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Technical Activities 1990
Surface Science Division

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National Institute of Standards
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ABSTRACT

This report summarizes technical activities and accomplishments of the NIST Surface Science Division during Fiscal Year 1990. Listings are given of publications, talks, and professional committee assignments, by the Division staff together with the Conferences and NIST seminars organized by the staff.

key words: surface chemistry; surface physics; surface science; surface standards

FOREWORD

This report is a summary of the technical activities and accomplishments of the NIST Surface Science Division for the period of October 1, 1989 to September 30, 1990. The report was prepared as part of the Annual Report of the NIST Chemical Science and Technology Program.

Overviews are presented of the Division and of its three constituent groups: Surface Dynamical Processes, Thin Films and Interfaces, and Surface Spectroscopies and Standards. These overviews are followed by reports of selected technical accomplishments during the year. A summary is given of Division outputs and interactions that includes lists of publications, talks, committee assignments, seminars (including both Division seminars and Interface Science seminars arranged through the Division), conferences organized, and a standard reference material certified. Finally, lists are given of Division staff and of guest scientists who have worked in the Division during the past year.

Further information on the technical activities can be obtained by contacting the scientists identified in each project report or by contacting Dr. C. J. Powell, Chemistry B-248, National Institute of Standards and Technology, Gaithersburg, MD 20899 (telephone, 301-975-2534).

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A. Division Overview

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) to perform experimental and theoretical research in surface science to provide a scientific base for the surface-measurement methodology; (2) to 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) to develop reference procedures, reference data, and reference materials in cooperation with national and international standards organizations; and (4) to develop expertise in selected new areas of surface science in order for NIST to provide measurement services where needs are anticipated in the near future.

Surface science is a multidisciplinary activity involving chemistry, physics, and materials science. Over the last decade, there has been a dramatic growth of surface science and its applications, as described in recent survey reports of the National Academy of Sciences (Opportunities in Chemistry, Physics through the 1990's, and Materials Science and Engineering for the 1990's) and the Department of Commerce (Emerging Technologies: A Survey of Technical and Economic Opportunities). The scientific growth has been stimulated by the development of new experimental and theoretical techniques for determining basic physical and chemical surface properties and processes at a fundamental atomic and molecular level. The growth in applications has been important in industrial areas, particularly for semiconductor devices, magnetic recording media, surface-modified materials, thin-film devices, anti-corrosion coatings, adhesion, wear, and lubrication, as well as for other applications of national concern, especially defense, energy, health and the environment.

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 currently 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. More details of the technical program are given in the following group overviews.

About one quarter of the Division's support is obtained through a Surface Science Competence Project established in 1984. This project has two main components, "Novel Two-Dimensional Materials" and "State Characterization of Energetic Species Ejected from Surfaces". Work on the former component is conducted in the Thin Films and Interfaces Group, while work on the latter component is performed partly in the Surface Spectroscopies and Standards Group and partly in the Surface Dynamical Processes Group.

Division staff have been active in submitting proposals for new Competence and Director's Reserve Projects during the past year. During FY90, the Director provided one-year funding from his reserve for work on "Magneto-Optical Data Storage Media"; he has similarly funded in FY91 a related project on "Magnetic Superlattices", and has provided equipment funds for the purchase of components to assemble a molecular beam epitaxy system for the fabrication of metallic superlattice and sandwich structures. The Division has been fortunate in obtaining the services of Dr. W.R. Bennett on a contract basis for this project. He has experience in the design and use of magneto-optical Kerr-effect equipment for characterizing the magnetic properties of ultrathin magnetic films, and has constructed a suitable system for magnetic films grown at NIST. We are also currently assembling improved instrumentation for determining the structural perfection of multilayer thin films using the electron forward-scattering technique, reflection high-energy electron diffraction, and low-energy electron diffraction.

Over many years, the Division has employed field-ion microscopy and, more recently, atom-probe field-ion microscopy for the microstructural and microcompositional characterization of a wide range of materials. This project was brought to a conclusion at the end of FY90 due to a shortage of funds. Arrangements have been made to loan the instrumentation to the University of Wisconsin at Madison, and it is expected that joint research projects with NIST personnel will be established.

The Division has been active in the organization of four Conferences during FY90. A conference on Quantitative Surface Analysis was held in Salem, Massachusetts on October 20-21, 1989; this conference, the third in a biennial series, is sponsored primarily by the American Vacuum Society. The annual Physical Electronics Conference was held at NIST on June 11-13, 1990; this Topical Conference of the American Physical Society is concerned with the fundamental physics and chemistry of solid surfaces and interfaces. A Workshop on Surface and Interface Characterization with High Spatial Resolution was held at the University of York, United Kingdom, on September 10-13, 1990; this meeting was sponsored by the International Union of Vacuum Science, Technique and Applications. The Sixth International Conference on Vibrations at Surfaces was held at Shelter Island, New York on September 10-14, 1990; this conference was sponsored by several societies and organizations.

Later sections of this report summarize the major technical accomplishments of the past year. Despite its small size, the Division has again been productive with 52 scientific papers published, 17 papers submitted or in press, and 2 other reports. Ninety-four talks have been presented to conferences or other groups, 57 by invitation. In addition to a series of Division seminars on surface science topics, the Division has been active in organizing a NIST-wide series of seminars on interface science. Division staff also interact with many professional groups.

It is a pleasure to report recognition of Division staff during the past year. Joseph Fine and Denes Marton (a former guest scientist from Hungary) were selected to receive an R&D 100 award, in the 1990 competition, for their invention of the scanning scattering microscope. This instrument produces a "roughness" image from a surface, using a measurement of the non-specularly scattered light intensity as a focussed laser beam is scanned across a specimen surface; a patent has also been awarded for this invention. A patent was also awarded to Terrence Jach (and J. Geist, D. Novotny, and G. Carver of NEL) for an integrated diffracting crystal and solid-state detector which facilitates maintaining the Bragg condition in x-ray monochromators. William Egelhoff and Daniel Steigerwald (a former postdoctoral research associate) were chosen by the American Vacuum Society to receive the Shopnote Award for their paper published in the Journal of Vacuum Science and Technology. Their paper described two simple, inexpensive but effective designs for metal vapor sources to produce thin films by molecular beam epitaxy. Richard Cavanagh was selected to receive a Department of Commerce Gold Medal in 1990. This award was made to recognize his achievements in using laser techniques to identify fundamental dynamical phenomena in molecule-surface interactions. Linda Johnson was chosen to receive a Deparment of Commerce Bronze Medal in 1990. She was cited for outstanding secretarial and administrative services to the Division over the past eight years.

1. Surface Dynamical Processes Group: Overview

The group conducts research to characterize the molecular and atomic level properties at surfaces. The program involves the use of a spectrum of surface-sensitive techniques, ranging from state-of-the-art laser diagnostics to dedicated synchrotron-based measurements. Topics of concern include the interactions of laser radiation, synchrotron radiation, and electrons with clean surfaces, and the corresponding interactions with adsorbed molecules. The measurements are designed to obtain information on electronic structure, reactivity, and the mechanisms and detailed processes involved in energy transfer at surfaces. Experiments are conducted with substrates of metals, semiconductors, oxides and high-temperature superconductors, and with selected deposited films and adsorbates.

Time-resolved studies of energy-transfer processes at surfaces are conducted in the nanosecond to femtosecond range using infrared and visible laser sources. Well-characterized surfaces, and the time resolution available from state-of-the-art lasers, are exploited in attempts to directly characterize chemical bond breaking at surfaces. Measurements by this group have recently been extended from high-surface-area materials to adsorbates on single-crystal surfaces. Experimental and theoretical advances have led to a clearer understanding of the dissipation of vibrational excitation in chemisorbed monolayers. The group is now well positioned to address the transient spectral response of these adsorbate systems. This work stands at the frontier in establishing the foundation for a thorough understanding of the pathways and mechanisms of energy flow at surfaces. Future work will extend the present activities to include the study of excited electronic states as surfaces through two-photon photoemission and visible-visible sum-frequency generation.

Insight into optically stimulated surface processes is obtained (from parallel measurements) from final-state-resolved measurements of the nascent products of surface processes such as laser-induced desorption. NIST staff have played a leadership role in the identification of optically generated excited carriers, in desorption experiments with metal surfaces, using state-resolved detection techniques. In the past year the role of surface-localized excited electronic states in optically driven desorption from semiconductor surfaces was established by this group. Such contributions to understanding laser-stimulated reactions at surfaces hold promise for indicating those reaction steps that might be most suitable for the low-temperature processing of semiconductors. The ability to successfully exploit lasers to initiate and control reactions in a manner not accessible under conventional thermal processing reactions remains an area of active research. These nonthermal events indicate that chemical reactions that are optically driven through substrate excitations may offer a readily accessible avenue for exploiting laser-surface chemistry. Future work is planned to assess the feasibility of using laser radiation to directly excite adsorbate-localized states. With this goal in view, we have recently developed the capability of measuring state-resolved CO populations associated with laser photolysis of metal carbonyls.

Growth and characterization of epitaxial thin films are critical to a wide range of technologies, but remain poorly understood from the perspective of both processing technology and fundamental science. The application of surface science diagnostics such as Auger Spectroscopy and Reflection High Energy Electron Diffraction are being explored to establish correlations between the atomic level characteristics of film growth and the resultant properties. Toward this goal, a small Molecular Beam Epitaxy (MBE) facility has been built in this group to explore the fabrication of thin films of multicomponent alloys. Currently this system allows deposition from three independent, computer-controlled sources and the initial emphasis is on the high-$T_c$oxide $Dy_1Ba_2Cu_3O_{7-x}$. Growth procedures for this material are currently under evaluation. In the future, application of the above-mentioned surface diagnostics, combined with in-situ synchrotron-based photoemission measurements of the electronic structure in these thin films, should result in greater control of growth conditions to produce the required high transition temperatures and current densities.

The electronic structure of materials and their surfaces holds the key to a large variety of phenomena. These phenomena include the performance of electronic devices and the possible mechanisms of energy transfer and absorption, which can guide chemical reactions at surfaces. Resonant photoemission experiments provide a window on the bulk and surface electronic structure of complex materials, surfaces and thin films. The facilities at the SURF-II synchrotron currently operated by this group include a dedicated beam line for the characterization of the valence electronic structure of these materials. Recent measurements at this facility have involved high-temperature superconductors and ferromagnetic alloys. Future measurements in the area will involve studies of ferroelectric oxides such as $BaTiO_3$and high-T_c materials from the Center for Superconductivity Research at the University of Maryland. These studies will provide information on the electronic structure that can be correlated with important material properties.

An Ellipsoidal Mirror Display analyzer, a new diagnostic tool for exploring interactions of radiation with clean and adsorbate-covered surfaces, was installed at SURF-II this past year. This analyzer was designed to characterize the energy and angular distributions of desorbed species, and will also be used both for angle-resolved and angle-integrated photoemission. While the photoemission techniques are sensitive to bulk and surface electronic structure, the stimulated desorption measurements provide structural and dynamic information on the adsorbate layers and mechanisms determining sensitivity to radiation damage. The performance of the instrument is presently being tested and refined, and images of ion and electron angular distributions are presently being obtained. Both synchrotron radiation and electron beams will be used in the future as probes of surface structure. Initial experiments, to be conducted in the fall of 1990, will focus on obtaining images of adsorbate chemical bonds that are revealed by the trajectories of ions that are produced when these bonds are ruptured.

The dynamics program relies heavily on interactions with theorists both within and external to NIST. Due to the complexity of the surface processes being addressed and the subtleties of the experimental diagnostics, a strong interdisciplinary effort is necessary. For instance, convergence on a complete picture of the laser-induced desorption process has been made possible by interactions with J.W. Gadzuk. Similarly, M.D. Stiles is providing support in the area of the excited-state response of coupled two-dimensional lattices. External theoretical support for the angular distribution measurements comes from IBM and Louisiana State University.

R.R. Cavanagh, Group Leader; J.D. Beckerle, E. Elizalde (Guest Scientist), T.J. Hsieh (Student,), L.T. Hudson, R.L. Kurtz, L.J. Richter, and S.W. Robey.

2. Thin Films and Interfaces Group: Overview

The group conducts research concerning the fundamental atomic and electronic structure of thin-film structures in order to relate these structural properties to important electrical and magnetic properties of the devices. Experiments and calculations are performed with epitaxial multilayer films and superlattices involving metals, alloys, and semiconductors. The experiments involve the fabrication and characterization of films and interfaces with layer thicknesses ranging from one to one hundred atomic layers and the development of improved characterization methods.

The members of the Group have common interests in the areas of epitaxial growth, artificially-structured or atomically engineered novel materials, electron transport across interfaces, and the structure of buried interfaces. A unifying theme within the Group is the recognition that structure, at the atomic level, is the key to the properties and performance of solid-state materials and devices. Each member of the Group is involved in developing an understanding of this relationship between structure and properties for a selected class (or classes) of materials. Progress in such understanding is essential, but is only a first step for developing new and improved solid-state materials and devices. The Group is also involved, as much as possible, in using the new understanding it has developed for the next step, the actual production of materials and devices with improved properties or, in the case of theoretical work, in the prediction of atomic structures needed for improved properties.

A major component of the Group's program is the investigation of the magnetic properties of thin-film sandwich and superlattice structures consisting of ferromagnetic and nonferromagnetic metals. The magnetic properties, however, are extremely sensitive to the film structure, which is determined by experimental conditions during film growth and subsequent processing. We have developed improved techniques for determining film structure and have developed procedures for growing thin-film structures of iron and copper of improved quality. As a result, we have been able to demonstrate that these films have novel magnetic properties.

During the past year, we have purchased components to replace the x-ray photoelectron spectrometer, which was eighteen years old and had been used to characterize film morphology through observations of the angular distributions of photoelectrons and Auger electrons. We expect that the new spectrometer will give both improved performance and improved reliability. With special support from the NIST Director, we have designed and installed magneto-optical Kerr-effect instrumentation to determine the magnetic properties of the thin-film-structures; previously, the magnetic properties of films we had prepared had been determined by collaborators in Canadian and British laboratories. With additional support from the Director, we are planning during FY91 to purchase components for a molecular-beam epitaxy system that will be used to fabricate thin-film structures with better control and performance than is possible with the equipment now in use.

Over the past few years, we have been constructing an instrument to make x-ray standing wave measurements in both the grazing angle and Bragg geometries, using x-rays from a synchrotron light source. This instrument will be used to determine the locations of adsorbate atoms on single-crystal surfaces, for example during deposition. It will also be possible to use this instrument to obtain the positions of atoms at buried interfaces. We expect to complete construction of this instrument during FY91 and to use it to examine adsorbate structures. We are also expecting to conduct resonant diffraction experiments using magnetic multilayers.

Theoretical studies are underway to investigate electron transport at interfaces, a topic important for improving the speed of semiconductor devices. In the past we have analyzed electron transport at certain metal-metal silicide interfaces and more recently have studied transport behavior at the interfaces of compound semiconductors. We have also investigated Coulomb charging effects in tunnel junctions with small dimensions.

W.F. Egelhoff, Jr., Group Leader; P.P. Camus, T. Jach, M.D. Stiles, W.R. Bennett (Guest Scientist), A.J. Melmed (Guest Scientist), and W. Schwarzacher (Guest Scientist).

3. Surface Spectroscopies and Standards Group: Overview

The Group performs theoretical and experimental research to make existing and emerging surface spectroscopies more reliable and develops standards to improve the accuracy and efficiency of surface analyses and related measurements of composition versus depth. Theoretical research is performed to improve understanding, at an atomic and molecular level, of spectroscopies involved in surface characterization. Experiments are performed to determine fundamental processes involved in ion-surface interactions, ion sputtering, ion-induced defect production, and ion-induced segregation. Reference data and standard reference materials are produced to assist in the calibration and optimization of sputter-depth-profiling equipment. Experiments are conducted to investigate electron-surface interactions, and calculations are performed to determine interaction parameters. This work is coordinated with related activities in other national standards laboratories, and with national and international standards groups.

Our theoretical work is directed towards 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. Measurement-process-specific quantities such as line shapes, satellite structures, etc., are analyzed to provide additional information on system dynamics.

Ion beams are now widely used to probe surface structure and composition by monitoring scattered ions, ejected ions from the specimen surface and, more recently, ejected neutral atoms. Surface layers are removed by ion impact and measurements are made of the composition of the exposed surface as a function of depth from the initial surface. Many of the basic physical phenomena that occur during ion bombardment are poorly understood and limit the full capability of many ion beam techniques. Such phenomena include the nature of excitation events occurring during the collision cascade, energy states and angular distributions of ejected ions and neutrals, and bombardment-induced defect effects such as diffusion and segregation. With the increased use of the more traditional ion beam techniques, as well as the emergence of new methods (such as sputtered neutral mass spectrometry), there is a growing need for fundamental understanding at the microscopic level of collisional processes occurring when surfaces are bombarded by ions. New calculations of momentum-transfer processes that occur during the first few collisional events have been carried out using a molecular dynamics simulation approach rather than the more simplified binary collision approximation. Our results indicate, for example, that collisional excitation is much more probable during the primary ion/surface encounter than in subsequent events. This rather unexpected result would suggest that even elementary ballistic processes need careful re-examination. To further investigate many of these basic mechanisms we are currently constructing a new instrument to measure the angular and energy distributions of sputtered atoms and ions and their states of excitation; the sputtered species will be detected by resonance multiphoton ionization and time-of-flight mass analysis.

Electron-spectroscopic techniques are extensively used for different types of surface characterization, particularly the measurement of surface composition, surface atomic structure, and surface electronic structure. Two techniques, Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) are in widespread use for measurements of surface composition on a wide range of materials. We are currently involved in calculations of electron inelastic mean free paths of 50-2000 eV electrons in solids, the range of practical interest for AES and XPS, in order that quantitative measurements of surface composition can be made by these techniques. We are also in the final stages of the analysis of high-accuracy measurements, recently done at NIST, of the binding energies of selected core levels in copper, silver and gold, and of the kinetic energies of certain Auger electrons from the same three metals. These values, together with independent measurements made at the UK National Physical Laboratory, will be used for the calibration of the instrumental energy scales of XPS and AES instruments.

Reference data, reference materials and reference procedures are required for the commonly used techniques of surface analysis. We are nearing completion of a compilation of evaluated ion sputtering yields for elemental solids and those ion species in common use. Technical advice is being provided for the further development and updating of the NIST X-ray Photoelectron Spectroscopy Database (a compilation of some 13,000 line positions, chemical shifts and splittings). This database originally was made available by the NIST Office of Standard Reference Data in 1989. In addition to efforts, described later, in characterizing a new batch of the NIST SRM 2135, we have completed the characterization of SRM 2136, a Cr/Cr_2O_3 multilayered thin-film structure consisting of seven, well-defined, thin oxide-marker layers (about three monolayers thick) separated by Cr films that are about 30 nm thick. This material should be useful as a depth-profile standard for secondary-ion mass spectrometry and a sensitivity standard for AES. We are currently developing a new SRM that will consist of Cu, Ag, and Au for the convenient calibration of the energy scales of AES and XPS instruments. Finally, we are active in the development of reference procedures for surface analysis through national and international standards groups.

C.J. Powell, Group Leader; J. Fine, J.W. Gadzuk, L. Tanovic (Guest Scientist), and N. Tanovic (Guest Scientist).

B. Selected Technical Reports

1. Time-Resolved Laser Probes of Vibrational Relaxation of Adsorbed Molecules

J.D. Beckerle and R.R. Cavanagh

Experiments in collaboration with the Molecular Physics Division have provided the first direct determination of the rate of energy transfer for vibrationally excited molecules adsorbed at well-characterized metal single-crystal surfaces. These experiments provide the capacity to address a variety of effects that have only been accessible through theoretical models or indirect measurements. The NIST experiments, performed with femtosecond laser pulses, have special significance because energy dissipation processes at surfaces are expected to play a profound role in the chemical and physical behavior of interfaces.

In these femtosecond infrared (IR) pump-probe experiments, an ordered monolayer of CO was adsorbed on a well characterized Pt(111) single crystal surface. An infrared pump pulse excited the adsorbed CO stretch mode (2105 cm^{-1}), and a second infrared probe pulse was used to characterize the time evolution of the excited state. Among the predicted effects which were observed was the rapid ($T_1{}^{a}3$ ps) decay of the excited state population. This decay was extremely rapid compared to that for CO oscillators in other materials, indicating that a mechanism unique to conducting surfaces is at work. Presumably, the energy is lost to electronic states of the metal (electron-hole pairs). It had been anticipated that this mechanism would give decay rates comparable to the observed rates, but the rapid decay had not been observed previously. In addition to the rapid decay, the experiments revealed a transient response characteristic of the dephasing time (T_2) of the CO oscillators (the time required for an ensemble of in-phase oscillators to lose its coherence), which is related to interactions among the oscillators. These time domain measurements of T_1 and T_2 were made possible by the use of laser pulses that were significantly shorter than either T_1 or T_2. The transient IR spectra also showed that the absorption frequency (2101 cm^{-1}) associated with the excited CO(v=1) oscillators is nearly the same as the fundamental absorption frequency (2105 cm^{-1}). This remarkably small anharmonic shift was unexpected and has yet to be fully explained. However, it is consistent with the presence of strong CO-CO coupling in the adlayer.

To pursue the above measurements of T_1, the experimental design was altered to incorporate subpicosecond IR pulses, and to also include spectral dispersion of the probe pulses. These measurements revealed that, when the IR pulse duration is less than T_2 (assumed to be reflected by the IR absorption lineshape), it is possible to extract T_1 and

T_2 from the time response. Models for this effect have been explored and are currently being extended to take into account the multilevel nature of the excited-state manifold in the Pt(111) experiments.

Due to the complexity of the adsorbate-coupling effects that are present in the adsorbed monolayer, combined with the fact that we were using new laser pulse-generation and detection facilities, the measurement technique was tested with a model inorganic compound, $Rh(CO)_2(acac)$ in $CHCl_3$ solution. This system has a T_1 time (70 ps) that is substantially longer than our pulse duration, has a line width and position that are essentially identical to those for CO/Pt(111), and overtone and combination bands that are significantly shifted from the fundamental transitions. These features allowed us to establish that the phenomena observed on the CO/Pt(111) sample were not artifacts of the single-reflection experiment, and we were able to demonstrate that the IR absorption linewidths were correlated with many of the unusual observations made for CO/Pt(111). These measurements have proven to be invaluable in mapping out the physics behind the observed optical transients, and they have now been confirmed by theoretical modeling.

These experiments have demonstrated the power of time-resolved measurements for directly monitoring energy redistribution amongst molecular bonds at surfaces. Such measurements promise to eludicate energy-transfer processes at surfaces, a field where direct information has been elusive. Future experimental work will extend the study to other metals, the role played by surface temperature in these relaxation processes, and the sensitivity to binding site of the adsorbed CO.

2. Laser-Driven Surface Chemistry at Semiconductor Surfaces

L.J. Richter, S.A. Buntin, and R.R. Cavanagh

Optically stimulated reactions are widely known and are important, for example, in the radiation damage of materials. There has been a flurry of activity in the past ten years to extend photochemical studies to the realm of the gas/solid interface. Several factors have propelled this interest, including the promise of materials with improved resilience, novel energy conversion systems, and non-thermal processing of semiconductors.

Recent collaborative work with the Molecular Physics Division has led to the first identification of an optically initiated chemical reaction that is driven by the creation of excited electronic states found only at surfaces. In these experiments, a Si(111) crystal was prepared in ultrahigh vacuum and covered with 0.05 of a monolayer of NO. A 10 nsec laser irradiated the surface, desorbing a small fraction of the bound NO. A second laser pulse was then used to identify the velocity and internal-state distribution of the ejected NO. Since the temperature of the surface increased by less than 1 degree Kelvin, it was apparent that the desorption was not thermally induced. By using quantum-state-specific detection of the desorbed NO, it was learned that the NO had an unusual internal energy content, exhibiting velocities which exceeded the surface temperature by up to a factor of fifteen, and a spin-orbit population which was not equilibrated with molecular rotation. Additional experiments, which probed the sensitivity of this optically driven desorption process to the wavelength of light used for irradiating the crystal, established that the desorption yield did not correlate with the bulk absorption properties, but were best accounted for by previously identified electronic states localized at the surface. The role of these surface states has now been confirmed by chemical titration of specific surface states.

In contrast to these low-coverage results, it appears that a different excitation/desorption process is operative at high NO coverages. When all the adsorption sites of the surface are saturated with NO, a much stronger dependence on desorption wavelength is found in the internal state populations and the kinetic energy distributions. At these high coverages, a $v=1/v=0$ population ratio of 0.6 is observed, again significantly greater than the result for low coverage. This high coverage process appears to be consistent with hot-carrier-mediated desorption.

The observation of optically driven, surface-state-mediated chemical reactions has interesting implications for the field of laser/surface processing. Reaction pathways involving optically accessed surface states can proceed with minimal substrate heating, providing new opportunities for low-temperature processing. Future experiments are being designed to explore adsorbate-localized, optically stimulated reactions.

3. Dynamics of Hot Electron-Ion Resonance Mediated, Non-Thermal Surface Reactions

J.W. Gadzuk, L.J. Richter, and R.R. Cavanagh

The promise of a truly novel, laser-induced surface photochemistry has been alive for nearly as long as photons have been aimed at surfaces. While the initial hopes undoubtedly were focussed on bond-selective chemistry, reality had it that the laser was mainly a large and expensive Bunsen burner, serving as an energy source for an esoteric thermal chemistry. Part of the problem arose from the deleterious influence of the surface. Basically, it served as a heat bath, draining off whatever energy was deposited locally in the surface-molecular complex before anything "of interest" happened.

Our experimental laser-induced desorption studies, initially for the system of adsorbed NO on Pt(111), in conjunction with our semiclassical wavepacket dynamics modeling, have provided some of the first evidence, and a plausible explanation, of laser-initiated, non-thermal surface reactions. The experimental results strongly suggest that the initial step in the reactions studied, specifically the desorption of internally excited NO, involved photon excitation of the Pt substrate conduction-band electrons. These hot electrons were then incident from within the substrate upon the adsorbed NO. An inelastic resonance scattering process occurs in which the NO-Pt chemisorption bond is compressed due to the formation of a temporary negative molecular ion. This compression provides a microscopic mechanism for redistribution of the incident hot-electron kinetic energy into molecular vibrations and translations. For those events in which energy in excess of the chemisorption energy is placed in the molecular center-of-mass motion, desorption follows and the product yields and internal state distributions can be measured. In addition to compression of the NO-Pt chemisorption bond, the formation of the resonance distorts the N-O intramolecular bond. This leads to vibrational excitation of the desorbed NO. The ability to self-consistently treat both the desorption yield and the vibrational excitation was a key feature of the modeling. Unlike the case in earlier laser/surface investigations, the substrate has been an all-important positive element in the surface photochemistry. It not only serves as an antenna for the incident radiation, but it also provides the source of excited photoelectrons which then induce the non-thermal reaction.

These initial studies demonstrate the ideal symbiotic relationship between experimental and theoretical inquiry. In this case, totally new and unexpected experimental findings on a specific system inspired a program of theoretical modeling, which in turn provided a basis for understanding the conditions under which the new hot electron-ion resonance mediated, non-thermal laser surface chemistry might be operative.

4. High Temperature Superconductor Thin Films

S.W. Robey, T.J. Hsieh, and R.L. Kurtz

Our efforts in the field of high-temperature superconductivity this year have been concentrated on development of the ability to produce thin films of these materials under carefully controlled conditions. It is widely accepted that the successful incorporation of the high Tc oxides into new and existing technologies will require the development of viable thin-film processing techniques, and thus an understanding of the multitude of growth and interface problems which will certainly appear. By developing the ability to produce thin-film structures under ultra-high vacuum conditions, we will be able to apply electron spectroscopic techniques to investigate these problems and seek routes toward, for instance, methods for improved epitaxy and orientation of particular crystalline axes, temperature regimes needed to reduce substrate interactions, and methods leading to reduced processing temperatures.

With these goals in mind, we have designed and built a small molecular beam epitaxy facility for depositing high-T_c oxides by coevaporation. This system is currently operational, and we are making our initial attempts to produce superconducting thin films. At this stage, we are attempting to produce $Dy_1Ba_2Cu_3O_{7-x}$ materials. These films are deposited under ultra-high vacuum conditions, and they can then be removed using a sample-insertion system for investigation with x-ray diffraction, Rutherford backscattering spectroscopy, electron microscopy, and transport techniques. An ozone distillation system has also been built and tested for use as an oxidizing source for in-situ production of thin films with superconducting properties at reduced temperatures. This system is important since it allows us to study films using electron spectroscopies, and it is necessary from a technological point of view to eliminate the need for high-temperature post-deposition anneals, which are incompatible with most thin-film applications.

We have also made valuable contacts with members of the Center for Superconductivity Research at the University of Maryland, which will allow us to collaborate on investigations of the correlation between growth and microstructure aspects of thin films and the resulting superconducting properties. The Center will provide us with interesting new superconducting oxides for studying the electronic structure of these materials by resonant photoemission, and the relation of the electronic structure to superconductivity.

5. Resonant Photoemission Studies of Half-Metallic Ferromagnetic Alloys

S.W. Robey, L.T. Hudson, R.L. Kurtz, and E. Elizalde

Over the past several years there has been a great deal of theoretical and experimental interest in the properties of magnetic Heusler alloys, in particular those with compositions of XMnY and with $C1_b$ crystal structures, where typically X=Ni,Co,Cu, ... and Y=Sn,Sb, In... . This interest has been generated by electronic structure calculations, which indicated that these materials should be half-metallic ferromagnets. The term half-metallic is used as a result of the prediction that majority-spin electrons in these materials have a metallic band structure, while minority electrons are semiconducting and have a small band gap at the Fermi level. This result is in contrast to the electronic structure found for the more thoroughly investigated class of alloys with compositions of X_2MnY and with $L2_1$ crystal structures, which are normal metallic systems. Aside from the purely scientific interest, the half-metallic character could induce very interesting, and possibly useful, transport and magneto-optic properties. For instance, the $C1_b$ alloy PtMnSb has the largest magneto-optic rotation measured for any material, and the half-metallic character has been offered as an explanation of this large effect. Understanding these materials could thus have great importance for magneto-optic recording technologies.

Over the past year, we have performed a series of experiments with the goal of investigating the electronic structure of the $C1_b$ alloy NiMnSb and comparing and contrasting this material with the "normal" alloy, Ni_2MnSb. These investigations employed resonant photoemission measurements at the SURF II synchrotron to provide information on the electronic densities of states in these materials and to determine the contributions from the different atomic constituents throughout the valence bands. Our main goal was to determine if any changes occur on going from the $L2_1$ to the $C1_b$ structure in the electronic density of states and, in particular, changes to the degree of hybridization of the Mn 3d levels.

We have found that both materials exhibit very similar densities of states consisting of a region from the Fermi level to about 2 eV binding energy comprised of a mix of Mn and Ni 3d states. The hybridization of Mn 3d states throughout this region appears to be similar in both materials as evidenced by the comparable degree of resonant enhancement seen around the Mn 3p core threshold. More localized, strongly resonating Mn 3d derived states are also present in both materials at about 3 eV below the Fermi level. The most evident difference observed is an increase in the density of states within about 1 eV of the Fermi level, and a somewhat larger-than-expected increase in resonant enhancement at the Ni 3p core threshold with increased Ni content in Ni_2MnSb. The lack of distinctive differences makes it difficult to establish directly the half-metallic character of NiMnSb. We are currently trying to understand the role of the observed subtle changes in revealing any differences in the electronic structure of these two materials.

6. Magnetic Engineering for Advanced Recording Media

W.F. Egelhoff, Jr., W.R. Bennett, and W. Schwarzacher

A recent DoC report "Emerging Technologies" identified high-density data storage, and in particular magneto-optical storage, as an area in which the U.S. is falling dangerously behind Japan. The importance of this technology is evident in the prediction by this report that, by the year 2000, U.S. sales will be in the range of \$10B-\$100B. This is a market that must not be lost to foreign competitors.

On the research front, an intense competition is developing among the U.S., Europe, and Japan for the development of magneto-optical recording media with improved properties. A principal goal of this research is to provide a fundamental scientific understanding of the relationship between the magneto-optical characteristics of the metallic thin films that form the active element of recording media and the structural properties of the film at the atomic level. The common view is that through such an understanding it will be possible to design and fabricate media with improved properties in a rational way. In view of this situation, it was decided in the past year to add a magneto-optical measurement capability to an existing thin-film growth facility. The latter facility has been used in recent years to develop techniques for improving the structural perfection of epitaxial thin films. A major part of this work has been the development of new approaches to structural measurements of epitaxial films, at the atomic level, using new techniques such as x-ray photoelectron and Auger-electron forward scattering, and reflection high-energy electron diffraction. As a result of this work we have a considerable body of expertise that can be utilized in efforts to understand the fundamentals of magneto-optical recording media.

The new magneto-optical measurement facility has been designed, constructed, tested, and used in preliminary experiments on our specially grown epitaxial Fe-Cu multilayer films. Even these preliminary results have shown an exciting and entirely unexpected new effect, an enhanced magneto-optical Kerr rotation in Fe-Cu films of particular thicknesses and of very high structural quality. Since Kerr rotation is the physical basis of signal generation in magneto-optical recording media, any method of enhancing it is of great interest.

We plan to follow up on this discovery by applying the same approach to other systems, such as Co-Pd and Co-Pt multilayer films, which are much closer to commercialization (2-5 years) as actual high-density data-storage media. If we can use our special film growth techniques to "engineer" enhanced magnetic properties, and hence enhanced signal strength, in these advanced recording media, the technology is expected to be of considerable value to U.S. industry.

7. Synchrotron X-ray Studies of Interfaces

T. Jach

The determination of electronic and structural properties of atoms located at interfaces has been one of the principal directions towards which surface science has moved in recent years. The development of new ways of investigating atomic growth in the process of molecular beam epitaxy (MBE) has been one of the main concerns of groups responsible for such work, including the MBE Group in the Semiconductor Devices Division and our Thin Films and Interface Group.

The purpose of the x-ray studies of interfaces with synchrotron radiation has been to develop the techniques of x-ray standing waves for the accurate location of atoms. We had previously been successful in applying this technique in a new way to determine the positions of atoms on metal-crystal surfaces. This year, the standing wave technique was developed in a new geometry to determine the positions of halogen atoms on semiconductors. The geometry of the new technique, grazing-angle diffraction, is totally different from that used in previous experiments. The merit of the new geometry is that, while it provides atomic positions of impurities with respect to the substrate of considerable accuracy (0.04 Å), it is not limited to atoms on surfaces.

During the past year, the theory of x-ray standing waves in grazing-angle diffraction was developed, which allowed extraction of data parameters similar to the parameters obtained from Bragg diffraction. Computer codes were then written to fit data obtained in the grazing-angle geometry, which requires fitting of twice the number of parameters of the previously used Bragg geometry. The agreement between theory and experiment was excellent over a wide range of experimental conditions. Data obtained experimentally at the Cornell High Energy Synchrotron Source were fitted to obtain the positions of iodine on germanium in a model-independent way. These results are a significant contribution to the ultimate goal of locating impurity atoms buried in a semiconductor interface; the previous x-ray standing wave techniques cannot be applied to this problem.

For purposes of extending these experiments to atoms in the process of deposition, an ultra-high vacuum chamber was assembled and tested. It will permit x-ray standing wave measurements in the grazing-angle and Bragg geometries during in-situ deposition on a synchrotron beamline. A separate x-ray diffractometer was constructed for the purpose of aligning crystals used in surface science experiments throughout NIST.

The ultimate development of this work will be to locate atoms in buried interfaces using x-ray fluorescence. Samples of GaAs have been prepared on which the MBE group of the Semiconductor Devices Division will deposit heterogeneous semiconductor interfaces of importance for device fabrication. These materials will be studied using our x-ray standing wave method.

8. Electron Transport in Ultra-small Devices

M.D. Stiles

As devices are made smaller and smaller, it becomes important to answer several questions to better understand how these devices operate. During the past year, a series of investigations have been conducted into some of these issues. These include the effect of Coulomb charging effects in tunnel junctions as the junctions (and leads) become smaller and smaller, the coupling between electrons associated with different minima in abrupt interfaces between gallium arsenide and aluminum arsenide, and the transmission of electrons across interfaces between silicon and nickel disilicide.

There is a particular energy associated with a capacitor being charged. When an electron tunnels across a junction, the junction is temporarily charged and the energy is raised by the charging energy. If the junction does not discharge quickly enough, this charging energy can "block" the tunneling, leading to an increase in the junction resistance. Only recently have devices become small enough for this effect to be observable; as devices become smaller this effect could degrade their performance. On the other hand, it may be possible to use this effect to construct a new current standard. In collaboration with people from several other institutions, a way of understanding these effects has been developed for model systems. The results of this study indicate when these effects might be important and when they can be ignored.

One proposal for the next generation of high-speed devices is based on the use of gallium arsenide-aluminum arsenide materials. Some of these devices use aluminum arsenide tunnel barriers. In collaboration with D.R. Hamann of AT&T Bell laboratories, a first-principles method has been applied to the problem of electron transmission across interfaces between these materials. A complication in this system is that the conduction band in the gallium arsenide is at the zone center and in aluminum arsenide it is at the zone boundary. We have shown that under some circumstances the behavior of electrons is dominated by the coupling between these different types of electrons. We have developed techniques that, by comparison with our detailed calculations, allow these effects to be calculated simply in many different situations.

Prompted in part by our previous calculations, recent measurements of the transmission of electrons across silicon-nickel disilicide and silicon-cobalt disilicide are being made using a technique called Ballistic Electron Emission Microscopy (BEEM). These new experiments have allowed us to extend our previous calculations to provide a more complete comparison with the experimental data. Neither the calculations nor the experiments are complete, but preliminary indications show that they agree in the most important details. This system provides the first good test of our understanding of metal-semiconductor interfaces, particularly electron transport across them.

9. Micro-Structural and Micro-Compositional Characterization of Novel Materials

P.P. Camus and A.J. Melmed

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 complementary 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 high-temperature superconductors, and of a NIST thin-film standard reference material. During the past year, we have added a reflectron ion-energy-compensation element to our probe-hole AP instrument, which increased its mass resolution from about 200 to over 1000.

We have previously shown that a stoichiometric Eu 1-2-3 superconducting material could lose oxygen from its outermost surface layers on exposure to a vacuum environment at room temperature. It had also been found that this surface was insulating, but the application of a strong negative electric field made the surface metallic-like; this change was thought to be due to diffusion of oxygen to the surface. We have made AP measurements of changes in the surface stoichiometry of Y 1-2-3 superconductors, following the application of both positive and negative electric fields to specimens at 85 K. No significant change in surface composition occurred with a positive field. A strong negative field (sufficient to cause field electron emission) applied for about 10 minutes caused a decrease in the oxygen and barium relative concentrations, and a surface enrichment in copper and yttrium. We have proposed a qualitative model to account for these results in terms of diffusivities of the species, the density of vacant sites, the resistivity of the near-surface off-stoichiometric layer, and the conductivity of the bulk. It would therefore be expected that different results could occur at other temperatures. Specifically, it might be possible to reduce the loss of surface oxygen by cooling the specimens to lower temperatures. Outward diffusion of oxygen, presumably by vacancy hopping, would still occur but field-assisted desorption of oxygen from the surface might be considerably reduced. The surface region might then become superconducting. It is believed that oxygen diffusion in the high-temperature superconductors most likely occurs through the end-plane positions in the unit cell. A novel model of the micromorphology of the Y 1-2-3 superconductor was proposed during the year. It was postulated that the material consisted of microdomains with dimensions of about 10 nm. Such a microdomain structure could account for conflicting observations, particularly through a hypothesis that ^{18}O-^{16}O isotopic exchange, which could occur in the domain interiors but not at the walls. We have attempted to observe isotopic effects of the type proposed, but have found no evidence for the existence of

^{18}O-depleted domain walls. Our work is preliminary, and it is possible that the amount of isotopic exchange may have been insufficient for an observable effect.

We have demonstrated the feasibility of FIM and AP characterization of the NIST multilayered Ni/Cr thin-film SRM 2135 (see also item 14). Several samples of the original and newest batches of material were examined. Interface widths, the compositions of individual layers, and measures of inhomogeneity within the layers were determined. Oxides were present at Ni-Cr interfaces and at Ni-Ni grain boundaries. Our measurements of layer composition and thickness were consistent with characterizations by sputter-depth-profiling with Auger-electron spectroscopy.

10. Calculations of Electron Inelastic Mean Free Paths in Compounds

C.J. Powell

Values of inelastic mean free paths (IMFPs) of low-energy (^{a}50-2000 eV) electrons in solids are needed for quantitative surface analyses by Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy, as well as for determining the surface sensitivity of other electron spectroscopies. Information is particularly desired on the dependence of the IMFP on material and electron energy. Unfortunately, it is not possible to make IMFP measurements with the needed accuracy, and it is therefore difficult to draw reliable conclusions on how the IMFP varies with material or electron energy, based on the available measurements which are of uncertain accuracy.

In a collaboration with Drs. D.R. Penn of the Electron and Optical Physics Division and S. Tanuma of the Nippon Mining Company, calculations have been made of IMFPs for 50-2000 eV electrons in a range of materials. We make use of experimental optical data for a given material to represent the inelastic scattering probability as a function of energy loss and, in the absence of experimental measurements, we use a theoretical function to represent the dependence of the scattering probability on momentum transfer. We initially made IMFP calculations for a group of 27 solid elements and were able to derive from these results an empirical equation that could be used to predict IMFP values in other materials. Although approximations have been made in developing our algorithm, these are expected to be systematic, and it is therefore believed that useful predictions of the dependence of IMFP on material parameters and on electron energy can be made from our empirical equation.

During the past year, we have made IMFP calculations for a group of 15 inorganic compounds (Al_2O_3, GaAs, GaP, InAs, InP, InSb, KCl, LiF, NaCl, PbS, PbTe, SiC, Si_3N_4, SiO_2, and ZnS). As we found in our analysis of the IMFP results for the group of elements, there are substantial differences in the shapes of the IMFP versus electron energy curves for the compounds in the 50-200 eV region. These differences can be understood in terms of the different inelastic scattering mechanisms in the various materials. We find that the predictive equation developed from our IMFP results for the elements provides a reasonable guide for predicting IMFP values in the compounds. This equation, however, is less accurate for the compounds then the elements because of the more complex inelastic scattering phenomena that can occur in the compounds. Nevertheless, our equation is believed to be more reliable for indicating IMFP dependences on material and energy than a simpler equation deduced previously from a group of experimental measurements with large measurement uncertainties.

11. Chaos in Coupled Molecule-Surface Dynamics

J.W. Gadzuk

Great strides have occurred in recent years in theoretical/numerical simulations of many dynamical phenomena involving the interaction of energetic molecule-surface systems. The processes that we have treated include hyperthermal-molecule-surface collisions, vibrational spectroscopy, and electron femtochemistry at surfaces. Depending upon the issues to be addressed, a wide range of tradeoffs between classical, semiclassical, and quantum dynamics of both the incident molecule and the target surface can be invoked while still maintaining the basic integrity of the study. Amongst the more important issues of inquiry are the factors responsible for various energy redistribution patterns in state-to-state monitored collisions, particularly the conversion of incident translation (T) energy into rotational (R), vibrational (V), or electronic excitations of the scattered, trapped, or dissociated molecule. With regards to collision phenomena, the relevant properties of the system energy enter into a dynamics simulation via the system-specific multi-dimensional potential energy surface (PES) used in the appropriate time-evolution equations. Within the context of gas-phase molecule-atom collisions, it is known that certain generic classes of PES topology give rise to definite classes of energy redistribution.

Our ultimate goal is to understand molecule-surface collisions routinely at the same level of generality as for gas-phase collision systems. In order to progress towards this goal, we have been studying various aspects of TRV energy distributions for a number of model PESs characteristic of specific systems. For at least three different reasons, we have directed particular attention on the role of chaos in the resulting non-linear time evolution equations used in classical trajectory simulations. In no particular order, the issues under study are:

i) Statistical vs. selective outcomes. A requirement for statistically distributed collision outcomes is ergodic behavior which in turn requires chaotic evolution. We are studying ways to defeat statistical outcomes in molecule/surface collisions.

ii) Numerical stability. Due to inherent roundoff errors in truncated numerical simulations, dynamics of coupled non-linear molecule-surface systems are subject to chaotic instabilities, whose existence and properties must be understood and dealt with.

iii) New methodologies: New techniques in numerical modeling and analysis of both conservative and driven physical systems are being developed in interdisciplinary chaos research throughout the world. These newly devised techniques are being applied to our problems in molecule-surface collisions, spectroscopies, and reaction rates.

12. Exactly Solvable Models in Electron-Phonon Systems at Surfaces

J.W. Gadzuk

In mathematical modeling of physical processes, one is always confronted with possibly conflicting drives, on the one hand towards numerical significance (usually at the expense of physical transparency and understanding) and on the other, towards simplicity, understanding, and elegance. The ultimate goal would be the attainment of exactly solvable model descriptions of the physics problems, thus providing numerical consequences without approximations, which are often times justified only on the basis that they make numerical evaluation possible.

The need for exactly solvable models of complex physico-chemical situations is more than a superfluous nicety. Such models serve as theoretical standards to which approximate numerical simulations can be compared to assess the "goodness" of a given numerical procedure.

A particular class of physical problems, with which we have been concerned in the recent past, involves the excitation of a phonon system due to the transient occupation of a localized-electron resonance state. Realizations of this abstract problem that we have focused on include resonance-assisted electron-stimulated desorption, laser-induced desorption, and inelastic resonant tunneling in quantum-well heterojunctions. In all three cases, an incident electron is trapped in a quasi-discrete bound state, either a molecular shape resonance or a quantum well state, where it displaces the phonon field or vibrational coordinates, the degree of excitation depending upon the lifetime of the resonance state in relation to the phonon period. Vibrational excitation, desorption, and/or phonon sidebands in junction current vs. voltage characteristics are the observable consequences of such processes.

We have provided exact solutions to various models for the just mentioned phenomena, first in terms of semiclassical Gaussian wavepacket dynamics, and second in terms of a transient displaced quantum harmonic oscillator. These models have been useful in assessing the limitations and domains of applicability of numerical simulations, have provided insight into the sensitivity to various system properties, and have successfully provided explanations and rationalizations for a considerable body of experimental desorption data.

13. Kinetic Processes Induced by Ion Bombardment

J. Fine, L. Tanovic, and N. Tanovic

Bombardment-enhanced mass transport processes are increasingly being recognized as an important factor contributing to increased interface broadening during sputter-depth profiling. Our previous work on enhanced segregation and diffusion at Ag/Ni interfaces dramatically demonstrated the importance of this type of transport process: we were able to demonstrate that, at elevated temperature (400-700 K), there was an abrupt transition in the enhanced diffusion, which decreased with increasing temperature. To explain this unprecedented result, we developed a complex-defect annihilation model which, in the case of Ag/Ni, indicates that the rate-controlling step is the dissociation of complex defects with increasing temperature.

As a test of this defect annihilation model, we have investigated the bombardment-enhanced segregation of Ag in Ni at elevated temperatures (400-700K). Preliminary analysis of this segregation data indicates that the segregation rate does decrease with increasing temperature, in keeping with our defect model. These data also suggest that, at elevated temperatures, silver diffuses over the surface at a rate that is distinguishable from the segregation rate. A more complete analysis is underway in order to characterize the temperature-dependent segregation rates, as well as the surface diffusion rate for silver.

Enhanced diffusion at Ni/Cr interfaces also was studied during the sputter-depth-profiling process of a multilayered Ni/Cr Standard Reference Material at elevated temperatures. Such diffusion is rather complex in the Ni-Cr system. Extensive, concentration-dependent diffusion of Cr into Ni was observed; however, very little diffusion of Ni into Cr was detected. This enhanced diffusion of Cr into Ni was dependent on ion-beam current density and, therefore, is consistent with other material systems that exhibit bombardment-enhanced diffusion (such as Ni/Ag).

In related work, performed in collaboration with Prof. M.H. Shapiro of the California State University at Fullerton and Mr. R.N. Freemire of the Scientific Computing Environments Division, multiple-interaction calculations have been made to simulate the dynamic phenomena occurring in the collision cascade following ion-surface collisions. We have recently completed an analysis for an Al(100) surface bombarded by 5 keV argon ions, and have examined the collisional mechanisms and trajectories of atoms in the cascade. In contrast to most previous studies, we find that essentially all atoms ejected from the surface with excitation of core electrons result from asymmetric collisions, that is, an incident ion colliding with a target atom rather than an excited target atom colliding with another target atom. We have been able to generate time-step trajectories that show the sequence of events; the trajectories have been color-coded according to their energies. Our computer graphics displays are being assembled for a movie and we anticipate that this will assist the communication and understanding of our simulations.

14. Reference Data and Reference Materials for Sputter-Depth Profiling

J. Fine, L. Tanovic, and N. Tanovic

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) 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. We also found that preferred yield data could be fitted to curves generated from the Sigmund sputtering theory and Ziegler-Biersack-Littmark nuclear stopping cross sections. These fitted curves have been used to obtain recommended values of sputtering yields for ion energies from 0.5 to 20 keV. Tables of these recommended values as well as graphs of fitted data have been generated and are being edited for publication. We anticipate that our evaluated yield data well be much more useful and reliable than the unevaluated data compilations that are now available.

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. 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.

This past year a large stock (about 800 pieces) of replacement thin-film materials was successfully prepared under contract with Comsat Laboratories in Germantown, MD. This stock consists of 8 batches; each batch of about 100 specimens was separately fabricated. Each of these batches has been characterized by Auger sputter-depth-profile analysis for both layer thickness uniformity and interface broadening as a function of sputtered depth. These new materials are of very high quality (uniformity of layer thickness is about ±2%) and should be quite suitable for sputtered depth calibration.

15. National and International Standards Activities

C.J. Powell and J. Fine

Three groups are currently active in the development of standards for surface analysis: ASTM Committee E-42 on Surface Analysis; the Surface Chemical Analysis Technical Working Party (SCATWP) of the Versailles Project on Advanced Materials and Standards (VAMAS); and the Subcommittee on Surface Analysis (SSA) of the International Union of Pure and Applied Chemistry (IUPAC) within Commission V.2 on Microchemical Techniques and Trace Analysis. We make contributions to projects organized by each group, and also provide a liaison function for the purpose of transferring status reports to ensure coordination and to minimize duplication of effort.

We summarize here project contributions that have been made during the past year. For the ASTM E-42 Committee, we are leading a task group in the calibration of energy scales for x-ray photoelectron spectrometers and Auger-electron spectrometers. This work is based on a VAMAS SCATWP project involving NIST and the UK National Physical Laboratory, in which each laboratory has made independent, high-accuracy measurements of the binding energies of selected core electrons of copper, silver and gold; similar measurements have been made of the kinetic energies of selected Auger electrons from the same three metals. These measurements are now undergoing final review and it is anticipated that joint recommendations will be prepared soon for values of the binding energies and kinetic energies to be used as reference values for the calibration of instrumental energy scales. An appropriate calibration procedure has been proposed to the ASTM E-42 Committee, and a formal document will be prepared during the current year. Such calibrations are needed to ensure reliability in the identification of chemical state from small shifts of measured binding energies or kinetic energies from elemental values. In addition, adequate calibrations are needed to enhance confidence in databases and compilations of measured binding energies and kinetic energies.

We are leading a VAMAS SCATWP project to evaluate an algorithm developed at NIST for fitting sputter-depth-profile data. A round robin has been designed in which participating laboratories will measure sputter depth profiles of a NIST multilayered nickel/chromium material; the profiles will then be analyzed with the NIST algorithm and the results compared. The round robin will enable an assessment to be made of the reliability of the algorithm in analyzing depth-profile data for well-characterized interfaces that were obtained on instruments with different geometries and sputtering conditions. Results have been obtained so far from nine laboratories, and these results will be analyzed during the coming year.

The ASTM E-42 Committee has developed definitions of terms commonly used in surface analysis and these are currently being analyzed by the IUPAC SSA for logical coherence and for consistency with definitions adopted by other standards bodies. It is expected that this effort will lead to modifications of the ASTM E-42 definitions and to enhancement of their value.

C. Outputs and Interactions

1. Publications

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Yarmoff, J.A., Joyce, S.A., Cartier, E., and McFeely, F.R., "Electron Attenuation Lengths at SiO_2/Si Interfaces," J. Elect. Spectr. 52, pp. 221-227 (1990).

Yarmoff, J.A., Joyce, S.A., Lo, C.W., and Song, J., "Photon Stimulated Desorption of Fluorine From Silicon Etched by XeF_2," in Desorption Induced by Electronic Transitions DIET-IV, G. Betz and P. Varga, Eds., Springer-Verlag, Berlin, pp. 65-74 (1990).

2. Talks

Beckerle, J.D., "Time-Resolved Studies of Vibrational Relaxation of CO(v=1) on Metal Particle Surfaces," American Vacuum Society Meeting, Boston, MA, October 26, 1989.

Beckerle, J.D., "Picosecond IR Studies of the Vibrational Dynamics of CO/Pt(111)," Vibrations at Surfaces VI Conference, Shelter Island, NY, September 10, 1990. Invited

Camus, P.P., "Performance of a Reflectron Energy Compensating Lens," International Field Emission Symposium, Albuquerque, NM, July 31, 1990.

Camus, P.P., "Application of Atom Probe Field Ion Microscopy," Department of Materials Science & Engineering, University of Wisconsin, Madison, WI, August 10, 1990. Invited.

Cavanagh, R.R., "Time-Resolved Studies of Vibrational Energy Transfer," AFOSR Molecular Dynamics Contractors' Conference, Sanibel Island, FL, October 30, 1989. Invited

Cavanagh, R.R., "Laser-Induced Desorption and State Specific Detection: Insight Into Carrier Driven Desorption From Metals and Semiconductors," 1989 International Chemical Congress of Pacific Basin Societies Meeting, Honolulu, HI, December 19, 1989. Invited

Cavanagh, R.R., "Vibrational Relaxation at Surfaces," Society of Photo-Optical Instrumentation Engineering (SPIE) Meeting, Los Angeles, CA, January 16, 1990. Invited

Cavanagh, R.R., "Laser-Induced Desorption: State-Resolved Evidence for Carrier Driven Processes," Society of Photo-Optical Instrumentation Engineering (SPIE) meeting, Los Angeles, CA, January 18, 1990. Invited

Cavanagh, R.R., "Laser-Induced Desorption: State-Resolved Evidence for Carrier Driven Pocesses," Chemical Physics Seminar, University of Oregon, Eugene, OR, January 22, 1990. Invited

Cavanagh, R.R., "Time Resolved Measurements of Vibrational Relaxation at Surfaces," Surface Science Division, IBM, Almaden, CA, January 24, 1990.

Cavanagh, R.R., "Time Resolved Measurements of Vibrational Relaxation at Surfaces," Western Spectroscopy Conference, Government Laboratory Representative in a Workshop: "Job Opportunities and How to Prepare for Them," Asilomar, CA, January 25, 1990. Invited

Cavanagh, R.R., "Real-Time Optical Studies of Surface Vibrations: C0/Pt(111)," Chemistry Department, University of Maryland, College Park, MD, April 18, 1990. Invited

Cavanagh, R.R., "Time Resolved Vibrational Relaxation: Molecules to Monolayers," Chemistry Department, Georgetown University, Washington, DC, May 1, 1990. Invited

Cavanagh, R.R., "Optically Driven Desorption: State-Resolved Evidence for Carrier Mediated Chemistry," American Chemical Society Meeting, Washington, DC, August 29, 1990. Invited

Egelhoff, Jr., W.F., "XPS and Auger Forward Scattering: A Probe for Optimizing the Structural Quality of Magnetic Films, Sandwiches, and Superlattices," IBM Almaden Research Laboratories, San Jose, CA, October 5, 1989. Invited

Egelhoff, Jr., W.F., "XPS and Auger Electron Forward Scattering: A Structural Tool for Ultra-Thin Films, Epitaxy, Surface Segregation, and Interdiffusion," American Vacuum Society Meeting, Boston, MA, October 25, 1989.

Egelhoff, Jr., W.F., "The Structure and Growth of Epitaxial Mn Films on Cu(100) and Ag(100) by XPS Forward Scattering," American Vacuum Society Meeting, Boston, MA, October 27, 1989.

Egelhoff, Jr., W.F., "Sandwiches and Superlattices of fcc-Fe on Cu(100): Growth Techniques for Optimizing Structural Quality and Magnetic Properties," American Vacuum Society Meeting, Boston, MA, October 27, 1989.

Egelhoff, Jr., W.F., "Surface Structural Studies of Epitaxial Growth," University of Maryland, College Park, MD, November 2, 1989. Invited

Egelhoff, Jr., W.F., "Surface Structural Studies of Epitaxial Films," Physics Department, Brookhaven National Laboratory, Islip, NY, December 14, 1989. Invited

Egelhoff, Jr., W.F., "XPS Forward Scattering: A Structural Tool for Studying Epitaxial Growth," American Vacuum Society Symposium on the Chemistry and Physics of Ultrathin Films, Rutgers University, Piscataway, NJ, March 7, 1990. Invited

Egelhoff, Jr., W.F., "XPS Forward Scattering: A Structural Tool for Surface Crystallography," American Physical Society Meeting, Anaheim, CA, March 13, 1990. Invited

Egelhoff, Jr., W.F., "XPS Forward Scattering," American Vacuum Society Symposium, Cleveland, OH, May 31, 1990. Invited

Egelhoff, Jr., W.F., "Angle-Dependent XPS and Auger Intensities: Forward Scattering or Shadowing?," International Conference on the Structure of Surfaces, University of Wisconsin, Milwaukee, WI, July 12, 1990. Invited

Fine, J., "Direct Laser Resonance Ionization of Atom Vaporization as a Probe of Chemisorption Mechanisms," First International Workshop on Post Ionization Techniques for Surface Analysis," Kaiserslautern, W. Germany, October 4, 1989.

Fine, J., "Ion Bombardment Induced Diffusion Processes at Ni/Ag Interfaces," Physics Faculty, University of Kaiserslautern, Kaiserslautern, W. Germany, October 5, 1989. Invited

Fine, J., "Evaluated Absolute Elemental Sputtering Yields for Surface Analysis," Quantitative Surface Analysis Conference, Salem, MA, October 20, 1989. Invited

Fine, J., "Scanning Scattering Microscope: A Novel Technique for Surface Studies," American Vacuum Society Meeting, Boston, MA, October 23, 1989.

Fine, J., "Multiphonon Resonance Ionization of Mg Vapor Pressure as a Probe for Oxidation Mechanisms on Polycrystalline Mg," American Vacuum Society Meeting, Boston, MA, October 24, 1989.

Fine, J., "Kinetic Energy Distribution of Magnesium Neutrals and Ions Ejected by a Pulsed Argon Beam," American Vacuum Society Meeting, Boston, MA, October 25, 1989.

Fine, J., "Resolution Limits of Sputter Depth Profiling," 16th DoE Surface Studies Conference, Golden, CO, June 7, 1990. Invited

Fine, J., " Evaluated Absolute Elemental Sputtering Yields for Surface Analysis," XVth International Symposium on the Physics of Ionized Gases," Dubrovnik, Yugoslavia, September 6, 1990.

Fine, J., "Trajectory Calculations of Collisionally Excited Atoms at Surfaces," XVth International Symposium on the Physics of Ionized Gases, Dubrovnik, Yugoslavia, September 7, 1990.

Fine, J., "Collisionally Excited Na Auger Transitions at Sodium Halide Surfaces," Eighth International Workshop on Inelastic Ion Surface Collisions," Vienna, Austria, September 18, 1990.

Fine, J., "A Molecular Dynamics Simulation of Collisional Excitation in Sputtered Aℓ," Eighth International Workshop on Inelastic Ion Surface Collisions, Vienna, Austria, September 20, 1990. Invited

Fine, J., "A Molecular Dynamics Simulation of Collisional Excitation in Sputtered Aℓ," Institute of Physics Seminar, Jagellonian University, Krakow, Poland, September 25, 1990. Invited

Gadzuk, J.W., "New Theoretical Aspects in DIET," Fourth International Workshop on Desorption Induced by Electronic Transitions-DIET V, Gloggnitz, Austria, October 2, 1989. Invited

Gadzuk, J.W., "Real-Time Dyanmics of Molecular Processes at Surfaces by Femtosecond Excitation," Physical Chemistry Colloquium, Fritz-Haber-Institute, Berlin, West Germany, October 13, 1989. Invited

Gadzuk, J.W., "Dynamics of Molecular Processes at Surfaces by Femtosecond Excitation," Department of Chemistry Colloquium, Duke University, Durham, NC, October 27, 1989. Invited

Gadzuk, J.W., "Dynamics of Molecular Processes at Surfaces," Physical Chemistry Colloquium, University of Delaware, Newark, DE, November 3, 1989. Invited

Gadzuk, J.W., "Dynamics of Molecular Processes at Surfaces by Femtosecond Excitation," Institut für Festkorperforschung, Jülich, West Germany, February 15, 1990. Invited

Gadzuk, J.W., "Fractals in Chaotic Molecule-Surface Collisions," American Physical Society Meeting, Anaheim, CA, March 13, 1990.

Gadzuk, J.W., "Laser-Excited Hot-Electron Induced Desorption: A Theoretical Model Applied to NO/Pt(111)," American Physical Society Meeting, Anaheim, CA, March 14, 1990.

Gadzuk, J.W., "Real-Time Dynamics at Surfaces by Femtosecond Excitation," IBM Almaden Research Center, San Jose, CA, March 19, 1990. Invited

Gadzuk, J.W., "Future Opportunities in Atomic Collisions and Surfaces," DoE Panel on Atomic and Molecular Physics at Surfaces, National Academy of Sciences, Washington, DC, March 26, 1990. Invited

Gadzuk, J.W., "Dynamics of Molecular Processes at Surfaces by Femtosecond Excitation," Physical Chemistry Seminar, University of Illinois in Chicago, Chicago, IL, April 12, 1990. Invited

Gadzuk, J.W., "Dissociation Bands, Fractals, and Chaos in Molecule-Surface Collisions," 50th Physical Electronics Conference, National Institute of Standards and Technology, Gaithersburg, MD, June 11, 1990.

Gadzuk, J.W., "Tunneling Time, Resonant Electron-Phonon Interactions, and Desorption," Surface Science Research Center, University of Liverpool, Liverpool, England, July 10, 1990. Invited

Gadzuk, J.W., "Electron Femtochemistry at Surfaces," American Chemical Society Meeting, Washington, DC, August 29, 1990. Invited

Gadzuk, J.W., "Resonant Tunneling with Electron Phonon Interactions: Some Exactly Solvable Model Applied to Desorption," Vibrations at Surfaces VI Conference, Shelter Island, NY, September 12, 1990.

Gadzuk, J.W., "Dissociation Bands, Fractals, and Chaos in Molecule-Surface Collosions," 7th Workshop on Interactions of Molecular Beams and Surfaces, Hindas, Sweden, September 25, 1990.

Gadzuk, J.W., "Resonant Tunneling with Electron Phonon Interactions: Some Exactly Solvable Models Applied to Desorption," Institute of Theoretical Physics Colloquium, Chalmers University, Goteborg, Sweden, September 28, 1990. Invited

Jach, T., "Comparison of Observed Au Thin-Film Growth on Amorphous Substrates with the Kinetics of Surface Growth," American Physical Society Meeting, Anaheim, CA, March 16, 1990.

Jach, T., "Determining Atomic Positions with X-Ray Standing Waves," Department of Physics, Michigan State University, East Lansing, MI, April 16, 1990. Invited

Jach, T., "Tests of Amorphous Semiconductor PIN X-Ray Photodetectors," Workshop on Magnetic X-Ray Scattering, Brookhaven National Laboratory, Islip, NY, May 16, 1990.

Jach, T., "The Instrumentation of Synchrotron X-Ray Detectors with PIN Diode Detectors," Seventh Symposium on Radiation Measurements and Applications, University of Michigan, Ann Arbor, MI, May 23, 1990.

Jach, T., "Grazing Angle Diffraction and X-Ray Standing Waves," Department of Physics, Brookhaven National Laboratory, Islip, NY, June 14, 1990.

Jach, T., "Grazing Angle Diffraction and X-Ray Standing Waves," Materials Science Division, Argonne National Laboratory, Argonne, IL, June 29, 1990. Invited

Jach, T., "Grazing Angle Standing Waves," 1990 International Conference on X-Ray Physics and Inner Shell Processes, Knoxville, TN, July 9, 1990.

Joyce, S.A., "The Influence of Coadsorbed Potassium on the ESD of PF_3 on Ru(0001)," American Vacuum Society Meeting, Boston, MA, October 24, 1989.

Kurtz, R.L., "Using Synchrotron Radiation to Probe the Surface Structure of Oxides," Physics Department, Louisiana State University, October 12, 1989. Invited

Kurtz, R.L., "Structure and Reactivity of TiO_2 as Revealed by Photoemission and Stimulated Desorption," Physics Department, Rutgers, The State University, Piscataway, NJ, January 25, 1990. Invited

Kurtz, R.L., "Dynamics Calculation of Stimulated Desorption from TiO_2," Surface Dynamics Laboratory, Rutgers, The State University, Piscataway, NJ, January 25, 1990. Invited

Kurtz, R.L., "The Role of Defects in H_2O Chemisorption on TiO_2 Surfaces," Gordon Research Conference on Fundamental Interactions of H_2O with Solid Surfaces, Meriden, NH, July 18, 1990.

Melmed, A.J., "Diffusion and Isotope Exchange in Y-Ba-Cu-O," International Field Emission Symposium, Albuquerque, NM, August 1, 1990.

Powell, C.J., "Electron Attenuation Lengths for Quantitative AES and XPS," Third Topical Conference on Quantitative Surface Analysis, Salem, MA, October 20, 1989. Invited

Powell, C.J., "Electronic Inelastic Mean Free Paths in Solids at Low Energies," American Vacuum Society Meeting, Boston, MA, October 24, 1989.

Powell, C.J., "International Efforts to Develop Reference Data for Surface Analysis: Contributions of M.P. Seah," American Vacuum Society Meeting, Boston, MA, October 25, 1989.

Powell, C.J., "Comparison of L_3-Shell Binding Energies in Six 3d Metals by X-Ray Photoelectron Spectroscopy, Appearance-Potential Spectroscopy, and Electron Energy-Loss Spectroscopy," Battelle Pacific Northwest Laboratories, Richland, WA, November 18, 1989. Invited

Powell, C.J., Reference Materials and Reference Data for Surface Analysis, University of Tokyo, Tokyo, Japan, November 20, 1989. Invited

Powell, C.J., Progress and Pitfalls in Quantitative Surface Analysis by AES and XPS, Nippon Steel Co., Tokyo, Japan, November 21, 1989. Invited

Powell, C.J., Electron Inelastic Mean Free Paths and Attenuation Lengths for Quantitative Surface Chemical Analyses by AES and XPS, Japanese National Research Institute for Metals, Tsukuba, Japan, November 22, 1989. Invited

Powell, C.J., Reference Materials and Reference Data for Surface Analysis, VAMAS Surface Chemical Analysis Group, Kyoto, Japan, November 25, 1989. Invited

Powell, C.J., Progress and Pitfalls in Quantitative Surface Analysis by AES and XPS, Japanese Microbeam Analysis Meeting, Osaka, Japan, November 27, 1989. Invited

Powell, C.J., Comparison of L_3-Shell Binding Energies in Six 3d Metals by X-Ray Photoelectron Spectroscopy, Appearance-Potential Spectroscopy, and Electron Energy-Loss Spectroscopy, Nippon Mining Co., Tokyo, Japan, November 28, 1989. Invited

Powell, C.J., "Progress and Pitfalls in Quantitative Surface Analyses by Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy," 10th Anniversary Symposium of the Surface Science Society of Japan, Waseda University, Tokyo, Japan, November 29, 1989. Invited

Powell, C.J., "Progress and Pitfalls in Quantitative Surface Analysis by AES and XPS," JEOL Company, Tokyo, Japan, December 1, 1989. Invited

Powell, C.J., "Accuracy and Precision of Quantitative Surface Analyses by Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy," National Physical Laboratory, New Delhi, India, June 20, 1990. Invited

Powell, C.J., "Attenuation Lengths and Inelastic Mean Free Paths of Low-Energy Electrons in Solids," National Physical Laboratory, New Delhi, India, June 21, 1990. Invited

Powell, C.J., "Reference Materials and Reference Data for Quantitative Surface Analyses," National Physical Laboratory, New Delhi, India, June 22, 1990. Invited

Powell, C.J., "Material Dependence of Electron Inelastic Mean Free Paths," Gordon Research Conference on Electron Spectroscopy," Wolfeboro, NH, July 17, 1990.

Powell, C.J., "Inner-Shell Ionization Cross Sections," International Congress on Electron Microscopy, Seattle, WA, August 13, 1990. Invited

Richter, L.J., "Laser-Induced Desorption of NO from Si(111): Effects of Coverage on NO Vibrational Populations," Vibrations at Surfaces VI Conference, Shelter Island, NY, September 10, 1990. Invited

Robey, S.W., "Resonant Photoemission in Ni_bMnSb Heusler Alloys," Gordon Research Conference on Electron Spectroscopy, Wolfeboro, NH, July 17, 1990.

Stiles, M.D., "Theory of Electron Transmission Through Epitaxial Interfaces," Department of Physics, University of Florida, Gainesville, FL, January 30, 1990. Invited

Stiles, M.D., "Theory of Electron Transmission Through Epitaxial Interfaces," 17th Conference on the Physics and Chemistry of Semiconductor Interfaces, Clearwater, FL, February 1, 1990.

Stiles, M.D., "Electron Transmission Through Interfaces, Workshop on Ballistic Electron Emission Microscopy," Jet Propulsion Laboratory, Pasadena, CA, March 9, 1990. Invited

Stiles, M.D., "Coulomb Blockade Effects in Transmission Lines," American Physical Society Meeting, Anaheim, CA, March 12, 1990.

Stiles, M.D., "Coulomb Blockade Effects in Transmission Lines," IBM, Yorktown Heights, NY, April 13, 1990. Invited

Stiles, M.D., "Theory of Ballistic Electron Emission Microscopy for $NiSi_2$/Si(111) Interfaces," 50th Physical Electronics Conference, National Institute of Standards and Technology, Gaithersburg, MD, June 13, 1990.

Stiles, M.D., "Theory of Ballistic Electron Emission Microscopy for $NiSi_2$/Si(111) Interfaces," Scanning Tunnelling Microscopy/90 Conference, Baltimore, MD, July 24, 1990.

Yarmoff, J.A., "Photon Stimulated Desorption of Fluorine From Surfaces Etched by XeF_2," 4th International Workshop on Desorption Induced by Electronic Transitions," Gloggnitz, Austria, October 3, 1989.

Yarmoff, J.A., "The Chemisorption of PF_3 on Ru(0001) Studied with Soft X-Ray Photoemission and Photon Stimulated Desorption," American Vacuum Society Meeting, Boston, MA, October 25, 1989.

3. Committee Assignments

R.R. Cavanagh
Local Co-Chairman, Physical Electronics Conference
National Measurement Laboratory Representative, NIST-NRC Postdoctoral Committee
Member, Organizing Committee, 6th International Conference on Vibrations at Surfaces
Member, Executive Committee, Surface Science Division, American Vacuum Society
Member, NIST Research Advisory Committee
Member, NIST 25/90th Anniversary Symposium Committee

J. Fine
Chairman of Sub-Committee Standard Reference Materials, ASTM Committee E-42 on Surface Analysis

J.W. Gadzuk
Member, Advisory Editorial Board, "Progress in Surface Science"
Member, International Advisory Committee, 6th International Conference on Vibrations at Surfaces
Member, Greater Washington Solid State Physics Colloquium
Member, Department of Energy Panel on Atomic and Molecular Physics at Surfaces
Advisor, SCIENCE Editorial Board Annual Meeting
Subject Specialist Consultant, NIST Information Resource Center
Outside Opponent for Doctoral Thesis Examination, Institute of Theoretical Physics, Chalmers University, Goteborg, Sweden

Cedric J. Powell
Immediate Past Chairman, ASTM Committee E-42 on Surface Analysis; Member, Executive Committee; and International Liaison
US representative and Vice-Chairman, Surface Chemical Analysis Technical Working Party, Versailles Project on Advanced Materials and Standards
Chairman, Applied Surface Science Division, International Union of Vacuum Science, Technique, and Applications
Co-opted Member, Subcommittee on Surface Analysis, Commission V.2 on Microchemical Techniques and Trace Analysis, International Union of Pure and Applied Chemistry
Co-opted Member, Selection and Scheduling Committee, Gordon Research Conferences
Member, International Program Committee and Advisory Board, Second International Workshop on Auger Spectroscopy and Electronic Structure
Member, Scientific Committee, European Conference on Applications of Surface and Interface Analysis
Chairman, Organizing Committee, 3rd Topical Conference on Quantitative Surface Analysis

Chairman, Organizing Committee, Workshop on Surface and Interface Characterization with High Spatial Resolution
Member, Editorial Board, "Applications of Surface Science"
Member, Editorial Board, "Surface and Interface Analysis"
Member, Editorial Board, "Methods of Surface Characterization"

4. Others

a. Seminars

October 10, 1989
L.J. Terminello, IBM T.J. Watson Research Center, Yorktown Heights, NY, "Chemistry of Surface Interaction Studies by VUV Photoemission". (Division Sponsor: S.W. Robey)

October 19, 1989
E.B. Stechel, Sandia National Laboratories, Albuquerque, NM, "Quantum Resolved Stimulated Desorption of Adsorbed Molecules: NO/Pt(111)". (Division Sponsor: J.W. Gadzuk)

November 6, 1989
J. Harris, Institut fur Festkorperforschung, Julich, Germany, "Dissociation at Surfaces". (Division Sponsor: J.W. Gadzuk)

November 28, 1989
L.T. Hudson, Vanderbilt University, Nashville, TN, "Stimulated Desorption of Atomic H from Alkali Halide Surfaces". (Division Sponsor: R.L. Kurtz)

January 16, 1990
P.A. Heimann, University of California, Lawrence Berkeley Laboratories, Berkeley, CA, "Vibrational Effects in Core Photoionization". (Division Sponsor: S.W. Robey)

February 23, 1990
S. Donner, Pennsylvania State University, University Park, PA, "Dynamical Effects in Epitaxial Growth From RHEED Oscillations". (Division Sponsor: W.F. Egelhoff)

March 8, 1990*
J.A. Venables, Arizona State University, Tempe, AZ, "Studies of Surface Diffusion and Crystal Growth by SEM and STEM". (Sponsor: R.J. Celotta, Electron and Optical Physics Division)

March 21, 1990
R. Smilgys, University of Colorado, Boulder, CO, "Laser Probing of Thermal Desorption Kinetics: As_4 Dissociation at Si(100)". (Division Sponsor: R.L. Kurtz)

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* Interface Science Seminar Series

April 17, 1990

J.A.D. Matthew, University of York, York, England, "4f-4f Excitations in the Rare Earths". (Division Sponsor: C.J. Powell)

May 9, 1990 *

W.A. Goddard III, California Institute of Technology, Pasadena, CA, "Simulation of Materials with Applications to Surfaces and Superconductors". (Division Sponsor: C.J. Powell)

May 11, 1990*

R. Clarke, University of Michigan, Ann Arbor, MI, "Interface Structure and Magnetic Properties of Co-Based Superlattices". (Division Sponsor: W.F. Egelhoff)

June 6, 1990

N. Sathyamurthy, Indian Institute of Technology, Kanpur, India, "Fractals in Atomic and Molecular Collisions". (Division Sponsor: J.W. Gadzuk)

June 14, 1990

B.D. Kay, Sandia National Laboratories, Albuquerque, NM, "State-to-State Molecular Beam Scattering From Surfaces,". (Division Sponsor: R.R. Cavanagh)

June 15, 1990

S. George, Stanford University, Stanford, CA, "Laser Induced Desorption Studies of Surface Reaction Kinetics". (Division Sponsor: R.R. Cavanagh)

June 21, 1990*

L.B. Freund, Division of Engineering, Brown University, Providence, RI, "Mechanics of Dislocations in Strained Epitaxial Layers and Other Issues Related to Thin Film Materials". (Sponsor: R. Thomson, Materials Science and Engineering Laboratory)

July 9, 1990*

P.F. Carcia, E.I. du Pont de Nemours & Company, Wilmington, DE, "Interface Design of Pt/Co and Pd/Co Thin Multilayers for Magnetic and Magneto-Optical Applications". (Division Sponsor: W.F. Egelhoff)

July 19, 1990*

M.K. Chaudhury, Dow Corning Corporation, Midland, MI, "Measurement of Interfacial Interaction Between Deformable Bodies". (Sponsor: T. Nguyen, Building Materials Division)

* Interface Science Seminar Series

August 9, 1990*

M. Weinert, Brookhaven National Laboratory, Islip, NY, "The Formation of Transition Metal Adlayers and Multilayers". (Division Sponsor: M.D. Stiles)

August 29, 1990

H.D. Bist, Indian Institute of Technology, Kanpur, India, "Laser Raman Spectroscopy and its Applications in Structural Phase Transitions". (Division Sponsor: R.R. Cavanagh)

August 27, 1990

F.P. Netzer, University of Innsbruck, Innsbruck, Austria, "Rare Earth Metal-Silicon Interfaces: Silicide Formation and Oxidation Reactions". (Division Sponsor: C.J. Powell)

September 4, 1990

B. Persson, Institut fur Festkorperforschung, Julich, Germany, "Topics in Molecular Vibrations at Surfaces: Relaxation, STM, Tunneling Times, etc.". (Division Sponsor: J.W. Gadzuk)

September 4, 1990*

E. Hasselbrink, Fritz-Haber-Institut der Max-Planck-Gessellschaft, Berlin, Germany, "Photoinduced Electron Chemistry at the Adsorbate-Metal Interface". (Division Sponsor: R.R. Cavanagh)

September 10, 1990*

R. Farrow, IBM Research Division, Almaden Research Center, San Jose, CA, "Seeded Epitaxy and its Application to Magnetic Metal Interfaces". (Division Sponsor: W.F. Egelhoff)

September 19, 1990*

G.A. Prinz, Naval Research Laboratory, Washington, DC, "Epitaxial Growth of Magnetic Films on Semiconductors". (Sponsor: D.T. Pierce, Electron and Optical Physics Division)

* Interface Science Seminar Series

b. Conferences Sponsored

October 20-21, 1989

C.J. Powell, 3rd Topical Conference on Quantitative Surface Analysis, Salem, MA

June 11-13, 1990

R.R. Cavanagh, 50th Physical Electronics Conference, NIST, Gaithersburg, MD

September 10-13, 1990

C.J. Powell, Workshop on Surface and Interface Characterization with High Spatial Resolution, York, United Kingdom

September 10-14, 1990

R.R. Cavanagh and J.W. Gadzuk, 6th International Conference on Vibrations at Surfaces, Shelter Island, NY

c. Standard Reference Material Certification

Thin Film

SRM 2136, Chromium/Chromium Oxide Marker Layer Thin-Film Depth Profile Standard

d. Faculty Appointment

R.L. Kurtz

Adjunct Associate Professor of Physics and Astronomy, Louisiana State University, Baton Rouge, LA.

D. Personnel

1. Surface Science Division Staff

As of September 30, 1990, the Surface Science Division was staffed as follows:

C. J. Powell, Chief
L. M. Johnson, Secretary

Surface Dynamical Processes Group

R. R. Cavanagh, Group Leader
J. D. Beckerle[*]
E. Elizalde[†]
T.J. Hsieh[†]
L.T. Hudson[*]
R.L. Kurtz
T.E. Madey[°]
D.E. Ramaker[°]
L.J. Richter
S.W. Robey
R.L. Stockbauer[°]

Thin Films and Interfaces Group

W.F. Egelhoff, Jr., Group Leader
W.R. Bennett[†]
T. Jach
A.J. Melmed[†]
W. Schwarzacher[†]
M.D. Stiles

Surface Spectroscopies and Standards Group

C.J. Powell, Group Leader
P.M. Connelly[#]
J. Fine
J.W. Gadzuk
R.L. King[+]
E.O. Neitzel[#]
L. Tanovic[†]
N. Tanovic[†]

[*] NIST-NRC Postdoctoral Research Associate
[†] Guest Scientist
[°] WAE, When Actually Employed
[#] Engineering Technican
[+] Electronics Technican

2. Guest Scientists

The Surface Science Division has been host during the past year to a number of scientists who have worked with the Division staff on problems of mutual interest.

Bennett, W.R., has worked at NIST for eleven months and prepared ultrathin films containing magnetic and nonmagnetic elements and measured magnetic properties of these films.

Elizalde, E., Applied Physics Department, University Autonoma of Madrid, Madrid, worked at NIST for six months on the production of thin-film high-temperature superconductors.

Hsieh, T.J., University of Maryland, College Park, worked at NIST for nine months to produce high-temperature superconducting thin films via molecular beam epitaxy.

Melmed, A.J., worked at NIST for eleven months on the microcompositional and microstructural characterization of high-temperature superconductors and composite thin films.

Schwarzacher, W., worked at NIST for eight months and prepared ultrathin films containing magnetic and nonmagnetic elements and characterized the structural and magnetic properties of the films.

Tanovic, L., Electrical Engineering Department, University of Sarajevo, Sarajevo, worked at NIST for eight months studying the interfacial structure of sputter-profiled Ni/Cr and Cr/Cr_2O_3 multilayers and characterizing a new batch of SRM 2135.

Tanovic, N., Physics Department, University of Sarajevo, Sarajevo worked at NIST for eight months studying the interfacial structure of sputter-profiled Ni/Cr and Cr/Cr_2O_3 multilayers and characterizing a new batch of SRM 2135.

3. Awards and Honors

Cavanagh, R. R.	Department of Commerce Gold Medal
Egelhoff, Jr., W.F.	Shopnote Award, American Vacuum Society
Fine, J.	R&D 100 Award for Scanning Scattering Microscope
	Scanning Scattering Microscope, U.S. Patent issued September 4, 1990, No. 4,954,722
Jach, T.	A Diffraction Device Which Detects the Bragg Condition, U.S. Patent issued April 16, 1991, No. 5,008,908
Johnson, L.	Department of Commerce Bronze Medal

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C. J. Powell, editor

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NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
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This report summarizes technical activities and accomplishments of the NIST Surface Science Division during Fiscal Year 1990. Listings are given of publications, talks, and professional committee assignments, by the Division staff together with the Conferences and NIST seminars organized by the staff.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)
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