

Tom Fleming (JILA) - A Search for Chromospheres in Late-M Dwarfs, October 19, 1988.

Don Luttermoser (JILA) - IUE Observations of Cool Carbon Stars, Part I, October 26, 1988.

Don Luttermoser (JILA) - IUE Observations of Cool Carbon Stars, Part II, November 2, 1988.

Fred Walter (JILA) - How Naked Are the Naked T Tauri Stars?, November 9, 1988.

Fred Walter (JILA) - What Do the Flux-Flux Relations Really Mean?, November 16, 1988.

Jeffrey Linsky (JILA) - What Einstein Has Taught Us About Stellar Coronae, November 22, 1988.

Karel Schrijver (JILA) - Farewell Address, November 30, 1988.

Fred Walter (JILA) - Discovery of Six Pre-Main Sequence Spectroscopic Binaries, January 4, 1989.

Don Luttermoser (JILA) The JILA/Iowa State Mira Star Collaboration, January 18, 1989.

Phil Judge (JILA) - The Real Interpretations of Chromospheric Emission Lines, February 1, 1989.

Don Luttermoser (JILA) - Radiative Transfer in Mira Atmospheres--The Colorado/Iowa State Collaboration, February 7, 1989.

Manfred Cuntz (JILA) - Extended Chromospheres and Mass Loss of Late-Type Giant Stars Due to Propagating Shock Waves, February 15, 1989.

Tom Ayres (CASA) - How Deep Can One See Into the Sun, February 22, 1989.

Jeff Linsky (JILA) - Radio Continuum Emission From Warm Supergiants, March 9, 1989.

Alec Brown (JILA) - Do A Stars Lose Moss, or is Lee Anne Willson Wrong Again, March 22, 1989.

Fred Walter (JILA) - Decay of Solar Activity With Time, March 22, 1989.

Bob Stencel (CASA) - Disk, Disk, April 5, 1989.

Don Luttermoser (JILA) - Semiempirical Models of Cool Carbon Star Chromospheres, April 12, 1989.

Manfred Cuntz (JILA) - The Present State of my Wave Models for the Chromospheres of Cool Giants, April 19, 1989.

Tom Fleming (JILA) - ROSAT Mission and His Role in This Project, May 3, 1989.

Phil Judge (JILA) - How Everything Correlates With Everything Else, June 14, 1989.

Jeff Linsky (JILA) - Astrophysics From the South Pole and Radio Observations of Magnetic B Stars, June 22, 1989.

Brian Patten (Iowa State University) - A Study of Main Sequence A and F Stars: Testing the Main Sequence Mass Loss Hypothesis, June 29, 1989.

Ivan Hubeny (HAO) - Influence of Radiation on the Structure of Accretion Disks, July 5, 1989.

Phil Judge (JILA) - Cooling Functions for a Hot Day, July 19, 1989.

Steve Skinner (JILA) - Nonthermal Radio Emission From the X-Ray Bright K5 Star 1E 1751 + 7046, July 26, 1989.

Chemical Physics Colloquia

George Schatz (JILA Visiting Fellow, Northwestern University) - Vibrational Relaxation of Highly Excited Polyatomic Molecules, October 7, 1988.

William Harter (University of Arkansas) - Computer Graphical Visualization of Molecule Rotations and Vibrations, October 14, 1988.

Robert Whetten (University of California, Los Angeles) - October 21, 1988.

Paul Barbara (University of Minnesota) - Microscopic Solvation Dynamics and Ultrafast Electron Transfer, October 28, 1988.

Michael Morse (University of Utah) - Spectroscopy and Electronic Structure of Small Metal Clusters, November 4, 1988.

Joseph Nuth (Goddard Space Flight Center) - Chemical Dynamics and the Formation of Circumstellar Grains, November 11, 1988.

Matthew Vernon (Columbia University) - Molecular Beam Studies of Organometallic Photodissociation Processes, November 18, 1988.

Kopin Liu (Argonne National Laboratory) - Cross Beam Studies of Radical Chemistry, December 2, 1988.

Robert Bernheim (Pennsylvania State, NBS Visitor) - Spin Orientation and the Law of Mass Action, December 9, 1988.

Robert Silbey (Massachusetts Institute of Technology) - January 20, 1989.

Kevin Lehman (Princeton University) - Spectroscopy and Intramolecular Dynamics of Ammonia, January 27, 1989.

David Kelley (Colorado State University) - Reaction Dynamics and Molecular Clusters, February 3, 1989.

James Meiss (University of Texas at Austin) - The Relationship Between Classical and Quantum Ionization Thresholds for MPI in Hydrogen, February 17, 1989.

Carleton Howard (NOAA) - The Chemistry of Sodium in the Upper Atmosphere, March 3, 1989.

Richard Gottscho (Bell Labs) - In Situ Diagnostics for Gas-Phase and Surface Processes in Reactive Plasmas, March 10, 1989.

David Chandler (Sandia National Labs) - Application of Two-Dimensional Imaging to the Study of Photochemistry, March 17, 1989.

Turgay Uzer (Georgia Tech) - Beyond Chirikov's Pendulum: The Geometry of Vibrational Mixing in Molecules, March 24, 1989.

Robert Littlejohn (University of California, Berkeley) - Maslov Indices and Semiclassical Dynamics, April 7, 1989.

Louis Rothberg (Bell Laboratories) - Photoexcitations of an Infinite Polyene Studied by Subpicosecond Spectroscopy, April 17, 1989.

Mark Smith (University of Arizona) - The Chemistry of Extremely Long-Lived Ion Collision Complexes, April 21, 1989.

Richard Saykally (University of California, Berkeley) - Ion and Cluster: Some New Experiments, April 28, 1989.

David Farrelly (University of California, Los Angeles) - Seeing Quantum

Interference Patterns with the Scanning Tunneling Microscope, May 5, 1989.

Chemical Physics After Dark Seminars

Stephen Klippenstein (University of Colorado) - Theoretical Studies of Unimolecular Dissociation Reactions, October 5, 1988.

Albert Stolow (University of Toronto) - Direct Observation of the Transition State in H + D_2, October 12, 1988.

Burkhard Brehm (JILA) - Doubly Charged Molecular Cations, October 19, 1988.

Kent Ervin (JILA) - Negative Ion Photoelectron Spectroscopy of Transition Metal Clusters and Reactive Intermediates, October 26, 1988.

Kermit Murray (JILA) - Photoelectron Spectroscopy of Halocarbene Anions, November 9, 1988.

Craig Taatjes (JILA) - Velocity - Changing Collisions of Br Atoms, November 16, 1988.

David Nelson (JILA) - The Dipole Moment Function and Absolute Vibrational Transition Strengths of the OH Radical, December 7, 1988.

Mark Nimlos (Colorado State University) - Vibrational Energy Flow and Vibrational Predissociation in van der Waals Clusters, December 14, 1988.

Dwayne Heard (Oxford Physical Chemistry Laboratories) - Time-Resolved FTIR Studies of Radicals, January 25, 1989.

Mark Nimlos (Colorado State University) - Vibrational Energy Flow and Vibrational Predissociation in van der Waals Clusters, February 1, 1989.

Eckart Ruehl (University of Colorado) - Coincidence Studies in Organic Molecules, February 8, 1989.

Doeke Oostra (JILA) - Laser Probing of the Interaction of Ga and In with Si (100) Surfaces, March 1, 1989.

Diane Szaflarski (JILA) - Photodissociation Dynamics and Mechanisms of Gas Phase Molecules Studied Using Multiphoton Ionization Mass Spectrometry, March 22, 1989.

Mark Johnson (Yale University) - Cluster Analogues of the Hydrated Electron, March 22, 1989.

Mark Jones (University of Colorado) - Chemistry of Bimetallic Surfaces: Structure and Chemistry of Bi on Ni(100), April 5, 1989.

Jorg Senekowitch (JILA) - Ab-initio Calculations of Rovibrational Spectra, April 12, 1989.

Debbie Parker (University of Colorado) - A Study of High Coverages of Atomic Oxygen on Pt (111), April 19, 1989.

Zamik Rosenwaks (Ben-Gunion University, Isreal) - Recent Advances in Short Wavelength Chemical Laser Research, April 26, 1989.

Aram Schiffman (JILA) - OH Kinetics the Infrared Way: Reactions - or - The Borneo Connection, May 4, 1989.

Michael Schuder (JILA) - Internal Dynamics of DCI - Containing van der Waals Molecules, May 10, 1989.

Joe Cline (JILA) - Diode Laser Probing of I Atom Doppler Profiles: Time Evolution of a Fast, May 17, 1989.

Informal Theory Seminars

John Briggs (JILA Visiting Fellow, Universitaet Freiburg) - Off-Shell Coulomb Wavefunctions and Their Applications, January 26, 1989.

Longhuan Kim (JILA) - Stable Negative Ions of the Heavy Alkaline Earth Atoms, February 2, 1989.

George Schatz (JILA Visiting Fellow, Northwestern University) - Quantum Scattering Studies of Orbital Alignment Effects in $Na(^2P)$ + He Fine-Structure Changing Collisions, February 8, 1989.

Sergei Ya Kilin - (Academy of Science, Minsk, USSR) Quantum Jumps and the Theory of Continuous Quantum Measurements, February 16, 1989.

Yurii Demkov (Leningrad Stae University, USSR) - Pseudo Crossings, the Adiabatic Approximation and Potential Curves, February 21, 1989.

Ugo Fano (University of Chicago) - Approaches to the Process of Fragmentation, February 23, 1989.

Sydney Geltman (JILA) - Collisions of Excited Na (3P) Atoms - Associative Ionization and Energy Transfer, March 2, 1989.

Dieter Witgen (Heidelberg) - Chaos and Quantum Mechanics, March 9, 1989.

Gunadya Bandarage (JILA) - Ionization in H + H^+ Collisions: A Classical Perspective, March 16, 1989.

Alfred Maquet (JILA Visiting Fellow, Universite Pierre et Marie Curie - Recent Developments in Perturbation Theory (with application to multiphoton processes in hydrogen), March 23, 1989.

Greg Snitchler (JILA) - Electron-Impact Vibrational Excitation of Small Molecules, April 6, 1989.

Marek Trippenbach (JILA) - Population Fluctuations in Raman Scattering, April 13, 1989.

Chris Greene (JILA Fellow) - Rydberg Spectra of the Rare Gas Dimers, May 4, 1989.

Gunadya Bandarage (JILA) - Ionization in H + H+ Collisions: A Theory of Molecular State Close-Coupling Including the Continuum, May 11, 1989.

Liwen Pan (University of Maryland and NIST) - Computation of High-Order Multiphoton Processes in Atomic Hydrogen, June 15, 1989.

G. S. Agarwal (University of Hyderabad, Hyderabad, India) - Quantum Noise Initiated Generation of Radiation at New Frequencies, June 22, 1989.

Leonid Presnyakov (Lebedev Physical Institute, Moscow) - Interaction of Highly-Charged Ions With Neutral Atoms, July 20, 1989.

Hot Stars Seminars

Jorge Sahade (University of Argentina) - Line Profiles in Variation in the Spectrum of Gamma2 Velorum, December 8, 1988.

Clint Poe (HAO/NCAR) - Steady and Unsteady Hot Star Winds: A Comparison With CAK and the Time-Dependent Model, December 15, 1988.

John Hillier (JILA) - Analysis of WC Stars: Implications for the Evolution of Massive Stars, January 26, 1989.

Joel Parker (CASA) - IMF in the MCs: Guilt by (OB) Association, February 9, 1989.

Ed Fitzpatrick (Princeton University) - Things He Is Doing, March 2, 1989.

Dennis Ebbets (Ball Corporation) - The High Resolution Spectrograph of the Space Telescope, March 16, 1989.

Werner Schmutz (JILA) - Supernova Atmosphere Models and Distance Determination, March 23, 1989.

Peter Conti (JILA) - Near IR Spectra of WR Stars, "So Many Types - So Little Time," April 20, 1989.

Bob Stencel (CASA) - Infrared Excess of Main Sequence Stars, May 4, 1989.

Bob Garrison - Spectral Classification, May 19, 1989.

Sally Heap (Goddard Space Flight Center) - Informal Luncheon Talk, May 26, 1989.

Ian Howarth (JILA) - Wibbly Wobbly Winds, and Other Odds and Sods, June 1, 1989.

Ed Fitzpatrick (Princeton University) - The HR Diagram of the LMC: Implication for Stellar Evolution, June 16, 1989.

Leo Bronfman (University of Chile) - Molecular CO Clouds in the Fourth Quadrant, August 3, 1989.

INVITED TALKS

Quantum Physics Division (577)

P. L. Bender, "Minimizing Test Mass Disturbances for a Laser Gravitational Wave Observatory in Space," Stanford Relativity Gyro Laboratory, Stanford University, Stanford, California, December 6, 1988.

G. H. Dunn, "Measurements on Very Low-Energy Collisions Using Ion Traps," at Sixteenth International Conference on the Physics of Electronic and Atomic Collisions, (ICPEAC), New York, New York, July 27, 1989.

J. E. Faller, "Precision Tests of the 5th Force Hypotheses," Physics Colloquium, Los Alamos National Laboratory, Los Alamos, New Mexico, December 1, 1988.

J. E. Faller, "Measurement of Absolute Gravity, Progress and Prospects," Canadian Gravity Division of Geological Survey, Ottawa, Canada, January 10, 1989.

J. E. Faller, "The Erie Tower Experiment," Moriond Conference, Les Arcs, Savoie, France, January 21-28, 1989.

J. E. Faller, "Rencontres De Moriond," Moriond Conference, Les Arcs, Savoie, France, January 21-28, 1989.

J. E. Faller, "The 5th Force Hypotheses," University of Wyoming, Laramie, Wyoming, March 29, 1989.

J. E. Faller, "The Measurement of Gravity, An Old Field, What's New," International Association of Geodesy Meeting, Edinburgh, Scotland, August 8, 1989 (Read by Chairman of the Session as Dr. Faller was called back to the States because of a death in the family).

A. C. Gallagher, "Gas and Surface Processes and Their Effect on Film Quality," at European Conference on Silane-Based CVD, Palaiseau, France, November 27, 1988.

A. C. Gallagher, "Silane Discharge Chemistry," Materials-Research Society Spring Meeting, San Diego, California, April 1989.

A. C. Gallagher, "Chemistry of Silane and Germane Discharges," SERI PV AR&D Review Meeting, Lakewood, Colorado, May 1989.

A. C. Gallagher, "Plasma Processes in Silane and Related Discharges," Kieo University, Tokyo, Japan, May 1989.

A. C. Gallagher, "Plasma Processes in Silane and Related Discharges," Tokyo Institute of Technology, Tokyo, Japan, May 1989.

A. C. Gallagher, "Plasma Processes in Silane and Related Discharges," Kyoto University, Kyoto, Japan, June 1989.

A. C. Gallagher, "Plasma Processes in Silane and Related Discharges," Kyoto Institute of Technology, Kyoto, Japan, June 1989.

A. C. Gallagher, "Plasma Processes in Silane and Related Discharges," Hiroshima University, Hiroshima, Japan, June 1989.

A. C. Gallagher, "Plasma Processes in Silane and Related Discharges," Sanyo Corporation, Kyoto, Japan, June 1989.

A. C. Gallagher, "Plasma Processes in Silane and Related Discharges," Japanese Symposium on Plasma Chemistry, Nagoya, Japan, June 1989.

A. C. Gallagher, "Deposition Plasma Chemistry," and "Experimental Methods and Diagnostics of Plasma Chemistry," NATO Advanced Study Institute, Maratea, Italy, June 1989.

J. L. Hall, "Testing Relativity With Stable Lasers," Department of Physics Colloquium, University of Colorado, Boulder, Colorado, January 18, 1989.

D. Hils and J. L. Hall, "Improved Kennedy-Thorndike Experiment--A Preliminary Report," given at the Ninth International Conference on Laser Spectroscopy, Bretton Woods, New Hampshire, June 1989. (Paper was presented by D. Hils).

S. R. Leone, "Laser Probing of Ga Interactions With Si(100)" Faraday Symposium, Julich, Germany, December 1988.

S. R. Leone, "Alignment Effects in Electronic Energy Transfer," Faraday Symposium, University of Freiburg, West Germany, December 1988.

S. R. Leone, "Alignment Effects of Sr $5_s 6_p$ $1p_1$ With Rare Gases," Faraday Symposium, Faraday Disc., Freiburg, Germany, December 1988.

S. R. Leone, "Time-Resolved Fourier Transform Emission Studies of Laser Photofragmentation," 18th Informal Photochemistry Meeting, Santa Monica, California, January 10, 1989.

S. R. Leone, "Optical Pumping and Probing of Hyperfine States and Velocity Distributions," NIST Workshop on Pump-Probe Techniques, Gaithersburg, Maryland, February 2, 1989.

S. R. Leone, "Pulsed Time-Resolved Fourier Transform Infrared Emission Spectroscopy," Optical Society of America's Topical Meeting on High Resolution Fourier Transform Spectroscopy, Santa Fe, New Mexico, February 14, 1989.

S. R. Leone, "Laser Probing of Alignment and Doppler Velocity Effects in Collision Dynamics," March 1989 American Physical Society Meeting, St. Louis, Missouri, March 20, 1989.

S. R. Leone, "Alignment, Mobility, and Velocity Effects in Collision Dynamics," Chemistry Department, University of California, Berkeley, California, March 1989.

S. R. Leone, "Laser Studies of Alignment Effects and Photofragmentation Dynamics," Chemistry Department, University of Rochester, May 1989.

S. R. Leone, "Laser Probing of Ion Velocity Distributions and Alignment Effects in Drift Collisions," Gordon Conference on Molecular Energy Transfer, Wolfeboro, New Hampshire, July 10, 1989.

S. R. Leone, "Time-Resolved FTIR Emission Studies of Photochemical Kinetics," 2nd International Conference on Chemical Kinetics, Gaithersburg, Maryland, July 24, 1989.

J. L. Linsky, "Einstein and Stellar Sources," From Einstein to AXAF: A Symposium to Celebrate the 10th Anniversary of the Launch of HEAO-2, The Einstein Observatory, Cambridge, Massachusetts, November 14, 1988.

J. L. Linsky, "The Next 30 Years in Space: Beyond NASA?" Boulder Space Society, CU Space Interest Group, Fiske Planetarium, University of Colorado, Boulder, Colorado, December 8, 1988.

J. L. Linsky, "High Resolution X-Ray Spectroscopy," Physics Department, University of Leicester, Leicester, England, May 3, 1989.

J. L. Linsky, "Solar and Stellar Physics," Astrophysics In Antarctica Meeting, Bartol Research Institute, University of Delaware, June 9, 1989.

J. L. Linsky, "Modelling of Coronae and Chromospheres of RS CVn Systems by the Analysis of UV, X-ray, and Radio Observations," NATO Advanced Study Institute on Active Close Binary Stars, Kusadasi, Turkey, September 19, 1989.

D. J. Nesbitt, "Spectroscopy in Slit Nozzles," Department of Chemistry, University of Maryland, College Park, Maryland, February 22, 1989.

D. J. Nesbitt, "Walking the Line Between Spectroscopy and Dynamics," Molecular Spectroscopy Division, NIST, Gaithersburg, Maryland, February 23, 1989.

D. J. Nesbitt, "Laser Studies of Vibrational Dynamics of Jet Cooled Molecules," Department of Chemistry, Princeton University, Princeton, New Jersey, March 2, 1989.

D. J. Nesbitt, "Laser Studies of Vibrational Dynamics on Slit Jet Cooled Molecules," Department of Chemistry, Yale University, New Haven, Connecticut, March 3, 1989.

D. J. Nesbitt, "Laser Studies of Vibrational Dynamics," IBM Research Laboratories, Yorktown Heights, New York, March 6, 1989.

D. J. Nesbitt, "Inter and Intra Molecular Dynamics in Slit Jet Cooled Molecules," Department of Chemistry, Ohio State University, Columbus, Ohio, May 22, 1989.

D. J. **Nesbitt**, "Intermolecular Potentials in Floppy Molecules," Nonlinear Dynamics Workshop, Telluride, Colorado, July 3, 1989.

TECHNICAL AND PROFESSIONAL PARTICIPATION AND LEADERSHIP

Quantum Physics Division (577)

P. L. **Bender**, Chairman, LAEOS-3 Science Advisory Group, NASA.

P. L. **Bender**, Member, Ultraviolet/Visible/Relativity Management and Operations Working Group, NASA.

P. L. **Bender**, Member, Ad Hoc Committee on Gravitational Physics and Astronomy, NASA.

P. L. **Bender**, Member, Crustal Dynamics Working Group, NASA.

P. L. **Bender**, Member, Interferometry Panel, Astronomy and Astrophysics Survey, National Research Council.

G. H. **Dunn**, Chairman, Division of Atomic, Molecular, and Optical Physics (DAMOP) of the American Physical Society, 1989-1990.

G. H. **Dunn**, Chairman, Program Committee of DAMOP, 1988-1989.

G. H. **Dunn**, Member, DAMOP Committee to Recommend Prize Structure in the field of AMO Physics.

G. H. **Dunn**, Vice-Chairman, Prize Selection Committee for the Davisson-Germer Prize of the American Physical Society.

G. H. **Dunn**, Vice-Chairman, Committee on Atomic, Molecular, and Optical Science of the National Research Council, NAS.

G. H. **Dunn**, Member, DOE Review Panel for Atomic Physics Program at Argonne National Laboratory.

G. H. **Dunn**, Member, DOE Review Panel for McDonald Physics Laboratory at Kansas State University.

J. E. **Faller**, Member, Working Group II of the International Gravity Commission.

J. E. **Faller**, Member, Special Study Group 3.86, "Estimation of Absolute Gravimetric Determinations," of the International Gravity Commission.

J. E. **Faller**, Member, Special Study Group 3.87, "Development of WorldWide Absolute Gravity Net," of the International Gravity Commission.

J. E. **Faller**, Member, U. S. Interagency Gravity Standards Committee.
J. E. **Faller**, Member, Management Operations Working Group on Lunar Ranging.

J. E. **Faller**, Member, International Program Committee.

J. E. **Faller**, Member, Directing Board of IGC (International Gravity Commission).

J. L. Hall, Delegate, Consultative Committee for the Definition of the Meter (BIPM), Sχvres, France, 1970 - present.

J. L. **Hall**, Chairman, International Steering Committee for Conferences on Laser Spectroscopy.

J. **L. Hall**, Member, NIST Committee for NIST Precision Measurement Grants.

J. **L. Hall**, Member, Nominating Committee, Optical Society of America.

J. **L. Hall**, Member, AMO Subcommittee of Physics Division, Academy of Science.

D. G. Hummer, Member, Editorial Board, Computer Physics Communications.

D. G. Hummer, Member, Steering Committee of the United Kingdom Collaborative Computational Project on Stellar Atmospheres.

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

D. G. Hummer, Member of Executive and Scientific Organizing Committees, NATO Advanced Research Workshop on "Stellar Atmospheres - Beyond Classical Models," Trieste, September 1990.

S. **R. Leone**, Member, Division of Chemical Physics, American Physical Society, 1988-1989.

S. R. Leone, Editorial Advisory Board, Chemical Reviews, 1982-1989.

S. R. Leone, Committee on Atomic and Molecular Science, National Research Council, 1986-1989.

S. **R. Leone**, Editorial Advisory Board, Journal of Physical Chemistry, 1984-1990.

S. **R. Leone**, Editorial Board, Progress in Reaction Kinetics, 1987-1989.

S. R. Leone, Editorial Board, Molecular Physics, 1988-1991.

S. R. Leone, Advisory Editorial Board, Chemical Physics Letters, 1987-1989.

J. **L. Linsky**, Member, Users' Committee, International Ultraviolet Explorer Satellite.

J. **L. Linsky**, Co-Investigator, High Resolution Spectrograph for the Hubble Space Telescope.

J. **L. Linsky**, Member, Lyman Far Ultraviolet Spectrograph Explorer Phase A Science Team.

J. L. Linsky, Member, NASA Astrophysics Data Program Proposal Review Panel.

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

J. L. Linsky, Member, Science Advisory Council, Mount Wilson Institute.

J. L. Linsky, Interdisciplinary Scientist on the Advanced X-Ray Astrophysical Facility (AXAF) and Member of the AXAF Science Working Group, NASA.

J. L. Linsky, Member, Astrophysics Council, NASA.

J. L. Linsky, Member, IUE Long Range Planning Committee.

J. L. Linsky, Chairman, Steering Committee, Synoptic High Resolution Spectroscopic Observing Group.

J. L. Linsky, Co-Investigator, Space Telescope Imaging Spectrograph for the Hubble Space Telescope.

J. L. Linsky, Chairman, Management Operations Working Group, Science Operations Branch, NASA.

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

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

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

J. L. Linsky, Chairman, Proposal Writing Team for the Advanced X-Ray Astrophysics Facility (AXAF) Science Data Center.

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

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

J. L. Linsky, Member, Status of the Profession Panel of the Astronomy and Astrophysics Survey Committee.

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

D. J. Nesbitt, Member, Organizing Subcommittee for IQEC '88, "Fundamental Laser Spectroscopy and Physics."

CONSULTING

Quantum Physics Division

A. C. Gallagher

Dr. Gallagher is consulting with the Lamp Division and Corporate Research Division of General Electric Corporation.

J. L. Hall

Dr. Hall is consulting with the Theoretical Astrophysics Group at Caltech in the area of laser techniques for gravity wave detection, and informally with colleagues in industry involved with stable laser design and application, and also consults with: Excel Precision Corporation, Santa Clara, California; and with ORE, Inc., Boston, Massachusetts, regarding data compression.

Advisory Committee to the Global Oscillation Network Group, National Solar Laboratory.

J. L. Linsky

Dr. Linsky consults with NASA concerning (1) future programs in the area of ultraviolet X-ray and infrared astronomy, (2) future programs in solar and heliospheric physics, (3) operations and long range planning for the International Ultraviolet Explorer satellite, (4) definition of the proposed LYMAN Far Ultraviolet Spectroscopic Explorer satellite, (5) definition of the Advanced X-ray Astronomical Facility, (6) calibration and initial operations of the Space Telescope High Resolution Spectrograph, (7) data operations for future missions, (8) interferometry from space, and (9) future infrared astronomy missions.

Dr. Linsky consults with the National Optical Astronomy Observatory (NOAO) and the Association of Universities for Research in Astronomy (AURA) concerning (1) operation of the National Solar Observatory and Sacramento Peak Observatory, (2) planning for coordinated ground-based and space observations, (3) potential need for a large-aperature ground-based solar telescope, (4) planning for synoptic high resolution spectroscopic observations, and (5) the long term goals of the NOAO.

Dr. Linsky consults with the Universities Space Research Association concerning the proposed AXAF Science Data Center.

D. W. Norcross

Dr. Norcross is consulting with the Theoretical Atomic and Molecular Physics Group at the Lawrence Livermore Laboratory on problems related to laser modeling, and is a Visiting Scientist (consultant) to Division T-4 of the Los Alamos Laboratory on problems related to electron collisions with atoms, ions, and molecules.

OTHER AGENCY RESEARCH

Quantum Physics Divison

P. L. Bender	NASA	Disturbance reduction system: conceptual design studies.
P. L. Bender	NASA	Regional translocation analysis: comparison of LAGEOS II and LAGEOS I results.
P. L. Bender	NASA	Integrated water vapor calibrator measurements.
P. L. Bender & R. Stebbins	NJIT	The study of the solar dynamo through the application of the theoretical and observational techniques of helioseimology.
G. H. Dunn	DOE	Cross sections and rates describing electron collisions with atoms and ions.
G. H. Dunn	DOE	Determine atomic, molecular, and nuclear data pertinent to the magnetic fusion energy program.
G. H. Dunn, J. Cooper & C. Lineberger	NSF	Research in atomic and molecular physics.
J. E. Faller	AFGL	Absolute gravity studies.
J. E. Faller	Belvoir RDEC	Gravity gradiometer
J. E. Faller	DMA	Gravimeter equipment support.
J. E. Faller	DMA-N	Absolute "G" co-op program.
J. E. Faller	NASA	Examination and evaluation of the laser lunar ranging multi-lens telescope.
J. E. Faller	NGS	Study of possible systemmatic error sources in JILA gravimeters.
J. E. Faller	NGS	Provide for repair of gravimeter.
J. E. Faller	NGS	Development of electronic and mechanical design of a new free-rise, free fall JILA absolute gravimeter system.
J. E. Faller & P. L. Bender	NSF	Development of very low frequency isolation systems for ground-based gravitational-wave interferometers.

A. C. Gallagher	AFWP	Activated-Surface Chemical Vapor Deposition.
A. C. Gallagher	DOE	Spectroscopic diagnostics of electron-atom collisions.
A. C. Gallagher	SERI	Diagnostics of glow discharges used to produce hydrogenated amorphous silicon films.
J. L. Hall	ONR	Generating high intensity squeezed light, with an optical parametric oscillator and electronic feedback.
J. L. Hall	ONR	Precision atomic beam spectroscopy using stabilized lasers.
D. G. Hummer	NASA	Awarded 16 hours of observing time on Hubble Space Telescope as member of Munich-Boulder team.
D. G. Hummer	NASA	High resolution spectrograph observing program.
D. G. Hummer	NASA	Co-investigator on Astrophysical Theory Grant.
D. G. Hummer & B. Bohannan	NSF	Optically-thick stellar winds and photospheres of hot stars.
S. R. Leone	AFOSR	Laser measurements of state-resolved Ga and atom scattering, sticking, and desorption on metal and semiconductor surfaces.
S. R. Leone	AFOSR	State-resolved dynamics of ion-molecule reactions in a flowing afterglow.
S. R. Leone	AFOSR	Theoretical/Experimental investigations of the structure and dynamics of highly energetic dication species.
S. R. Leone	AFOSR	Theoretical/Experimental investigations of the structure and dynamics of highly energetic dication species - Equipment.
S. R. Leone	AFWL	Diode laser probing of iodine atoms; optically pumped SO laser.
S. R. Leone	ARO	Surface deposition and etching interactions of laser-generated translationally hot atoms and radicals.

S. R. Leone	DOE	Fourier transform infrared spectroscopy and dynamics of combustion - Equipment.
S. R. Leone	DOE	Time-resolved FTIR emission studies of laser photofragmentation and chain reactions.
S. R. Leone	NSF	State-resolved molecular dynamics.
J. L. Linsky	NASA	Interdisciplinary scientist on the Advanced X-ray Astrophysical Facility (AXAF).
J. L. Linsky	NASA	Hubble Space Telescope Imaging Spectrograph
J. L. Linsky & T. Fleming	NASA	X-ray observations of late-type stars using the Rosat all-sky survey.
J. L. Linsky	NASA	International Ultraviolet Explorer studies of astronomical sources.
J. L. Linsky & A. Brown	NASA	Ultraviolet observations of selected astronomical sources.
J. L. Linsky	NASA	Basic research in solar physics.
J. L. Linsky	NASA	Hubble Space Telescope High Resolution Spectrograph.
J. L. Linsky K. Schrijver	NASA	Coronal temperature cool stars.
J. L. Linsky	NASA	Measurements of stellar magnetic fields.
J. L. Linsky	NASA	Science Operations Branch Management Operations Working Group.
D. J. Nesbitt	AFOSR	Infrared transition moments and collisional dynamics.
D. J. Nesbitt	NATO	van der Waals dynamics.
D. J. Nesbitt	NSF	Direct IR laser absorption spectroscopy in linear jets: Vibrational dynamics of van der Waals molecules.
D. J. Nesbitt	SLOAN	SLOAN Research Fellowship.
D. J. Nesbitt	BiNat'l Israeli-US,NSF	Vibrational Dynamics in Jet Cooled Clusters.
D. W. Norcross	DOE	Atomic and molecular collision processes.

D. W. Norcross	DOE	Electron impact excitation of atomic ions.

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	M. Winters Physics Department, University of Colorado	
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	H. Jin Physics Department, University of Colorado	
	Chris Oates Physics Department, University of Colorado	
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S. R. Leone	Final Ph.D. Defense Committee for: L. Cousins Chemistry Department, University of Colorado JILA Data Center Committee. JILA Visiting Scientists Office.
J. L. Linsky	University Space Science and Policy Task Force Search Committee for a faculty position in Theoretical Astrophysics, Department of Astrophysical, Planetary, and Atmospheric Sciences Thesis Committees for: S. Skinner Physics Department, University of Colorado A. Veale Physics Department, University of Colorado
D. J. Nesbitt	JILA Data Center Advisory Committee Library Committee, Department of Chemistry Physical Chemistry Graduate Admissions Committee

D. W. Norcross — JILA Data Center Advisory Committee.

Thesis Committee for:

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H.-L. Zhou
Physics Department, University of Colorado

GRADUATE STUDENTS AND POSTDOCTORAL RESEARCH ASSOCIATES SUPERVISED

Quantum Physics Division (577)

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J. E. Faller	H. Godwin M. McHugh	
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J. L. Hall	M. Eickhoff H. Jin C. Oates S. W. Swartz M. Winters M. Zhu	P. Busch P. J. Martin (NRC) M. C. Noecker
D. G. Hummer	A. Hayden	J. Hillier W. Schmutz
S. R. Leone	M. Bastian L. Cousins K. Knutsen L. Kovalenko S. Rogers R. Smilgys C. Smith C. Taatjes E. Woodbridge	H. Beijers V. Bierbaum (25%) J. Cline R. Fletcher R. Levis H. Miller P. Miller (NRC) D. Oostra S. Penn (NRC) R. Robinson

	Graduate Students	Postdoctoral Research Associates
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D. J. Nesbitt	R. Lascola C. Lovejoy A. McIlroy M. Robinson A. Schiffman M. Schuder	E. Kruus (NSERC) D. Nelson (NRC)
D. W. Norcross	T. Gorczyca H.-L. Zhou	A. Pradhan G. Snitchler

COURSES TAUGHT AT UNIVERSITY OF COLORADO

Quantum Physics Division (577)

S. R. Leone	Chemistry 4551 - Physical Chemistry (Spring 1989)
D. J. Nesbitt	Chemistry 558 - Quantum Chemistry (Fall 1988)
	Chemistry 4531 - Quantum Chemistry (Fall 1989)

ACRONYMS

AES	Auger Electron Spectroscopy
AFGL	Air Force Geophysical Laboratory
AFOSR	Air Force Office of Scientific Research
AIP	American Institute of Physics
AP	Atom Probe
APS	American Physical Society
AT&T	American Telephone and Telegraph
ATD	Above Threshold Dissociation
ATLAS	Argon Tandem Linac Accelerator System
BBIR	Broadband Infrared
BCD	Binary Coded Decimal
BIH	Bureau International de l'Heure
BIPM	Bureau International des Poids et Mesures
CAMO	Center for Atomic, Molecular, and Optical Physics
CARB	Center for Advanced Research in Biotechnology
CCD	Charge Coupled Device
CCDS	Consultative Committee on the Definition of the Second
CCE	Consultative Committee on Electricity
CCG	Calibration Coordination Group
CCIR	Consultative Committee for International Radio
CEL	Correlated Spontaneous Emission Laser
CEP	Compact Effective Potentials
CERN	Conseil Europeen pour la Recherche Nucleaire
CFA	Center for Astrophysics
CGS	Centimeter-gram-second
CIPM	Consultative Committee of Weights and Measures
CMA	Chemical Manufacturer's Association
CNRF	Cold Neutron Research Facility
CODATA	Committee on Data for Science and Technology
COMSAT	Commercial Satellite
CPEM 90	1990 Conference on Precision Electromagnetic Measurements
CRR	Center for Radiation Research
CU	Colorado University
CVD	Chemical Vapor Deposition
DMA/NGS	Defense Mapping Agency/National Geodetic Survey
DOD	Department of Defense
DOE	Department of Energy
EELS	Electron Energy Loss Spectrum
EEP	Einstein Equivalence Principle
ENS	Ecole Normale Superieure
ERC	Electron Cyclotron
EROS	Electric-Resonance Optothermal Spectroscopy
ESDIAD	Electron Stimulated Desorption Ion Angular Distributions
ESR	Experimental Storage Ring

FCPM	Fundamental Constants and Precision Measurements
FIM	Field Ion Microscopy
FTIR	Fourier Transform Infrared
FTMW	Fourier Transform Microwave Spectroscopy
GAMS-4	Gamma-Ray Spectrometer - Fourth Machine
GOES	Geostationary Operational Environmental Satellites
GPS	Global Positioning System
GSI	Gesselschaft für Schwerionenforshung
HRS	High Resolution Spectrograph (on the Hubble Space Telescope)
IAEA	International Atomic Energy Agency (Vienna)
IBM	International Business Machines
IEC	International Electrotechnical Commission
IEEE	Institute of Electrical and Electronic Engineers
ILL	Institut Laue Langevin
IMFP	Inelastic Mean Free Path
IR	Infrared
ISO	International Standardization Organization
IUE	International Ultraviolet Explorer Satellite
IUPAC	International Union of Pure and Applied Chemistry
JGR	Journal Geophysical Research
JILA	Joint Institute for Laboratory Astrophysics
JPL	Jet Propulsion Laboratory
LAGOS	Gravitational-wave Observatory in Space
LANL	Los Alamos National Laboratory
LASP	Laboratory for Atmospheric and Space Physics
LEAR	Low Energy Anti-Proton Ring
LID	Laser Induced Desorption
LIF	Laser Induced Fluorescence
LMR	Laser Magnetic Resonance
MBE	Molecular Beam Epitaxy
MCDF	Multiconfiguration Dirac-Fock
MILSTAR	Military Satellite System
MIM	Metal-Insulator-Metal
MRG	Materials Research Group
MW	Microwave
NAS/NRC	National Academy of Sciences/National Research Council
NASA	National Aeronautics and Space Administration
NATO	North Atlantic Treaty Organization
NCSL	National Conference of Standards Laboratories
NDAB	National Data Advsiory Board
NEXAFS	Near Edge X-Ray Absorption Fine Structure
NIST	National Institute of Standards and Technology
nm	Nanometer

NOAA	National Oceanic and Atmospheric Administration
NRAO	National Radio Astronomical Observatory
NRC	National Research Council
NRL	Naval Research Laboratory
NSERC	National Sciences and Engineering Research Council
NSF	National Science Foundation
NSLS	National Synchrotron Light Source
NSLS	National Synchrotron Light Source (Brookhaven)
OMA	Optical Multichannel Analyzer
OMEGA	
OSRD	Office of Standard Refernce Data
PEP	Pauli Exclusion Principle
PMG	Precision Measurement Grant
PNMS	Phase Noise Measurement Systems
PSD	Photon Stimulated Desorption
PSD	Photon Stimulated Desorption
PTB	Physikalisch-Technische Bundesanstalt
QED	Quantum Electrodynamics
QMD	Quantum Metrology Division
QPD	Quantum Physics Division
REDA	Resonant-Excitation-Double-Autoionization
REDAI	Resonant-Excitation-Auto-Double-Ionization
RETA	Resonant-Excitation-Triple-Autoionization
RF	Radio Frequency
RHEED	Reflection High Energy Electron Diffraction
RIMS	Resonance Ionization Mass Spectrometry
RIS	Resonance Ionization Spectroscopy
SEM	Scanning Electron Microscope
SEMPA	Scanning Electron Microscopy with Polarization Analysis
SI	International System of Units
SPIPES	Spin Polarized Inverse Photoemission
SRM	Standard Reference Material
SSM	Scanning Scattering Microscope
STM	Scanning Tunneling Microscope
SURF	Synchrotron Ultraviolet Radiation Facility
SURF	Synchrotron Ultraviolet Radiation Facility
TAI	International Atomic Time Scale
TEM	Transmission Electron Microscopy
TOF	Time of Flight
TuFIR	Tunable Far-Infrared
UHV	Ultra High Vacuum
UPS	Ultraviolet Photoemission Spectroscopy
USNC	U.S. National Committee
USNO	U.S. Naval Observatory
USSR	Union Soviet Socialist Republic

UTC	Universal Time Coordinated
UV	Ultraviolet
VAMAS	Versailles Project on Advanced Materials and Standards
VDW	van der Waals
VLA	Very Large Array
VUV	Vacuum Ultraviolet
XPS	X-Ray Photoelectron Spectroscopy
XROI	X-Ray Optical Interferometer
XSW	X-Ray Standing Waves
XUV	Soft X-Ray and Ultraviolet Wavelength Range, 4-50 nm

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