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Technical Activities 1988
Surface Science Division

C. J. Powell, Chief

U.S. DEPARTMENT OF COMMERCE
National Institute of Standards and Technology
(Formerly National Bureau of Standards)
National Measurement Laboratory
Center for Atomic, Molecular, and Optical Physics
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National Bureau of Standards became the National Institute of Standards and Technology on August 23, 1988, when the Omnibus Trade and Competitiveness Act was signed. NIST retains all NBS functions. Its new programs will encourage improved use of technology by U.S. industry.

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U.S. DEPARTMENT OF COMMERCE
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Ernest Ambler, Acting Undersecretary for Technology
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
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ABSTRACT

This report summarizes technical activities of the NIST Surface Science Division during Fiscal Years 1987 and 1988. These activities include surface-standards work, experimental and theoretical research in surface science, the development of improved measurement methods, and applications to important scientific and national problems. A listing is given of publications, talks, professional committee participation, and professional interactions by the Division staff.

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

FOREWORD

This report is a summary of the technical activities of the NIST Surface Science Division for the period October 1, 1986 to September 30, 1988. The report was prepared as part of the Annual Report of the Center for Atomic, Molecular, and Optical Physics within the National Measurement Laboratory of NIST.

The technical work of the Division is separated formally into three main program areas: Surface Standards, Surface Measurements, and Surface Competence. Reports are given in sections 2, 3, and 4 of work performed in these three program areas. For each area there are a number of separate technical projects and information is given on project objectives, results obtained during the past two years, and the nature of planned activities.

Sections 5 and 6 of the report contain listings of papers published, papers submitted for publication, and talks presented during the year. Talks presented at the Division's seminars at NIST are given in section 7. Information on conferences organized or hosted by Division staff is summarized in section 8. The involvement of Division staff on professional committees is shown in section 9 while internal and external scientific collaborations are described in section 10. Visiting scientists who have worked in the Division during the year are identified in section 11 and the Division staff is listed in section 12.

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

NOTE: Certain commercial equipment, instruments, or materials are identified in this report in order to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

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SURFACE SCIENCE DIVISION

SUMMARY OF ACTIVITIES
Fiscal Years 1987 and 1988

1. Introduction

A. Background

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

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

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

B. Goal, Objectives and Division Programs

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

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

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

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

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

The Division addresses these objectives by means of three principal program activities for which there are technical reports in the following three sections. Information on the Surface Standards Program (objective (3)) is given in section 2, the Surface Measurements Program (objectives (1) and (2)) is described in section 3, and a report on the Surface Competence Program (objective (4)) is presented in section 4.

The Division's programs are supported financially by other NIST offices and by other Federal agencies. These arrangements enable the Division to meet NIST objectives and standards needs and also to contribute its expertise and facilities to important national programs. During FY87 and FY88, support was received from the following offices and agencies:

Office of Standard Reference Data

- o Surface Science: Sputtering Yield Data

Office of Standard Reference Materials

- o Fabrication, Characterization, and Certification of Additional Lots of SRM 2135
- o Characterization and Certification of Cr/Cr_2O_3 Thin Film Depth Profile Material (SRM 2136)

Department of Energy

- o Structure and Reactivity of Chemisorbed Species and Reaction Intermediates
- o Laser Studies of Chemical Dynamics at the Gas-Solid Interface (joint with Molecular Spectroscopy Division)

Air Force Office of Scientific Research

- o Picosecond Laser Studies of Vibrational Energy Transfer in Molecules on Surfaces (joint with Molecular Spectroscopy Division)

Office of Naval Research

- o Surface Characterization of High-T_c Superconductors and Other Oxides using Synchrotron Radiation

U.S.-Spain Joint Committee for Scientific and Technological Cooperation

- o Structure and Reactivity in Catalysis by Metals and Oxides

C. Highlights

The Division staff have been productive over the past two years, as can be judged from the following narrative reports, the lists of publications and talks, and the involvement with standards and professional groups. There have also been successful collaborations with scientists in many other institutions and with guest scientists in our own laboratories.

We mention here some highlights of the past two years; further details of these accomplishments are given in the indicated sections of this report.

- The discovery of the new high-T_c superconducting materials has generated intense activity at NIST as at many other laboratories. Division staff have contributed in two areas. Photoelectron spectroscopy with synchrotron radiation has been used to investigate the electronic structure and chemisorption properties of these materials (section 3.A). Field-ion microscopy has been successfully employed to characterize their microstructure; the images have an unusual striped pattern, not seen in any other type of material (section 4.A.3)

- New calculations have been made of electron inelastic mean free paths for 200-2000 eV electrons in 31 materials from which a general predictive formula has been derived (section 2.A.2(a))

- New high-accuracy measurements have been made of core-level binding energies and Auger-electron kinetic energies in copper, silver and gold for the calibration of the energy scales of x-ray photolectron and Auger-electron spectrometers (section 2.A.3)

- We have developed an _in situ_ method for measuring changes in surface roughness due to ion bombardment (section 2.B.2)

- We have developed a new complex-defect model to describe radiation-enhanced diffusion due to ion bombardment (section 2.B.3)

- A new suite of cooperative projects to develop standards for surface analysis on an international basis has been developed under the Versailles Project on Advanced Materials and Standards (VAMAS) and coordinated with parallel activities of ASTM Committee E-42 on Surface Analysis and of groups of the International Union of Pure and Applied Chemistry (Sections 2.C.2 and 2.C.3)

- Successful conferences on quantitative surface analysis have been held in 1986 and 1987, each attended by about 100 scientists (section 2.C.4)

- Division staff have authored 22 review articles during the past two years (section 2.D)

- We have developed improved instrumentation for photoemission and other experiments using synchrotron radiation (section 3.B)

- New grazing-angle x-ray diffraction experiments have been conducted and have shown the existence of surface-trapped diffraction waves. In addition, the registration of halogen atoms on a germanium single crystal has been established using x-ray standing waves excited under grazing-incidence conditions (section 3.D)

- We have invented a monochromator crystal for synchrotron radiation experiments that incorporates a detector for the x-rays in order to facilitate monochromator alignment. We expect a patent to be issued for this device (section 3.E)

- We have investigated fundamental mechanisms for several surface reactions important in semiconductor processing (Section 3.F)

- We have found unusual chemical properties of thin films of platinum deposited on single-crystal tungsten surfaces (section 3.H)

- We have demonstrated the first negative-ion ESDIAD (electron-stimulated desorption ion angular distributions) experiment. Results to date indicate that negative-ion ESDIAD is a useful complement to positive-ion ESDIAD (section 3.J)

- We have measured the laser-induced desorption of NO from Pt(111) and found non-thermal distributions for some of the desorbing molecules. These molecules appear to have been excited by optically excited hot electrons in the substrate (section 3.K.1)

- We have made direct measurements of the decay of vibrationally excited populations ranging from metal-cluster carbonyls to CO adsorbed on small metal particles (section 3.K.2)

- Studies have been made of the role of chaos in surface dynamics and its effects on lineshapes of vibrational spectroscopies for adsorbed molecules (section 3.L.1)

- We have investigated how selectivity can be controlled in several types of molecule-surface interactions (section 3.L.2)

- We have fabricated novel thin-film sandwich and superlattice structures which have been shown to have novel magnetic properties (section 4.A.2)

- We have constructed and tested a new instrument to measure the kinetic energy distributions of sputtered atoms and ions and their states of excitation (section 4.B.1)

2. SURFACE STANDARDS PROGRAM

G. P. Chambers, W. F. Egelhoff, Jr., N. E. Erickson, J. Fine, T. Jach,
I. Jacob, S. A. Joyce, R. L. Kurtz, T. E. Madey, D. Marton, C. J. Powell,
R. Stockbauer, S. Tanuma, Q. Wang, and J. A. Yarmoff

The term "surface standards" is intended to cover a broad range of activities that are directed to improving the quality of surface-characterization measurements through: (1) development of needed reference data and standard reference materials; (2) leadership in standards-committee activities, the development of reference procedures, and other actions to improve the accuracy and reliability of surface-analysis measurements; and (3) publication of review articles and books that enable scientists to make surface-characterization measurements of the needed quality.

Standards are needed for the many measurement techniques used for surface characterization. The most critical needs, however, exist for standards in surface analysis, by far the most commonly made measurement. Reference data, reference materials, and reference procedures are particularly needed for reliable and efficient measurements by Auger-electron spectroscopy and x-ray photoelectron spectroscopy and in the use of these and other techniques to acquire composition-versus-depth information as a specimen is ion bombarded. Requirements in these areas are assessed through surveys of user groups (the ASTM Committee E-42 on Surface Analysis and the VAMAS Working Party on Surface Chemical Analysis) and through focussed discussions at workshops and conferences (Workshop on Quantitative Surface Analysis, NIST, October 24, 1986; NPL-VAMAS Workshop on Quantitative Surface Analysis, National Physical Laboratory, London, November 17, 1986; Second Topical Conference on Quantitative Surface Analysis, Monterey, CA, October 30-31, 1987; and evening workshops on specific topics sponsored by the ASTM Committee E-42 on Surface Analysis and the Applied Surface Science Division of the American Vacuum Society (AVS) at the fall AVS National Symposium and the spring AVS Applied Surface Analysis Symposium). Three articles describing recent progress in the provision of standards and current needs are listed in section 2.D.

The Division's efforts to provide needed reference data and reference materials are summarized in sections 2.A and 2.B., respectively. The Division also contributes to coordinated international efforts to develop reference data and reference materials in surface analysis (section 2.C). Reference procedures are developed in conjunction with three active standards groups, as described in section 2.C. Division staff authored a large number of review articles which summarize recent advances and guide scientists in making reliable measurements by particular surface techniques; these articles are listed in section 2.D.

A. Reference Data

1. Sputtering Yield Data Compilation
(J. Fine and G. P. Chambers)

Sputtering techniques for depth-profile analysis are presently being used in conjunction with a number of surface analytical methods to analyze compositional changes of materials at surfaces and at interfaces. Many of these techniques have now progressed to the point of being able to provide quantitative sputter-depth-profile information yet the necessary sputtering yield data is not readily available in easy-to-use, evaluated form.

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

The HP-1000 Data System in the Center for Chemical Technology is being used for the data compilation. Dr. D. Neumann and members of his group have provided guidance as well as technical assistance with the software development.

Extensive use has been made of on-line abstract searching capability in order to bring our reference files up to date. Abstract searching has been completed and checked for completeness by making selected author searches. Sputtering yield papers have been identified and compiled, and data has been abstracted and entered into our data base. Certain experimental parameters needed for evaluating the reliability of the sputtering yield data have also been entered into our data base.

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 "reliable" (consistent) than others. Based on the setting of such limits and on the total ion dose used to obtain the measurement, we have been able to show that subsets of the yield data exist which are quite reasonable in the scatter of the data and which have the "proper" dependence on ion energy. Computer fitting routines are being developed which take into account the impacting ion and target atom masses in order to produce the "proper" shape curve for those data sets which do not contain sufficient data for fitting purposes. On completion of this phase of our evaluation scheme, we will complete the data compilation and will provide both tabular as well as graphical output of what we find to be the more reliable yield data.

2. Inelastic Mean Free Paths and Attenuation Lengths of Low-Energy Electrons in Solids

(R. L. Kurtz, T. E. Madey, C. J. Powell, R. L. Stockbauer, S. Tanuma, Q. Wang, and J. A. Yarmoff)

Values of inelastic mean free paths (IMFPs) and attenuation lengths (ALs) of low-energy (often 50-2000 eV) electrons are required in quantitative surface analysis by Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) for correction of so-called matrix effects. These parameters also define the surface sensitivity of these and other electron-spectroscopic methods of surface characterization. The AL is distinguished from the IMFP by the fact that AL values are usually derived from overlayer-film experiments on the basis of a model in which elastic electron scattering has been assumed to be insignificant. The IMFP, on the other hand, is usually obtained from theory. IMFP values will therefore be systematically greater than AL values by up to about 15-30%, the difference being greatest for high atomic numbers and low electron energies.

Accurate values of IMFPs and ALs are urgently required for a range of materials and for electron energies of practical interest in AES and XPS. AL measurements of high accuracy are generally difficult since the values are typically in the range 3 to 30 Å and specimen characterization on this scale (morphology, thickness, homogeneity, uniformity, etc.) is difficult. Calculations of IMFPs are also difficult since approximations, particularly for electron energies below about 200 eV, may not be valid. Useful formulas are needed to enable useful predictions to be made of AL or IMFP values in materials for which no measurements or calculations have been made. Reliable predictions of this type require knowledge of the dependence of AL or IMFP on electron energy and on material parameters (e.g., density, atomic or molecular weight). It is also desired to be able to convert data for IMFPs to ALs and vice versa so that IMFP calculations can be compared simply with AL experiments and that IMFP models can, when validated, be used to predict AL values for a useful range of materials and electron energies. Finally, knowledge is needed of the extent to which concepts (and data) developed for polycrystalline or amorphous materials break down in single-crystal materials.

We report below on efforts to address some of the above-mentioned needs.

(a) Calculations of Inelastic Mean Free Paths in 31 Materials

(C. J. Powell and S. Tanuma)

We have calculated IMFPs for 200-2000 eV electrons in 27 elements (C, Mg, Al, Si, Ti, V, Cr, Fe, Ni, Cu, Y, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Hf, Ta, W, Re, Os, Ir, Pt, Au, and Bi) and 4 compounds (LiF, SiO_2, ZnS, and Al_2O_3). These calculations are based on an algorithm recently developed by Dr. D. R. Penn (Radiation Physics Division) in which experimental optical data are used to give information on the inelastic scattering probability as a function of energy loss and in which theory is used to describe the dependence of the scattering probability on momentum transfer. This hybrid approach enabled us to take advantage of the available optical data (that can be checked for internal consistency by various sum rules) and avoids the necessity for making assumptions about the relative strengths of various valence-electron and core-electron excitations.

The calculated IMFPs λ_i were found to be well described by the Bethe equation for inelastic electron scattering in matter:

$$\lambda_i = E/[E_p{}^2 \beta \ell n(\gamma E)] \quad \text{Å} \tag{2.1}$$

where E is the electron energy (in eV), E_p is the free-electron plasmon energy for the material (in eV), and β and γ are two parameters. The plasmon energy is $E_p = 28.8\ (N_v \rho/A)^{1/2}$ where N_v is the number of valence electrons per atom or molecule, ρ is the bulk density (in g cm^{-3}), and A is the atomic or molecular weight. The inelastic scattering is mostly due to valence-electron excitations; for materials with shallow core levels (binding energies less than about 30 eV), these also contribute to the inelastic scattering and the plasmon energy should be calculated with the number of these core electrons and the number of valence electrons. We have found empirically that the two Bethe parameters could be simply related to other material constants:

$$\beta = -2.52\text{x}10^{-2} + 1.05/(E_p{}^2 + E_g{}^2)^{1/2} + 8.10\text{x}10^{-4}\rho \tag{2.2}$$

$$\gamma = 0.151\ \rho^{-0.49} \tag{2.3}$$

where E_g is the bandgap energy for nonconductors (in eV).

Fig. 2.1 shows an illustrative plot of our results for aluminum. The solid line shows the IMFP results calculated with the Penn algorithm and the curve labelled TPP is a plot of Eqs. (2.1)-(2.3) using parameter values for aluminum. The dashed line shows an IMFP formula due to Szajman et al, and the dot-dashed curve gives results from the widely used empirical AL formula of Seah and Dench. In the case of Al, there is good agreement between our IMFP calculations the results calculated from Eqs. (2.1)-(2.3), the Szajman et al. formula, and the AL experimental data; the Seah and Dench formula agrees with the other results for E < 500 eV but diverges at higher energies.

For the 31 materials we have investigated so far, the rms difference between the individual IMFP values for a particular material and the values calculated from Eqs.(2.1)-(2.3) for that material was about 12%. This level of consistency was considered satisfactory considering the uncertainties in the optical data and the empirical nature of Eqs. (2.1)-(2.3). Equations (2.1)-(2.3) are therefore believed to be a useful general formula for predicting IMFPs in other materials and to be a reasonable but more approximate guide to AL values. The approximations in the Penn algorithm are likely to give systematic uncertainties in the calculated IMFPs so the new general formula is believed to be particularly useful for predicting the IMFP dependence on electron energy for a given material and the material-dependence for a given energy.

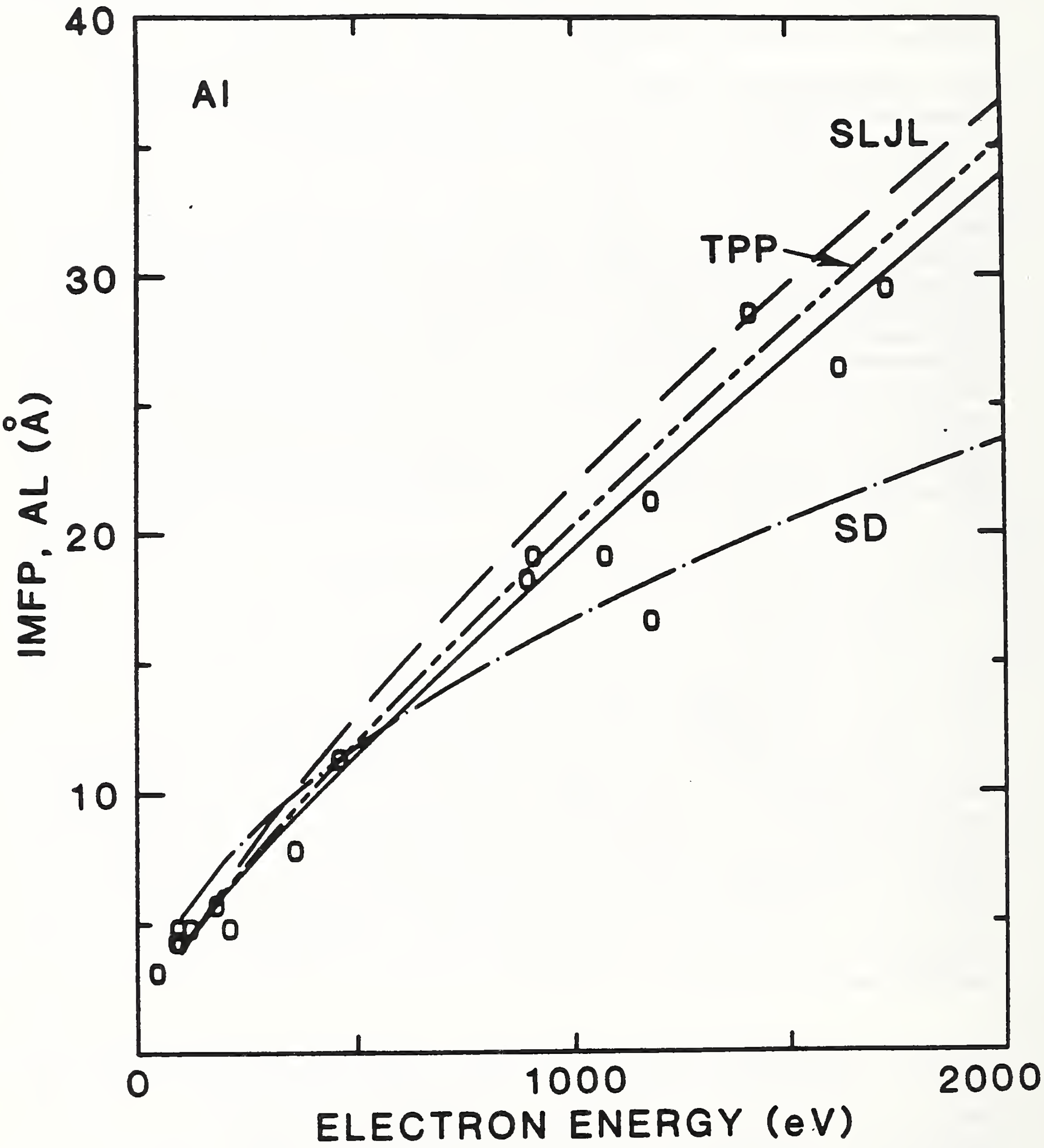

Fig. 2.1. Comparison of IMFP and AL results for aluminum. The solid line shows the calculated IMFPs and the curve labelled TPP is the general IMFP formula, Eqs. (2.1)-(2.3), using parameter values for Al. The curve labelled SLJL is an IMFP formula due to Szajman et al. and the curve denoted SD is the AL formula of Seah and Dench. The open circles are the AL values of Tracy.

Penn has developed a more complex algorithm with which IMFP calculations can be made for electron energies down to about 50 eV. Additional IMFP calculations with this algorithm are in progress and it is hoped to extend Eqs. (2.1)-(2.3) to correspondingly lower energies. It is also planned to extend the calculations to other materials for which the optical data are available over a substantial photon energy range (typically about 1-1000 eV).

(b) Measurements of Electron Attenuation Lengths in Condensed Molecular Solids

(R. L. Stockbauer, R. L. Kurtz, Q. Wang, and T. E. Madey)

We have continued to improve a method developed earlier for measuring electron attenuation lengths in condensed molecular solids. In this method, electrons emitted from a substrate are attenuated by a condensed film of the sample material. Variable wavelength photoemission spectroscopy using synchrotron radiation is able to distinguish the electrons emitted by the substrate from those emitted by the overlayer. Changing the incident photon energy changes the kinetic energy of the emitted electrons allowing the measurements to be made as a function of electron kinetic energy over the range available at the synchrotron.

Since the thickness of the overlayer is critical to the measurement, three independent methods are used to determine this quantity: a measure of the number of molecules condensed on the surface, a shift of the photoemission spectral features between the first and subsequent layers, and different thermal desorption temperatures for different layers. The three methods give consistent results within experimental error.

Improvements in the experiment have been made in several areas. The first was moving the instrument to beamline 1 at SURF-II where the higher photon flux, lower second-order light, and broader energy range of the monochromator allow faster, lower-noise and lower-background measurements. With this monochromator, the energy range of the measurements was doubled to nearly 200 eV. The second improvement was to mask the energy analyzer to permit only electrons emitted normal to the surface to be detected. This eliminated the necessity for correcting the data for electrons emitted off-normal, a correction which has questionable applicability in our previous work. The third was to continually dose the sample while the photoemission data were being accumulated. This eliminated a background correction and reduced the data acquisition time by a factor of 5. Lastly, two different substrates were used in the present measurements, Cu(100) and Ni(100), to investigate effects of the substrate on overlayer growth. No significant differences were observed.

To date, measurements have been made on water, methanol, ethanol, and acetone. These condensed molecular solids were selected for measurement since there are very few measurements of attenuation lengths for organic solids. Semilog plots of the substrate intensity versus film thickness were linear over two decades which indicated layer-by-layer growth of the overlayer as opposed to three-dimensional island growth. The attenuation length as a function of electron energy appeared to follow the empirical universal curve proposed by Seah and Dench for organic molecules. They were somewhat lower than our previous results and results obtained by several other groups. A series of experiments are being planned to determine the source of the differences.

The measurements will be expanded to include atoms and molecules which are not condensable at liquid nitrogen temperature by using a new helium-cooled cold stage. Attenuation length measurements of rare gases and simple diatomic molecules (O_2, N_2, and CO, for instance) should enable assessment of IMFP calculations for these solids based on atomic excitations and ionizations. In addition, beam time has been scheduled for experiments to be performed at our Brookhaven NSLS beamline to allow the electron energy range to be extended to 600 eV.

(c) Measurements of the Attenuation Lengths of Very Low Energy Electrons in Silicon Oxide and of the Relative Si 2p Photoemission Cross-Sections at the SiO_2/Si Interface as a Function of Oxidation State and Final-State Energy

(J. A. Yarmoff and S. A. Joyce)

Core-level soft x-ray photoemission is an ideal technique for the study of interfaces owing to its ability to distinguish between the oxidation states of an atom. This technique is ideally performed with synchrotron radiation, since the tunability of the synchrotron allows for the collection of spectra with differing electron kinetic energies. As the attenuation length of electrons traveling through solids is a function of the kinetic energy, an effective depth profiling can be achieved by comparing spectra collected at different photon energies. This rather simple picture is complicated, however, by the fact that photoemission cross-sections are also functions of the photon energy, and that these functions can vary with the oxidation state of a particular atom. It is thus of importance to perform accurate measurements of both electron attenuation lengths and photoemission cross-sections as functions of electron or photon energy.

The SiO_2/Si interface is one of the most important systems for study in terms of current materials used in the fabrication of semiconductor devices. Core-level soft x-ray photoemission is an ideal technique to properly understand the structure of this system, as the interface constains three sub-oxide peaks which can be clearly resolved. In addition, films of SiO_2 can be grown of varying thickness without changing the properties of the interface.

In order to measure attenuation lengths for electrons photoemitted from these surfaces, photoelectron spectra were collected in the constant-final-state mode; that is, the energy analyzer was set to a constant kinetic energy and the photon energy was then varied. This insured that all of the electrons measured in a given spectrum have suffered the same average inelastic loss, i.e., have originated from the same average depth. Spectra were collected for kinetic energies ranging from 6 to 100 eV. The changes in intensity of each peak that are observed when varying the electron kinetic energy of detection are due to a combination of cross-section and electron scattering effects. The analyzer for these experiments accepted electrons emitted over a large solid angle so the inelastic scattering parameter meaured is an average escape depth rather than an attenuation length for a particular takeoff angle.

The average escape depth was determined by comparison of data collected from two samples with significantly different oxide thicknesses. In this case, the ratio of the silicon core-level peaks for SiO_2 and bulk Si was monitored as a function of detection energy for both samples. The difference in this ratio for the two samples is purely a result of the additional scattering occurring in the extra SiO_2 of the thicker sample. The analysis of this data produced the distribution shown in Fig. 2.2. This curve shows a local minimum at ~ 35 eV, which is most likely the result of scattering due to a bulk plasmon. The curve also contains the surprising result that at very low electron energies (< 10 eV), the

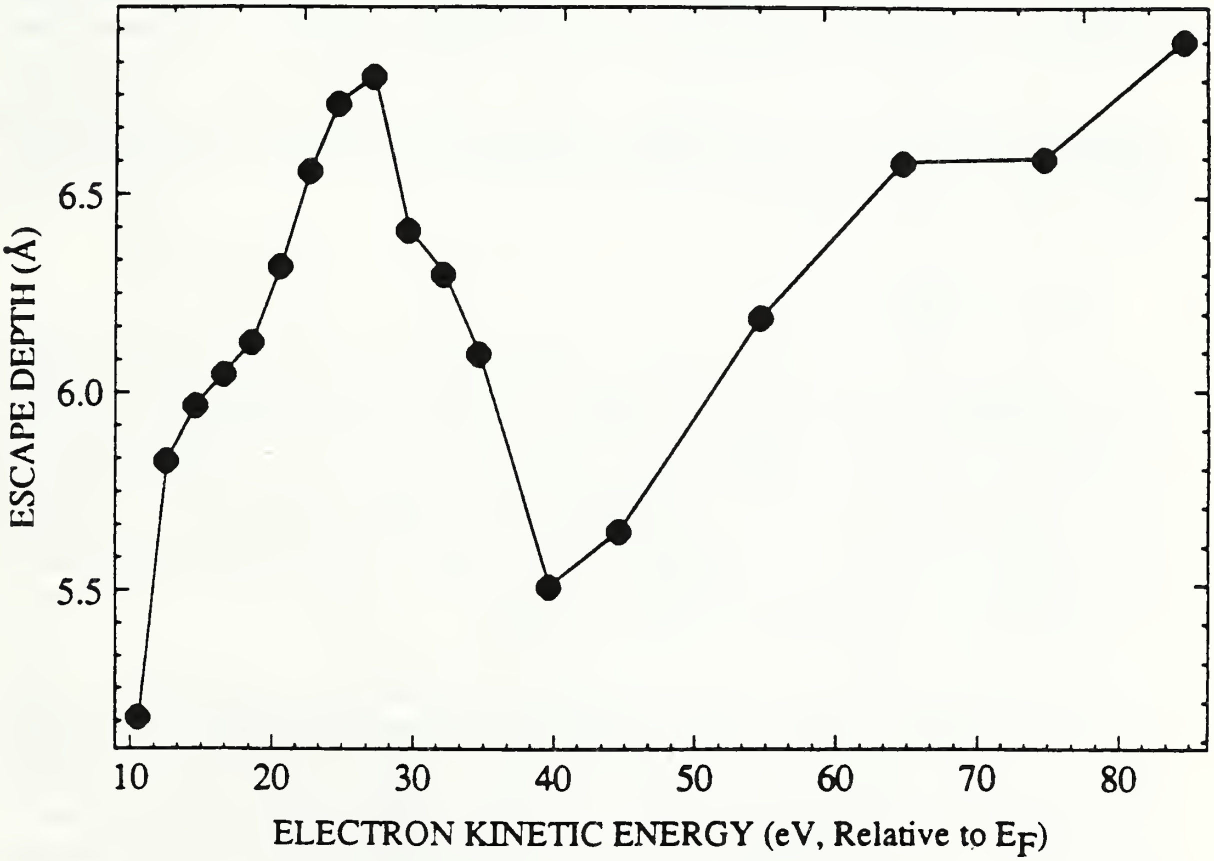

Fig. 2.2 The average escape depth determined for electrons traveling through SiO_2 as a function of electron kinetic energy.

escape length for electrons traveling through SiO_2 decreases with decreasing energy. This decrease in escape depth can be attributed to excitation of phonon modes in the SiO_2, for which there is a very large cross section. This conclusion is supported by the fact that the bulk Si photoelectron peak seen in spectra collected at very low electron energies is apparently broadened and shifted towards an apparently higher binding energy in the thicker samples. The bulk Si peak observed in the thicker samples is thus a convolution of the actual Si photoelectron peak and its loss function.

The photoemission cross-sections as a function of the electron kinetic energy were measured by preparing a sample that contained only a single monolayer of oxygen atoms. This was done by room temperature exposure of a clean Si surface to 200 Langmuirs of oxygen, which forms a surface containing all four oxidation states of Si. Since this oxide is less than a monolayer thick, a measurement of the absolute photoemission intensity from each oxidation state as a function of electron kientic energy (or final-state energy) would in essence be free of any effects of changing escape depths. This measurement showed that the photoemission cross-sections can be enhanced by as much as a factor of 2 in going from the +1 to +3 oxidation states at certain photon energies.

This work is a collaboration with Dr. F. R. McFeely of the IBM Watson Research Laboratory, and has been performed at the National Synchrotron Light Source at Brookhaven National Labortory.

(d) Universal Curves for Electron Inelastic Mean Free Paths and Attenuation Lengths

(C. J. Powell)

Since reliable knowledge of ALs and IMFPs is important for determining the surface sensitivity of various electron spectroscopies and for quantitative analyses by AES and XPS, there has been considerable interest in obtaining so-called universal curves to guide users in determining IMFP and AL values for particular materials and energies. The phrase "universal curve" came into vogue in the mid-1970s when it appeared that early AL data for different materials clustered about a common curve when the AL was plotted against electron energy. Later work, however, showed considerable scatter about the presumed universal curve.

A review article has been written that evaluates a number of proposed universal curves. Due to the difficulties in making accurate AL measurements and IMFP calculations, it is not surprising that there is a substantial scatter in data from different sources. Empirical guides, based on limited data, are convenient and useful but may be inaccurate for some conditions. A new formula, Eqs.(2.1)-(2.3) in section (a) above, is considered to be a useful guide for the IMFP dependences on material and electron energy in the range 200-2000 eV since it is based on application of a common algorithm and evaluated optical data for 31 materials. This formula is expected to be a reasonable but more approximate guide to ALs and it is hoped that it can be evaluated with AL data measured with higher accuracy than has been common in the past.

3. High-Accuracy Measurements of XPS Binding Energies and AES Kinetic Energies for Copper, Silver, and Gold

(N. E. Erickson and C. J. Powell)

The energy scales of x-ray photoelectron spectroscopy (XPS) and Auger-electron spectroscopy (AES) instruments need to be calibrated so that measurements of core-electron binding energies (BEs) by XPS or electron kinetic energies (KEs) by AES can be transferred meaningfully from one laboratory to another. The principal motivation of many practical BE and KE measurements is in the determination of the so-called chemical shifts in the energies from which chemical-state information can be obtained. Calibration of the XPS and AES energy scales enables reliable use of the available BE and KE data (if these have been acquired on calibrated instruments). The accuracy required in the calibration of the BE scales in XPS is typically 0.1 eV or better and of the KE scales in AES is typically 1 eV or better. Round robins conducted by NIST staff members about eight years ago indicated that the accuracies of BE and KE measurements then could be appreciably inferior to those required for valid chemical-state identification. In the meantime, BE data for Cu, Ag, and Au have been published by the National Physical Laboratory (NPL) and similar AES KE measurements there have recently been concluded. While we believe the NPL measurements to be of high quality, we consider that independent measurements at NIST are important to ensure maximum user confidence, particularly since there is still a discrepancy in some recently published high-accuracy measurements.

We had originally planned to calibrate the energy scale of our double-pass cylindrical-mirror analyzer (CMA) by measuring the positions of elastic peaks with electrons of known energy. By adjusting the voltage applied to the electron gun so that the elastic peak from a specimen closely overlapped the position of an AES or XPS peak from that material, it would be possible to determine the energy of electrons in the AES or XPS peak from an accurate measurement of the gun voltage and a separately measured instrumental constant (associated mainly with the selected analyzer pass energy and the work functions of cathode and analyzer). It was found, however, in a series of test measurements that the measured positions of the elastic peaks did not track accurately the voltages applied to the gun cathode. The observed deviations appear to be due to a recoil energy loss occurring with the elastic scattering process. These recoil losses depend on incident electron energy and range up to 0.2 eV for incident energies between 50 and 1250 eV with slight differences in magnitude, up to about 30 meV, for copper, silver, and gold.

The origins of the observed recoil energy losses are not clear. Published work with 20-40 keV electrons has indicated recoil losses of up to 4 eV that could be interpreted in terms of single Rutherford scattering. At the lower incident energies of present interest, the Rutherford scattering formula indicates the trends but greatly underestimates the magnitudes of the recoil losses. Other scattering mechanisms therefore have to be considered, such as those associated with phonon excitations. The observed elastic peaks probably are the envelopes of various (unresolved) phonon scattering modes for our polycrystalline foil specimens.

We have subsequently made use of accurate measurements of the voltage applied to the CMA inner cylinder corresponding to particular AES and XPS spectral features (e.g., peak maxima). XPS data were measured with a constant voltage between the outer and inner cylinders, corresponding to an analyzer pass energy of about 50 eV, and with magnesium characteristic x-rays. The binding energies of the principal peaks for Cu, Ag, and Au were measured with respect to the Fermi level of a nickel specimen, located from the position of the peak in the derivative of the spectrum in the Fermi-edge region.

Our preliminary binding energy results are shown in Table 2.1 and compared with corresponding results from NPL. Also shown are the positions of two Auger-electron peaks with reference to the binding-energy scale for magnesium characteristic x rays. The uncertainties in the NIST data represent the combined uncertainties of voltmeter calibration (5 meV) and the precision in locating the position of each peak and the Fermi level (typically between 5 and 15 meV). The NIST results agree with those of NPL within the combined uncertainties.

Table 2.1. Comparison of core-level binding energies (in eV) for the designated core levels of copper, silver, and gold as measured at NIST and NPL. The positions of two Auger-electron peaks are also shown on the binding energy scale using magnesium x rays.

Line	NIST	NPL
Au $4f_{7/2}$	84.01±0.01	84.00±0.01
Cu L_3VV	334.98±0.02	334.95±0.01
Au $4d_{5/2}$	335.19±0.02	
Ag $3d_{5/2}$	368.31±0.02	368.29±0.01
Ag M_4VV	895.75±0.03	895.76±0.02
Cu $2p_{3/2}$	932.71±0.02	932.67±0.02

We have made similar measurements of the Auger-electron peaks for copper, silver, and gold. Absolute kinetic energies were obtained by associating the magnesium characteristic x-ray energy with the observed position of the nickel Fermi edge. Our preliminary values are shown in Table 2.2. The low-energy lines of copper and gold are doublets and the two entries refer to the positions of the line components. There is again agreement between the NIST and NPL data within the combined uncertainties.

Table 2.2. Comparison of Auger-electron kinetic energies for copper, silver, and gold (in eV) as measured at NIST and NPL. The first stated uncertainty refers to the precision of measurement and the second uncertainty to the accuracy in establishing the absolute energy scale.

Line	NIST	NPL
Cu $M_{23}VV$	61.20±0.02±0.04	61.17±0.04±0.02
	63.48±0.02±0.04	63.45±0.04±0.02
Au $N_{67}VV$	70.20±0.15±0.04	70.12±0.04±0.02
	72.18±0.04±0.04	72.26±0.04±0.02
Ag M_4VV	357.85±0.03±0.04	357.87±0.01±0.02
Cu L_3VV	918.61±0.02±0.04	918.68±0.01±0.02
Au $M_5N_{67}N_{67}$	2015.71±0.04±0.04	2015.56±0.02±0.04

The new XPS binding energy and AES kinetic energy data for copper, silver, and gold appear to be satisfactory for checking and calibrating the energy scales of AES and XPS instruments.

4. Reference Data for X-Ray Photoelectron Spectroscopy and Auger-Electron Spectroscopy

(C. J. Powell and N. E. Erickson)

A project was initiated in FY82 with funding by the NIST Office of Standard Reference Data (OSRD) to prepare compilations and evaluations of core-electron binding energies and of the kinetic energies of selected Auger electrons for a wide range of elements and compounds. In particular, data are being compiled of the "chemical shifts" that can give useful information on the chemical state of a particular element. Data of this type are now scattered throughout the scientific literature but there is a need both for a convenient single source and for evaluation of the sometimes conflicting data. The reference data are being compiled by Dr. C. D. Wagner, a contractor to NIST, and the Surface Science Division is providing technical review.

The compilation and evaluation of these data have been completed. The resulting data base consists of some 13,000 entries and is to be published shortly in the Journal of Physical and Chemical Reference Data.

OSRD is currently developing a data system so that the data base can be accessed from computer terminals.

5. Composition Depth Profiles and Inelastic Background Subtraction in XPS

(W. F. Egelhoff, Jr., and I. Jacob)

It is well known in x-ray photoelectron spectroscopy (XPS) that the primary photoelectrons undergo inelastic losses as they propagate through the specimen material. These inelastic scattering events result in an inelastic tail that begins under the main XPS or elastic peak and trails to lower kinetic energies. The deeper the emitting atom is located in the specimen, the greater is the intensity of this inelastic tail relative to the elastic peak. Theoretical work by Dr. S. Tougaard of Odense University, Denmark has indicated that the relative strengths of the elastic peaks and the inelastic tails might be used as a method of non-destructively obtaining compositional depth profiles. However, there has so far been no standard reference materials available to evaluate this theoretical work.

A collaboration has been initiated with Dr. Tougaard to evaluate his proposed method. We are making angle-resolved XPS measurements of the elastic peaks and inelastic tails for epitaxial sandwich structure in which a single atomic layer of one element, e.g., Cu, is sandwiched between epitaxial layers of a different element, e.g., Fe. Marked changes occur in the relative elastic to inelastic intensities as a function of depth for the XPS peaks of the single layer. Using carefully controlled epitaxial growth, samples are being grown that provide data in a form ideally suited to evaluation of the theory and its parameters. This work is expected to lead to improved theoretical models for inelastic scattering in XPS, accurate prediction of the shape of inelastic tails, and improved background subtraction algorithms for quantitative XPS compositional measurements and depth profiling. This work is contributing to the VAMAS project described in more detail in section 2.D.2.

6. Uncertainties in Quantitative Surface Analyses by Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy

(C. J. Powell)

The two most popular techniques used to make quantitative analyses of surfaces are Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS). Such analyses are frequently used to identify the surface phases present on a specimen, to determine the concentrations of elements or compounds in those phases, and to measure the variation of composition as a function of position (both parallel or normal to the surface). A surface analysis comprises a series of operations that typically includes instrument setup, specimen positioning, data acquisition, data manipulation, and data analysis. These operations involve a sequence of measurements that are combined and/or compared with other data to yield an experimental result. This result could be the detection of a particular element or compound, the distribution of a species across a surface or with depth, the comparison of a spectrum from one specimen with that of a reference (a specimen from a different batch or a published result), or a quantitative analysis. The final result of the surface analysis has an uncertainty that reflects the separate random and systematic uncertainties in the various measurements and sources of data.

In a collaboration with Dr. M. P. Seah of the UK National Physical Laboratory, a detailed analysis has been made of the individual steps in AES and XPS analyses and of the various sources of uncertainty. Although adequate repeatability (precision) is often achieved, there are many sources of systematic uncertainty that make accuracy statements very difficult. The major sources of systematic uncertainty are associated with the complexity of typical specimens, with knowledge of instrument performance, and with limitations of current methodology and data. We have identified the sources of uncertainty in these areas and the extent to which there are adequate sources of reference data, reference materials, and reference procedures to guide analysts in making measurements of the desired accuracy. Although the details of the analysis are specific to AES and XPS, many aspects are applicable to other techniques of surface analysis.

7. PIN Diode Detectors for Synchrotron X-Rays
(T. Jach)

The use of PIN silicon photodiodes as a replacement for ion chambers in x-ray synchrotron radiation experiments was pioneered at NIST. The original work included performance data on five different commercially available photodiodes at x-ray energies of 1.2-3.0 keV. The diodes offer important advantages over ion chambers and their use has spread in the synchrotron community.

We have expanded the previous work by additional characterizations of commercial photodiodes in energy response and spatial resolution. The work was performed in collaboration with Drs. J. P. Kirkland and R. A. Neiser of the Naval Research Laboratory and experiments were carried out using the X-23B beamline at the Brookhaven National Synchrotron Light Source. This beamline offered orders of magnitude improvement over the previous measurements done in the laboratory with an x-ray tube in terms of x-ray flux, energy range, and freedom from harmonic contamination. We have published data on the response of four commercial photodiodes in the energy range 3.6-11 keV, as well as response curves for sensitivity vs. illumination position for one type of diode. The work has led to a model of how these diodes, which are designed to respond to visible light, perform at x-ray energies.

The use of PIN silicon photodiodes (both commercial and our own specialized devices) has become common for x-ray detection experiments performed at synchrotron sources by several groups at NIST and elsewhere. We intend to continue characterizing and modeling appropriate types both to assist the synchrotron community and to further our own applications in experiments.

B. Reference Materials

1. Developments and Production of Standard Reference Materials for Sputter-Depth Profiling)

(J. Fine and D. Marton)

The objective of this project is to develop standard reference materials (SRMs) that will allow convenient determinations of ion-beam sputter-removal rates in commonly used surface-analysis instrumentation. Thin-film reference materials of known thickness will be used to calibrate ion-gun current densitites for particular operating conditions. This information together with sputtering-yield data for a range of materials will establish depth scales in the measurement of depth profiles.

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 to achieve maximum depth resolution. The material consists of nine alternating metal thin-film layers, five layers of Cr and four of Ni, sputter deposited onto one side of a polished Si(100) substrate. With support from the NIST Office of Standard Reference Materials, SRM 2135 has been certified for total Ni and total Cr content, individual layer uniformity and Ni + Cr bilayer uniformity, and individual layer thickness.

SRM 2135 was issued in the fall of 1985 and by the spring of 1986, our initial stock of 80 specimens was sold. Since then, we have calibrated and put in stock two additional batches: SRM 2135a (1986) and SRM 2135b (1988). The last batch of Ni/Cr, SRM 2135b, was certified for total Ni and Cr using methods different from those we had previously used (polarography and plasma spectroscopy instead of neutron activation analysis). We were able to show that these new methods are adequate for future Ni and Cr certification.

The total sales of SRM 2135 is now more than 140. The material has been sold to many US laboraories and to institutions in other countries. In addition to its intended purposes, SRM 2135 has been used as a test material for sputtering studies, for laboratory intercomparisons, and for performance of commercial equipment.

Work is now in progress on the fabrication of a large additional stock (600-900 pieces) of SRM 2135. Because the fabrication facility used previously is no longer available, we are developing new fabrication techniques at the Comsat Laboratories in Germantown, MD. We anticipate that their planar magnetron sputter-deposition apparatus will produce satisfactory materials and that the film thickness uniformity will also be satisfactory. At present, prototype materials are being fabricated in order to evaluate interface structure and sample-to-sample film-thickness uniformity.

A new "marker-type" SRM has been under development along with improved Auger profiling techniques necessary for its characterization. This Cr/Cr_2O_3 multilayered thin-film structure consists of 6 well-defined, thin oxide marker layers (about 3 monolayers thick) separated by Cr films which are about 40 nm thick. The uniformity of the marker layer spacing is better than 3% (one standard deviation); it should be very useful both as a depth profile standard for secondary-ion mass spectrometry analysis as well as a sensitivity standard for Auger analysis. Certification is now almost complete and we anticipate that this SRM will be ready for issue in December 1988.

We are planning to develop a new SRM consisting of Cu, Ag, Au, and Si. This material is intended as a convenient means for calibrating the energy scales of Auger-electron spectrometers (AES) and x-ray photoelectron spectromers (XPS). It is being developing in response to our recent survey (section 2.B.4) and will provide a simple means of using the new high-accuracy XPS binding-energy and AES kinetic-energy data obtained at the UK National Physical Laboratory and at NIST (section 2.A.3) for Cu, Ag, and Au. Recently, it has been suggested that Si would be a useful calibration material for AES. The material should also be useful in checking analyzer intensity scales.

We plan to fabricate this SRM by sputter-depositing each element on a silicon wafer in an ultrahigh vacuum environment and at rates such that the films will have very fine grains (i.e., be nearly amorphous). Each film will be separately deposited and positioned adjacent to each other so that users can clean the surfaces easily by ion bombardment. We anticipate that the main development effort will be in producing films sufficiently fine grained that electron diffraction effects will be negligible.

2. Sputtering-Induced Surface Microroughness of Metallic Thin Films

(J. Fine and D. Marton)

Changes in surface microtopography which often occur during sputter-depth-profile analysis can significantly affect the measured depth resolution of interfaces. To better understand the importance of this roughening effect on interface analysis, we have correlated measurements of surface roughness obtained while Auger sputter-depth-profiling thin metallic multilayered systems with that of the observed Auger interface widths.

We have measured r.m.s. roughness of three test surfaces <u>in situ</u> using optical total-integrated-scattering (TIS) techniques. In this method, the specimen is illuminated with a collimated light beam and the off-specularly reflected light is related to the surface roughness and to the reflectivity of the investigated surface. The light scattering and Auger measurements were both carried out in an Auger-electron spectrometer used for depth profiling experiments. A light beam from a He-Ne laser source (λ = 632 nm) was directed perpendicular to the specimen surface and an ellipsoidal (or hemispherical) mirror was used to collect the off-specular light. Measurement of the off-specular light intensity was obtained with a Si detector using lock-in techniques.

We have made test measurements on three different metallic thin-film multilayer structures: SRM 2135 consisting of Ni and Cr; an Ag/Ni test structure; and the Cr/Cr_2O_3 material that is to be issued as an SRM shortly (section 2.B.2). The details of these structures are shown in Table 2.3.

Measurements of the r.m.s. surface microroughness for the three materials as a function of sputtered depth are shown in Fig. 2.3 for bombardment by argon ions of 1 and 4 keV energy. We find that the surface roughness increases with sputtered depth as well as with the energy of the impacting ions.

Table 2.3. Specimen structures used for measurement of sputtering-induced surface microroughness.

Specimen	Layer type	Number of layers	Single-layer thickness [nm]
Ni/Cr	Cr	5	50
	Ni	4	63
Ag/Ni	Ni	6	50
	Ag	5	4
Cr/Cr_2O_3	Cr	8	40
	Cr_2O_3	7	1-2

The data in Fig. 2.3 were fitted to the equation:

$$R_q = b <z>^a \qquad (2.4)$$

where R_q is the r.m.s. roughness, <z> the average sputtered depth, and b a constant. The exponent a was found to be between 0.42 and 0.51 for the Ni/Cr and Ag/Ni materials, and 0.83 for the Cr/Cr_2O_3 material. For the Ni/Cr and Ag/Ni samples, a is close to the expected value of 0.5 for a random distribution of surface areas of different sputtering yields. In the case of the Cr/Cr_2O_3 sample, the depth dependence is close to linear, although it is expected that the microstructure of the Cr layers of this sample is similar to that of the Ni/Cr sample. The presence of the Cr-oxide layers may be responsible for the rapid increase of the surface roughness.

The surface roughness measurements of the Ni/Cr and Ag/Ni specimens have been correlated with depth-resolution (interface-width) measurements obtained on the same samples by Auger depth-profiling and show that the surface topography developed due to ion bombardment is a major cause of

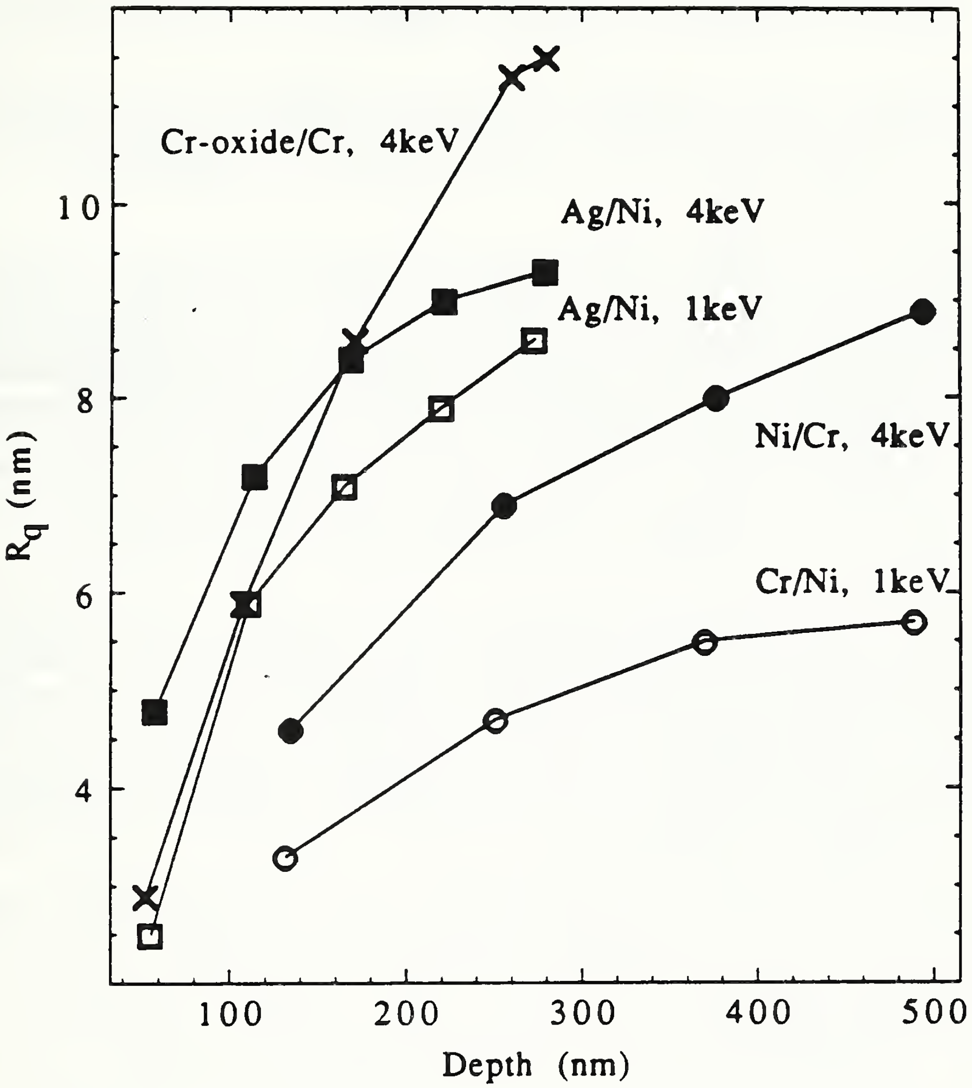

Fig. 2.3. Variation of r.m.s. surface microroughness of Ni/Cr, Ag/Ni, and Cr/Cr_2O_3 multilayer films as a function of sputtered depth under argon ion bombardment at the indicated energies.

interface broadening in sputter-depth profiling. These results are in good agreement with the predictions of a statistical model which considers differences in sputtering yields for the differently oriented crystallographic planes present in polycrystalline metallic layers. The data presented are the first direct quantitative measurement results on surface topography developed due to ion bombardment and measured without breaking the vacuum.

3. Radiation-Enhanced Diffusion During Sputter-Depth Profiling (J. Fine, D. Marton, and G. P. Chambers)

Radiation-enhanced diffusion (RED) is believed to be an important factor contributing to increased interface broadening during sputter-depth profiling. We describe here two series of experiments to characterize this phenomenon in more detail, one at room temperature and the other at elevated temperatures.

In our first series of experiments, we have investigated the interface broadening in Auger-electron sputter-depth profiling measurements on Ni/Ag multilayered thin-film structures (section 2.B.2). The interface broadening observed in this system is determined by a number of factors, the main two being roughening and RED. These two factors can be separated using the assumption that roughness leads to a symmetric profile shape, while an asymmetric shape is caused by RED. This concept is confirmed by interface broadening results which increase with depth (for subsequent Ag layers) for surface roughness, but remain independent of depth for diffusion.

We have found effective diffusion rates of Ag in Ni substantially greater than the grain-boundary diffusivity at room temperature when the thin-film structures were bombarded by argon ions of 1 and 4 keV energy. The observed diffusion rates were found to depend linearly on sputtering rate and thus on ion current density; the diffusion rates were also greater for 4 keV ion bombardment than 1 keV bombardment. The linear dependences on ion current density suggest that the observed diffusion rates are dependent on defect concentration.

In our second series of experiments, we have measured depth profiles while sputtering the Ni/Ag thin-film structures at different temperatures. At about 130°C, we find an abrupt transition at which the Ag profiles become very sharp and more well defined. This new and unprecedented result has enabled us to develop a new model for RED based on a complex defect mechanism. We propose that the complex defects can be long-lived (minutes), that the defects can diffuse long distances (~ 20 nm) much greater than the range of ion mixing, and that they can dissociate at elevated temperatures and give rise to a temperature dependence in RED which depends on the difference between the defect binding energy and the solute migration energy along these defects. At temperatures between 400 and 600 K, it appears that dissociation of the complex defects occurs at a rate faster than can be compensated for by the increased mobility of the Ag atoms. Such individual defect properties have previously been observed in a number of separate experiments but have not previously been found to be consistent with one set of results.

We believe that our new way of probing RED mechanisms allows us to observe, in real time, phenomena which have not been so clearly characterized. We have then been able to develop a new complex-defect model that may provide a general description of RED due to ion bombardment. Our observations also indicate that it may, by appropriate temperature control, be possible to control transport processes in RED and to achieve improved depth resolution at interfaces during sputter-depth profiling.

4. Survey of Needs for Standard Reference Materials in Surface Analysis

(J. Fine)

We have recently completed a survey in which users of surface analysis equipment were asked to assess needs for additional standard reference materials. This survey was conducted among the membership of ASTM Committee E-42 on Surface Analysis and the national representatives and participants in the VAMAS Surface Chemical Analysis Working Party (section 2.C.2). Each person was asked to give their opinions on the desirability of a number of possible types of reference materials using a numerical scale ranging from 1 (low interest) to 5 (high interest).

The survey results are summarized in Tables 2.4 for sputter-depth profiling (SDP) and in Table 2.5 for Auger-electron spectrosocpy (AES), x-ray photoelectron spectroscopy (XPS), and secondary-ion mass spectrometry (SIMS). For SDP applications, participants suggested that a single-layer thin-film system would be suitable for the first need in Table 2.4, a single- or multi-layer thin-film system for the second need, a multi-layer or marker-type thin-film system for the third need, and a multi-layer thin-film system for the fourth need. The most commonly sought types of material systems were metal-metal interfaces (by far), metal oxide-metal interfaces, semiconductor-semiconductor interfaces, semiconductor oxide-semiconductor interfaces, and metal-semiconductor interfaces.

Table 2.4. Summary of survey responses for reference materials in sputter-depth profiling (69 responses).

Need	Average Rating
1. Calibration of depth scale and erosion rate	4.0
2. Measurement of interface resolution	3.9
3. Optimization of sputtering conditions to produce narrowest interface widths	3.8
4. Verification of constancy of erosion rate (test for stability of ion-beam current density)	3.1

For applications in AES, XPS, and SIMS, a variety of types of materials were suggested ranging from single elements (line energies or mass scale; analyzer transmission function and energy resolution in AES and XPS; relative line intensities in SIMS), to metal alloys (relative line intensities; analyzer transmission function and mass resolution in SIMS; homogeneous multicomponent system for AES, XPS, and SIMS; and detection limits in AES and XPS), monolayer metal films on a single-crystal substrate (fractional or complete monolayer calibrations), ion implants in semiconductors (detection limits in XPS and SIMS; relative line intensities in SIMS), and mixed oxides (homogeneous multicomponent system for SIMS).

C. Standards Committee Activities

Division staff members are active on the ASTM Committee E-42 on Surface Analysis and with two international groups, the Surface Chemical Analysis Working Party of the Versailles Project on Advanced Materials and Standards (VAMAS) and the International Union of Pure and Applied Chemistry (IUPAC).

Table 2.5. Summary of survey responses for reference materials in AES, XPS, and SIMS

Need	Average Rating by Technique		
	AES	SPS	SIMS
A. Number of responses	35	33	22
B. Needs			
1. Spectrometer Calibration			
(a) Line energies (or mass scale)	3.3	3.6	3.0
(b) Relative line intensities	4.1	3.9	3.8
(c) Analyzer transmission function	2.8	3.0	3.5
(d) Energy or mass resolution	3.0	3.1	2.9
2. Calibration of Surface Composition			
(a) Fractional monolayer on a substrate	3.2	3.2	2.4
(b) Complete monolayer or bilayer	3.4	3.4	2.8
(c) Homogeneous multicomponent system	3.9	3.7	3.8
3. Detection Limits	3.2	2.8	4.2

Summaries are given here of recent activities of these organizations. Three articles have also been published recently (section 2.D) that give overviews of the work of these organizations in developing reference procedures together with information on sources and needs of reference data and reference materials for surface analysis.

1. ASTM Committee E-42 on Surface Analysis
(C. J. Powell, J. Fine, and N. E. Erickson)

The ASTM Committee E-42 on Surface Analysis, founded in 1976, now has some 120 members; in addition, a larger number of non-members, both within the U.S. and throughout the world, participate in Committee activities. The purpose of the Committee is to advance the field of surface analysis and the quality of surface analyses through the development of appropriate standards, standard practices, reference data, reference materials, round robins, symposia, workshops, and publications.

Some activities of the E-42 Committee during the past two years are listed below.

- Approval of three new standards:

  E-1127 Standard Guide for Depth Profiling in Auger Electron Spectroscopy

  E-1162 Standard Practice for Reporting Sputter Depth Profile Data in Secondary Ion Mass Spectroscopy (SIMS)

  E-1217 Standard Practice for Determination of the Specimen Area Contributing to the Detected Signal in X-Ray Photoelectron Spectroscopy and Auger Electron Spectroscopy

- Revisions and additions to the following standards:

  E-673 Standard Definitions of Terms Relating to Surface Analysis

  E-902 Standard Practice for Checking the Operating Characteristics of X-Ray Photoelectron Spectrometers

- Review of the following proposed standards:

  - Standard Guide to Charge Referencing Techniques in X-Ray Photoelectron Spectroscopy

  - Standard Guide to Enhancing the Depth Resolution of a SIMS Instrument

  - Standard Guide to Reporting SIMS Imaging Data

  - Standard Practice for Reporting SIMS Mass Spectral Data

  - Standard Practice for Analytically Describing Sputter-Depth Interface Data in Order to Obtain a Systematic Parameterization of Interface Regions

  - Recommended Practice for Fitting Depth Profile Interface Data to the Logistic Function by Means of a Specialized Computer Algorithm, LOGIT

- Discussion of standards in the following areas:
  - Calibration of energy scales (AES)
  - Instrument performance (AES)
  - Signal-to-noise measurements (AES)
  - Selected area XPS
  - Useful ion yields for elements in different matrices (SIMS)
  - Background subtraction algorithms (ISS)
  - Standard ISS spectra
- Regular reviews of standards activities of the VAMAS and IUPAC groups
- Survey of needs for standards in ion-scattering spectroscopy
- Survey of needs for different types of reference data in surface analysis
- Survey of needs for different types of reference materials in surface analysis (survey results summarized in section 2.B.4)
- Sponsorship of evening workshops at major meetings to discuss current specific problem areas in surface analysis
- Sponsorship of a symposium at the annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy
- Publication of a separate compilation of E-42 standards by ASTM
- Arrangements for republication of E-42 standards in the journal Surface and Interface Analysis
- Manuscript describing round robin of SIMS depth-profile measurements of B implanted in Si submitted for publication.

2. Surface Chemical Analysis Working Party of the Versailles Project on Advanced Materials and Standards (VAMAS)

(C. J. Powell and J. Fine)

The "Versailles Agreement" arose from a meeting of the Heads of State or Government (Economic Summit) of industrialized nations at Versailles in 1982. The participants represented Canada, the Federal Republic of Germany, France, Italy, Japan, the United Kingdom, the United States of America, and the Commission of the European Communities (CEC). A Summit Working Group on Technology, Growth, and Employment was established consisting of government science advisers. This group established international committees in eighteen areas such as photovoltaic solar energy, food technology, advanced robotics, biotechnology, high speed trains, remote sensing from space, and advanced materials and standards. The Versailles Project on Advanced Materials and Standards (VAMAS) has now evolved into a separate international cooperation involving the same seven nations and the CEC.

VAMAS supports international trade through projects aimed at providing the technical basis for drafting Codes of Practice and Specifications in Advanced Materials. The scope of the collaboration embraces all agreed aspects of enabling science and technology--data bases, test methods, design methods, materials technology--which are required as a precursor to the drafting of standards in advanced materials. VAMAS activity emphasizes collaboration on pre-standards measurement research, intercomparison of test results, and consolidation of existing views on priorities for standardization action. Through this activity, VAMAS fosters the development of internationally acceptable standards for advanced materials by the various existing national standards agencies.

The Surface Chemical Analysis (SCA) Working Party of VAMAS is one of thirteen such groups that have been approved to date. The main objective of the SCA working party is to produce, by coordinated effort, the reference procedures, data, and materials necessary to establish standards for surface chemical analysis. This effort is expected to lead to the international coordination of standards-related activities before national standards are adopted and to the development of standards on an international level.

The SCA Working Party was established in 1984 with C. J. Powell appointed as Chairman for 1984-87 and M. P. Seah (UK National Physical Laboratory) as Chairman for 1987-90. The most urgent needs for standards in surface analysis pertain to the commonly used techniques of Auger-electron spectroscopy (AES), x-ray photoelectron spectroscopy (XPS), secondary-ion mass spectroscopy (SIMS) and sputter-depth profiling (SDP). Specific needs for these techniques have been identified. The general requirements are as follows:

(1) an agreed based of principles, definitions of terms, and equations to relate the techniques and procedures to the measurement;

(2) reference procedures specifying how to measure intensities and spectral features;

(3) reference procedures, reference data, and reference materials for calibrating instruments, determining instrument functions, and inter-relating instruments of different designs;

(4) reference data of elemental sensitivity factors, matrix terms, information depths, libraries of chemical-state spectra, information on ion-sputtering rates, radiation damage, etc.; and

(5) standard methods of specifying an analysis.

Table 2.6 shows current VAMAS SCA projects and project leaders. These projects have been initiated at various times since the SCA group was formed. Some projects, such as projects 1 and 10, are close to completion; other projects, such as projects 2, 9, 16, and 17, are well-advanced while others are in early stages of project planning. Typically, a project will start in one institution and then later involve scientists with appropriate expertise in other states. Other projects are under discussion.

The projects listed in Table 2.6 are mutually independent and have been designed so that useful progress can be made by small groups in a reasonable time. There are, however, many significant inter-relationships among the projects which enhance the value and impact of this VAMAS activity. For example, calibration data for AES energy scales (project 2) and related work to align instruments will form the basis of the interlaboratory comparison (project 9), will be important in acquiring AES backscattering data (project 7), and will be valuable in tests of quantitative AES analyses of alloys (project 17). Similarly, the improved characterization of a Ta_2O_5 on Ta reference material (project 1) will form a basis for new measurements of sputtering rates in oxides (project 8) and will be a reference in the round robin of Al/Mg oxides (project 16).

NIST staff are leading three of the SCA projects. The work in project 2, led jointly with Dr. Seah, is directed to obtaining high-accuracy reference data for the calibration of energy scales in AES instruments; a progress report of the NIST work is given in section 2.A.3. Work for project 3 is currently in abeyance pending completion of project 16 in which oxide films on Al/Mg oxides are being characterized. If these materials are shown to be suitable, it is planned to use them as test specimens in an interlaboratory comparison of angular XPS measurements and derived film stoichiometries. Project 18 is an interlaboratory comparison of the use of LOGIT, a computer algorithm developed at NIST, for fitting the interface regions of SDP data measured with a Ni/Cr thin-film test specimen (NIST SRM 2135). Letters inviting participation in this intercomparison have been sent to scientists in the USA, UK, France, Federal Republic of Germany, Canada, Japan, and Switzerland.

Although scientists can arrange ad hoc individual international collaborations at any time, the formation of the VAMAS SCA group has stimulated interest and enthusiasm in many of the VAMAS states for the development of needed standards in surface analysis. There is a general recognition that the needs are so great that they are unlikely to be met in a reasonable time by even a few organizations. It is believed that the VAMAS SCA group was formed at an opportune time by providing a convenient mechanism and stimulation for international cooperations. Such cooperations are enabling standards to be developed more efficiently, more rapidly, and without unnecessary duplication of effort.

Table 2.6. Current projects of the VAMAS Surface Chemical Analysis Working Party. The names of project leaders are shown in parentheses.

1. Development of thin oxide films as references materials (Seah)
2. Development of calibration data for the energy scales of Auger-electron spectrometers (Seah, Powell)
3. Procedures for quantitative x-ray photoelectron spectroscopy (Powell)
4. Measurement of spatial resolution in AES (Prutton)
5. Development of reference materials prepared by ion implantation (Gries, Gould)
6. Development of polymer reference materials (Le Gressus)
7. Correction methods for backscattering in AES (Langeron)
8. Reference data for sputtering rates in oxides (Grabke)
9. Intercomparison of Auger-electron energy and intensity measurements (Seah)
10. Development of a standard data transfer format (Seah)
11. Multitechnique characterization of vacancies in alumina (Le Gressus)
12. Calibration of surface layers by nuclear reaction analysis (Davies)
13. Tests of algorithms for data processing in AES (Underhill)
14. Tests of algorithms for data processing in XPS (Tougaard)
15. Evaluation of SIMS sensitivity factors (Anderle)
16. EFC round robin of Al/Mg oxides (Marcus)
17. Quantitative AES of Au/Cu alloys (Shimizu)
18. Evaluation of LOGIT, an algorithm for fitting sputter-depth profile data, for the measurement of interface widths of an NIST thin-film reference material (Fine)

3. International Union of Pure and Applied Chemistry (C. J. Powell)

The International Union of Pure and Applied Chemistry (IUPAC) has several objectives, one of which is to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification. Recommendations concerning terminology, symbols, units, and how to make reliable measurements are made by different IUPAC Commissions organized to cover various fields of chemistry.

Three IUPAC Commissions now have activities in which surface analysis standards are being developed. Efforts are made to coordinate these activities with the VAMAS and ASTM E-42 groups.

(a) Subcommittee on Surface Analysis of Commission V.2 on Microchemical Techniques and Trace Analysis.

This Subcommittee has prepared five reports during 1983-87 with the general title "Standards and Calibration Methods for Surface Analysis I: Semiconductors". The five reports are:

Part A: "A Concise Report on the Use of Ion Implantation for Standardization"

Part B: "Characterization of the Superficial Area of Solids by Means of Nuclear Analytical Techniques. Application to Semiconductors"

Part C: "Critical Evaluation of Calibration Procedures for Distribution Analysis of Dopant Elements in Silicon and Gallium Arsenide"

Part D: "Distribution Analysis of Major and Trace Elements through Semiconductor Layers of Changing Matrix Using SIMS"

Part E: "Critical Evaluation of Calibration Procedures for Analysis of Thin Dielectric Films on Silicon by AES and XPS"

Part D has been published in Pure and Applied Chemistry and the other documents are in various stages of review. In 1985, the Subcommittee initiated the following two projects:

- "Trace Element Analysis in Monolayers"

- "Terminology for Surface Characterization"

At its most recent meeting in 1987, the Subcommittee approved the following new projects:

- "Effects of Radiation on Chemistry in the Solid State and its Analytical Implications: Part I - Ion Irradiation"

- "Preparation of Biological Samples for Ion Microscopy"

- "Determination of the Depth of Origin of Sputtered Atoms. A Critical Evaluation"

- "MeV Ions for Surface Analysis. A Critical Evaluation"

As an example of coordination among the several standards groups, definitions of terms relating to surface analysis that have been prepared by the ASTM E-42 Committee are being reviewed through the IUPAC Subcommittee to ensure consistency with similar definitions in other fields and compliance with universal terminology criteria. A status report of this IUPAC project was presented at a recent meeting of the ASTM E-42 Terminology Subcommittee.

(b) Commission I.6 on Colloid and Surface Chemistry Including Catalysis

This Commission has a Subcommittee on Thin Films which is planning to document thin-film terminology, methods for thin-film preparation and characterization, and applications of thin films. Another group is surveying experimental techniques in surface chemical physics.

(c) Commission I.5 on Molecular Structure and Spectroscopy

This Commission has groups developing a descriptive classification of the electron spectroscopies, summarizing acronyms and abbreviations in surface spectroscopy, documenting symmetry and selection rules in surface spectroscopy, and developing recommendations for SIMS.

(4) Conferences on Quantitative Surface Analysis
(C. J. Powell)

Two conferences on Quantitative Surface Analysis have been organized in the USA, the first at NIST on October 24, 1986 and the second at Monterey, CA on October 30-31, 1987. Each conference has been cosponsored by the Applied Surface Science Division of the American Vacuum Society, ASTM Committee E-42 on Surface Analysis, and the VAMAS Surface Chemical Analysis Working Party; the first conference was also cosponsored by the NIST Offices of Standard Reference Data and Standard Reference Materials.

Each conference was organized to provide a forum for discussion on recent advances and current problems in the quantitative aspects of surface analysis with emphasis on reference data, reference materials, instrument calibration, computer software, and reference procedures. The conferences were each attended by about 100 scientists and were judged to be very successful. It is now planned to hold the conferences on a two-year cycle with the next to be held in Salem, MA on October 20-21, 1989.

D. Review Articles and Books

1. Review Articles

Staff members in the Division author many review articles and book chapters that provide information on measurement methods, relevant reference data, reference materials, theories of the measurement process for any surface spectroscopies, and surface standards.

Division staff members have authored 22 review articles recently. The titles and abstracts of review articles published during the past two years are listed below:

(a) "Electron and Photon Stimulated Desorption: Probes of Structure and Bonding at Surfaces", T. E. Madey, Science 234, 316 (1986)

Techniques for analyzing the structure and composition of solid surfaces using electron and photon beams often suffer from difficulties due to radiation damage. Damage-producing processes compete with information-producing events during measurements, and beam damage can be a serious perturbation in quantitative surface analysis. However, there are also substantial benefits of electron and photon stimulated damage processes for studying molecules adsorbed on surfaces. Direct information about the geometrical structure of surface molecules can be obtained from measurements of the angular distributions of ions released by electron- or photon-stimulated desorption. The directions of ion emission are determined by the orientation of the surface bonds which are ruptured by beam irradiation. Moreover, photon-stimulated desorption studies using synchrotron radiation are revealing the fundamental electronic excitations which lead to bond-breaking processes at surfaces. These measurements are providing new insights into radiation-damage processes in areas as diverse as x-ray optics and semiconductor electronics.

(b) "Field Emission Microscopy - Trends and Perspectives", A. J. Melmed, Chemistry and Physics of Solid Surfaces VI, (Springer-Verlag, New York), 325 (1986).

The author's view of the role of surface microscopies, in particular the field emission microscopies, is given. Brief outlines of the historical development and nature of field-electron emission microscopy (FEEM) and field-ion microscopy (FIM) are given and selected examples are presented to illustrate the scope of research in FEEM and FIM. Research trends are described and some projections for the future are made.

(c) "Core-Level Binding-Energy Shifts in Solids and at Surfaces", W. F. Egelhoff, Jr., Surface Sci. Reports 6, 253 (1987)

This review presents an overview of the theory and of various successful approaches to the interpretation of core-level binding-energy shifts observed in photoelectron spectroscopy. The theoretical background is presented at a level readily accessible to the general reader. Particular attention is paid to the relative merits of two basically different conceptual frameworks for interpreting core-level binding-energy shifts, the initial-state--final-state approach and the equivalent-core Born-Haber cycle approach.

(d) "Excitation Mechanisms in Vibrational Spectroscopy of Molecules on Surfaces", J. W. Gadzuk, in Vibrational Spectroscopy of Molecules on Surfaces, J. T. Yates, Jr. and T. E. Madey, eds., Vol. 1 of Methods of Surface Characterization (Plenum, New York), 49 (1987).

An introduction to the theoretical basis of vibrational excitation mechanisms and processes relevant to vibrational spectroscopy of adsorbed molecules is presented.

(e) "Incoherent Neutron Inelastic Scattering: Vibrational Spectroscopy of Adsorbed Molecules on Surfaces", R. R. Cavanagh, J. J. Rush, and R. D. Kelley, in Vibrational Spectroscopy of Molecules on Surfaces, J. T. Yates, Jr., and T. E. Madey, eds., Vol. 1, of Methods of Surface Characterization (Plenum, New York), 183 (1987).

An introduction to neutron scattering as a probe of adsorbates at surfaces is presented. Emphasis is placed on experimental aspects of triple-axis and time-of-flight techniques along with a single-photon model for the spectral features. Wilson FG methods for constructing molecular force fields relevant to the molecular modes of the adsorbate are presented. The applicability of neutron scattering for exploring rotational diffusion and adsorbate torsions is also examined.

(f) "Mechanisms and Applications of Electron Stimulated Desorption in Surface Science", T. E. Madey, Vacuum (TAIP) 37, 31 (1987).

The principles and mechanisms of electron-stimulated desorption and the utility of the electron-stimulated desorption ion angular distributions (ESIAD) method as a tool for determining the structure of surface molecules have been described in several recent books and review articles. The present article is intended to provide a guide to the relevant literature, and to outline briefly some recent work relating to the uses of ESDIAD for determining the structure of surface molecules.

(g) "The Interaction of Water with Solid Surfaces: Fundamental Aspects", P. A. Thiel and T. E. Madey, Surface Sci. Reports 7, 211 (1987).

The purpose of this review is to compare and discuss recent experimental and theoretical results in the field of H_2O-solid interactions. Emphasis is placed upon adsorption studies performed on well-characterized, single-crystal surfaces of metal, semiconductors and oxides. We discuss the factors which influence dissociative vs. associative adsorption pathways. When H_2O adsorbs molecularly, it tends to form three-dimensional hydrogen-bonded clusters, even at fractional-monolayer coverages, because the strength of the attractive interaction between two molecules is comparable to that of the substrate-H_2O bond. The template effect of the substrate is important in determining both the local and long-range order of H_2O molecules in these clusters. The influence of surface additive atoms (e.g., O, Br, Na, K) on the surface structure and chemistry of H_2O is examined in detail. Results on single crystal substrates are compared with earlier available measurements of H_2O adsorption on high-area materials.

(h) "Core Level Spectroscopy: A Dynamics Perspective", J. W. Gadzuk, Physica Scripta 35, 171 (1987).

Various aspects of the dynamics of time-dependent localized potentials and intersections in solids and at surfaces, as they might relate to the fundamental screening and relaxation processes involved in core-level spectroscopies, are explored.

(i) "Dynamics of Molecular Collisions with Surfaces: Excitation, Dissociation, and Diffraction", S. Holloway, M. Karikorpi, and J. W. Gadzuk, Nuclear Instruments and Methods B 27, 37 (1987).

Aspects of molecular collisions are discussed which are important in the chemically relevant energy range of ~ 1-10 eV. In particular, the role of charge transfer, potential-energy-surface topology, and intra-molecular ground-and excited-state potential curves are investigated as they pertain to internal vibrational excitation, dissociative adsorption or scattering, and diffractive scattering. The modeling and analysis are based on classical trajectories and semi-classical wavepacket dynamics, both for intra-molecular and translational motion.

(j) "Neutron Scattering Studies of Hydrogen in Catalysts", T. J. Udovic and R. D. Kelley, in Hydrogen Effects in Catalysis: Fundamentals and Practical Applications, Z. Paal and P. G. Menon, eds. (Marcel Dekker, New York), 167 (1988).

Neutron scattering studies of hydrogen in catalysis are reviewed. Techniques applicable to catalysis studies (incoherent inelastic neutron scattering (IINS), quasielastic neutron scattering (QNS), and powder neutron diffraction) are introduced. Selected examples are presented with an emphasis on illustrating the utility of these neutron scattering techniques for probing the vibrational, diffusive, chemical, and structural behavior of hydrogen on catalyst surfaces.

(k) "Radiation Damage in Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy", T. E. Madey, in Analytical Electron Microscopy-1987, D. C. Joy, ed. (San Francisco Press, CA), 345 (1987).

This paper addresses the physical processes in radiation damage by electrons and photons in surface analysis, with emphasis on the microscopic mechanisms. Surface analysis techniques such as electron-excited Auger electron spectroscopy, AES, and x-ray photoelectron spectroscopy, XPS, are often plagued by radiation damage effects that change the surface structure and/or chemical composition. Damage-producing excitations compete with information-producing excitations in the surface layer during measurements, and the resultant beam damage can be a serious perturbation in quantitative surface analysis. The following aspects of radiation damage are discussed: the role of valence- and core-electron excitations in bond-breaking and desorption; cross sections for damage and the critical radiation dose for damage; relative damage rates in AES and XPS; examples of beam damage in surface analysis; and remedies for minimizing beam damage.

(l) "Reference Materials, Reference Data, and Reference Procedures for Surface Analysis: National and International Standards Activities", C. J. Powell, in Electronic Materials and Processes, eds. N. H. Kordsmeier, C. A. Harper, and S. M. Lee (Society for the Advancement of Material and Process Engineering, Covina, CA), 252 (1987).

As the use of surface analysis increases, the need for reference materials, reference data, and reference procedures becomes more urgent. A brief description is given of the needs for surface-analysis standards and of recent efforts to develop such standards. Emphasis is given to the work of two national laboratories, the US National Institute of Standards and Technology and the UK National Physical Laboratory, and of three standards organizations. The three standards organizations are the ASTM Committee E-42 on Surface Analysis, the Surface Chemical Analysis Working Party established by the Versailles Project on Advanced Materials and Standards (a cooperation of seven nations and the Commission of the European Communities), and the Surface Analysis Working Group of the International Union of Pure and Applied Chemistry.

(m) "The Quest for Universal Curves to Describe the Surface Sensitivity of Electron Spectroscopies", C. J. Powell, J. Electron Spectrosc. 47 197 (1988).

An overview is given of data for electron attenuation lengths (ALs) and inelastic mean free paths (IMFPs) in the energy range of interest for electron spectroscopy of surfaces with emphasis on the search for so-called universal curves. Reliable knowledge of ALs and IMFPs is important for determining the surface sensitivity of electron spectroscopies and for quantitative surface analysis by AES and XPS. Suitable formulas for ALs and IMFPs are needed as user guides but existing formulas are of limited accuracy due to problems in AL measurements and approximations in IMFP calculations. AL measurements and the various AL and IMFP formulas are critiqued. A new formula due to Tanuma et al. shows promise of being a useful guide to the energy- and material-dependences of IMFPs and may be a reasonable though less accurate guide for ALs.

(n) "The Development of Standards for Surface Analysis"; C. J. Powell, Surf. Interface Anal. 11, 103 (1988).

As the use of surface analysis increases, the need for standards (reference procedures, reference data, and reference materials) becomes more urgent). This article describes activities and current plans of three organizations that are active in developing standards for surface analysis: Committee E-42 on Surface Analysis of the American Society for Testing and

Materials; the Surface Chemical Analysis Working Party of the Versailles Project on Advanced Materials and Standards (VAMAS); and the Working Group on Surface Analysis of the International Union of Pure and Applied Chemistry.

(o) "Synchrotron Radiation Studies of the Electronic Structures of High-T_c Superconductors", in Thin Film Processing and Characterization of High-T_c Superconductors, J. M. E. Harper, R. J. Colton, and L. C. Feldman, eds., American Vacuum Society Series 3 (American Institute of Physics, N.Y.), 222 (1988).

Experimental measurements of the electronic structure of the high-T_c superconductors $La_{2-x}[Sr,Ba]_xCuO_4$ and $YBa_2Cu_3O_{7-x}$ are reviewed and discussed in the context of determining the strengths of the interactions within the valence bands. It is concluded that the Cu 3d - O 2p valence bands are highly hybridized and there are strong electron-electron correlations. It is shown that the Cu^{3+} configuration ($3d^8$) is energetically unfavorable and the systems are best thought of as having an approximate valence of Cu^{2+}. The influence of surface stoichiometry on the electronic structure is discussed and preliminary molecular adsorption studies are reported.

2. Review Articles in Publication

We list below the titles and abstracts of review articles in the course of publication.

(a) "Cross Sections for Inelastic Electron Scattering in Solids," C. J. Powell, Ultramicroscopy

An overview is given of available information on cross sections for inelastic electron scattring in solids with emphasis on the needs for cross-section data in electron energy-loss spectroscopy (EELS), x-ray emission spectroscopy (XES), and Auger-electron spectroscopy (AES). After a brief survey of the relevant theory, information is given on inelastic mean free paths of 200-2000 eV electrons in solids (AES), total inner-shell ionization cross sections (AES and XES), and partial inner-shell ionization cross sections (EELS).

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

A quantitative surface analysis by Auger-electron spectroscopy (AES) or x-ray photoelectron spectroscopy (XPS) requires a series of operations that typically includes instrument setup, specimen positioning, data acquisition, data manipulation, and data analysis. These operations involve a sequence of measurements which are combined and/or compared with other data to yield an analysis. The final result has an uncertainty that reflects the separate random and systematic uncertainties in the various measurements and sources of data. We identify the major steps in typical analyses and comment on the major sources of uncertainty. Systematic uncertainties generally exceed random uncertainties and are associated with the complex morphology of typical specimens, with adequate knowledge of instrument performance, and with limitations of current methodology and data. We review general measurement principles, the development of a suitable analytical strategy, and identify and discuss the many sources of uncertainty. The discussion is specific to AES and XPS but many of the issues are relevant to other techniques. Finally, some examples are presented to illustrate the sources and magnitudes of uncertainties in typical types of surface analyses by AES and XPS.

(c) "Electron and Photon Stimulated Desorption", Benefits and Difficulties", T. E. Madey, A. L. Johnson, and S. A. Joyce, Vacuum

Some of the benefits and pitfalls of electron and photon-stimulated desorption (ESD/PSD) processes at surfaces are described. Useful information about the local structure of surface molecules is provided by electron stimulated desorption ion angular distributions (ESDIAD). ESDIAD is an effective surface structural tool because the directions of ion desorption are determined by the orientation of the surface bonds ruptured by electron or photon bombardment. Other benefits of electron and photon-stimulated damage processes at surfaces include electron and photon beam lithography in microelectronics. The pitfalls of ESD/PSD include beam damage in surface analysis (by Auger electron spectroscopy, x-ray photoelectron spectroscopy, and high resolution transmission electron microscopy), the PSD of gases from vacuum walls in fusion reactors and synchrotron radiation sources, and false pressure readings due to ESD effects in ionization gauges.

(d) "The Semiclassical Way to Molecular Dynamics at Surfaces", J. W. Gadzuk, Annual Reviews of Physical Chemistry

Time-dependent molecular dynamics at surfaces is considered within the framework of semiclassical wave packet dynamics of Heller. Aspects of photoemission spectroscopy, stimulated desorption, electron energy loss spectroscopy, and molecule/surface collisions are considered within a unified picture.

(e) "Epitaxy of Metals on Metal Substrates: The Contributions of Field Emission Microscopy", A. Ciszewski and A. J. Melmed, Appl. Surface Science

The contributions to the literature on the epitaxial growth of metals on metal substrates made by research using the field emission (electron and positive-ion) microscopies are reviewed. In addition to a large amount of information about specific metal/metal pairs, some generalities have emerged. It is especially striking that in many cases of metal/metal epitaxy, the dominant factor determining the epitaxial relationship is the alignment of close-packed atomic rows in low-index crystallographic planes of each metal.

(f) "Molecular Desorption from Solid Surfaces: Laser Diagnostics and Chemical Dynamics", D. S. King and R. R. Cavanagh, Advances in Chemical Physics: Molecule-Surface Interactions

The energy content of molecules as they leave surfaces provides a detailed signature of the dynamics of the desorption process. In this article, the utility of laser-based diagnostics for characterizing the ensuing state specific populations is illustrated. Specific examples are taken from thermally driven desorption processes and contrasted with non-thermal processes. By restricting the systems of interest to a single desorbed species (NO), and a single substrate (Pt), the rich variety of desorption dynamics becomes apparent. Over 80 references are provided to provide access to the broader literature which deals with laser diagnostics of molecular desorption.

(g) "The Status of Reference Data, Reference Materials, and Reference Procedures in Surface Analysis", J. T. Grant, P. Williams, J. Fine, and C. J. Powell, Surf. Interface Anal.

A brief synopsis is given of recent developments and current needs for reference data, reference materials, and reference procedures in surface analysis. This assessment is based largely on the presentations and discussion at the Second Topical Conference on Quantitative Surface Analysis held at Monterey, California on October 30-31, 1987. While a reasonable start has been made in recent years in providing needed data, materials, and procedures, many important needs remain.

3. Books

(C. J. Powell and T. E. Madey)

While there are many books and review articles on different aspects of surface science and its applications, there is a dearth of information on how to make reliable surface-characterization measurements. There is, in essence, a large information gap between review articles in which the latest scientific advances are discussed and manufacturers' handbooks in which the operation of commonly used surface-characterization equipment is described. Arrangements have been made with a commercial publisher to produce a series of books, "Methods of Surface Characterization," which will address this need. Two Division staff members (Powell and Madey) and three other scientists (A. W. Czanderna at the Solar Energy Research Institute; D. M. Hercules and J. T. Yates, Jr., at the University of Pittsburgh) constitute an editorial board that will oversee the production. A series of four volumes is currently planned which will describe the principles, techniques, and methods considered important for surface characterization. It is intended to describe how important surface-characterization measurements are made and how to ensure that the measurements and interpretations are satisfactory (to the greatest extent possible). The approach of the series will be pedagogical or tutorial.

The first volume in the series, "Vibrational Spectroscopy of Molecules on Surfaces," was published in 1987. This volume contains descriptions of the major methods used to measure vibrational spectra of surface species. The emphasis of the volume is on the basic concepts and experimental methods rather than an extensive survey of literature in the field. Chapters in the volume and their authors are as follows:

1. Normal Modes at Surfaces (N. V. Richardson and N. Sheppard)
2. Excitation Mechanisms in Vibrational Spectroscopy of Molecules on Surfaces (J. W. Gadzuk)
3. Infrared Spectroscopy of High-Area Catalytic Surfaces (A.T. Bell)
4. Inelastic Electron Tunneling Spectroscopy (P. K. Hansma)
5. Incoherent Inelastic Neutron Scattering: Vibrational Spectroscopy of Adsorbed Molecules on Surfaces (R. R. Cavanagh, J. J. Rush, and R. D. Kelley)
6. Electron Energy Loss Spectroscopy (N. R. Avery)
7. Reflection Absorption Infrared Spectroscopy (B. E. Hayden)
8. Raman Spectroscopy (A. Campion)
9. Infrared Spectroscopy of Adsorbates on Metals: Direct Absorption and Emission (P. L. Richards and R. G. Tobin)

Three other volumes of the series are at an advanced stage of preparation. Two volumes will describe the techniques and methods for electron spectroscopy and ion spectroscopy, respectively, and will concentrate on techniques for which commercial instrumentation is available. The other volume will contain descriptions of techniques for specimen handling and depth profiling together with information on the common artifacts and problems associated with the bombardment of surfaces by electrons and ions.

3. SURFACE MEASUREMENTS PROGRAM

J. D. Beckerle, S. A. Buntin, R. R. Cavanagh, R. A. Demmin, J. W. Gadzuk, T. J. Jach, A. L. Johnson, S. A. Joyce, R. D. Kelley, R. L. Kurtz, T. E. Madey, J. M. Nicol, D. E. Ramaker, L. J. Richter, S. W. Robey, S. M. Shivaprasad, and R. L. Stockbauer

A. Photoemission Studies of the Electronic Structure and Chemisorption Properties of High-Temperature Superconducting Materials

(R. L. Kurtz, R. L. Stockbauer, and S. W. Robey)

The recent discovery of superconducting materials with critical temperatures in the range 90-120 K has generated intense interest and activity. Many scientists are trying to understand the physical properties and the mechanisms of superconductivity in the various copper oxides; others are trying to develop the materials so that they can be used successfully in devices.

We have initiated a project in which photoelectron spectroscopy is being applied to understand the electronic structure and to investigate the chemisorption properties of the new high-T_c materials. Our work has been expedited by a combination of relevant experience and of available equipment. We have previously studied metal oxide systems and know how to handle and prepare samples for measurement as well as how to interpret photoemission data. We are aware of the pitfalls one encounters in making photoemission measurements at low temperature, such as the propensity for samples at low temperature to adsorb water present in trace amounts from the background gas in the vacuum chamber. Our experience with dosing clean surfaces with controlled amounts of gas allows us to make quantitative measurements of the initial stages of degradation of these materials. We have a dedicated beamline at the NIST synchrotron light source SURF-II. This has enabled us to perform new experiments quickly and to continue the experiments for as long as necessary to answer the questions which present themselves during the experimental run, a luxury not available to most other synchrotron groups. Finally, we are one of the few groups which had a sample mount which was coolable to liquid nitrogen temperature which allowed us to make measurements above and below the critical temperature.

This project has been supported in part during FY88 by the NIST initiative on High Temperature Superconductors and in part by the Office of Naval Research.

1. Photoemission Studies of 1-2-3 Superconducting Compounds

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

Having the facilities to obtain photoemission spectra on cold samples, we were one of the first groups to publish spectra obtained with sample temperatures above and below T_c. Contrary to earlier reports, there was no change in the spectra with temperature.

Comparison of the spectra for a series of Sr-doped La superconductors as well as with Ho and Y compounds showed that their valence band structures were nearly identical, all having a low density of states at the Fermi level and a broad valence band consisting of mixed Cu 3d and O 2p states. This low density of states at the Fermi level did not agree with band structure calculations. The discrepancy was explained by the fact that these materials are highly correlated compounds in which electron-electron interactions are strong and therefore one-electron models would not be expected to adequately describe the system.

We were the first to publish resonant photoemission spectra of the 1-2-3 compounds, i.e., spectra as a function of incident photon energy. By observing the photon energy at which valence spectral features are enhanced, we were able to associate each of the multitude of peaks with the particular elemental component of the compound. Without this added degree of sophistication, such identifications are, at best, tenuous.

From knowledge of the photon energy at which two copper satellite features resonated as well as their binding energy, it was possible to determine that the dominant valence state of Cu in the 1-2-3 compounds was 2+. This was contrary to proposals at the time based on formal charge balance that 1/3 of the copper should be in a 3+ state. The explanation is that these are covalent compounds rather than ionic and therefore the concept of formal charge balance does not apply.

One of the features in the valence band spectra has as yet not been fully characterized. This feature at 9.5 eV binding energy appears in most of the materials and resonates with the onset of O 2s core excitations near a photon energy of 20 eV. This resonant behavior is very sensitive to the amount of oxygen in the high-T_c material. Details of the nature of the electronic states involved in this transition are currently being investigated.

2. Surface Degradation Studies Using Controlled Dosing of Atmospheric Gases

In the course of the resonant photoemission experiments at low temperature, it was realized that the high-T_c materials were very susceptible to adsorption of background gases in the ultrahigh vacuum chamber. It was also well known that the 1-2-3 compounds rapidly degraded when exposed to air. Photoemission spectra were obtained from freshly scraped samples before and after exposure to measured amounts of atmospheric gases. It was found that the 1-2-3 compounds react rapidly with H_2O with a sticking probability of nearly 1 to form hydroxide compounds. This is apparently the initial step in the degradation process and is why the samples degrade so rapidly in air. The reaction with CO_2 to form carbonates is less likely but still significant and points out that storage in desiccators as has been the common practice may not be sufficient for long-term protection. CO is less reactive by several orders of magnitude as is O_2. This latter result is a bit surprising since these compounds take up and lose oxygen so readily.

This study also pointed an error in several publications that claim to observe reversible changes in the photoemission spectra of the 1-2-3 material related to the superconductivity as the samples were cycled from 90 K to room temperature. These changes are now thought to be solely due to the reversible adsorption of background gases in the analysis chamber.

We have emphasized the importance of in-situ sample preparation in our publications and in our comments on the copious number of papers we are asked to review for major journals. Many of these reported changes as the samples are temperature cycled are due to lack of in-situ sample cleaning and to background gas adsorption.

3. Studies of New High-T_c Materials

Our most recent endeavors concern measurements on the new bismuth and thallium based superconductors. While these results are preliminary and we will repeat the experiments with better characterized materials when they are available, we do find some differences from the 1-2-3 compounds. The samples appear to be more susceptible to radiation damage from both electron and photon beams. This indicates that experiments using even a relatively low electron or photon beam flux (electron-excited Auger spectroscopy, inverse photoemission, or x-ray fluorescence, for instance) are likely to induce enough surface damage to produce erroneous results during the short time needed to acquire data.

Controlled adsorption experiments on the Tl-based compound produced results similar to those from the 1-2-3 compounds. H_2O adsorption produced an hydroxide species while CO_2 and CO produced a carbonate species. However, it appears that this surface is at least an order of magnitude less reactive than the 1-2-3 compounds.

4. Thin Film Evaporation Facility

One of the most important uses of the new high-T_c materials will be as thin films in electronic devices. We expect that the evolution of such devices will be similar to that of thin-film semiconductors. Since surface science played such a crucial role in semiconductor development, we expect that it will play as important a role in the superconductor device development. The primary thrust of our efforts in the future, then, will be directed toward the characterization of the electronic structure and chemisorption properties of high-T_c superconducting thin films.

To date, the primary experimental problem of high-T_c thin films has been surface preparation. Films are usually produced in one chamber and then transported through air to a second chamber for analysis. Since the normal surface preparation techniques of ion sputtering and annealing destroy the surface stoichiometry of these multi-component systems, there is no satisfactory method of cleaning the films once they are in the analysis chamber. Our present technique used on bulk samples of scraping to obtain a clean surface cannot be applied to the films since they are not thick enough to survive this macroscopic treatment.

To overcome this problem, we plan to attach a thin-film deposition chamber to our photoemission analysis chamber so that, with a sample transfer system, the freshly made films can be delivered directly to the analysis chamber without exposure to air. This will be a valuable facility for studying the surface properties of thin films. We should emphasize that we will not undertake an extensive program on the methodology for growing high-T_c thin films but rather we will use recipes developed by others to produce the films. We will concentrate on their characterization.

Our current plans call for a chamber containing 6 evaporation sources with independent evaporant beam monitors and controllers. This number is adequate for deposition of the currently known high-T_c compounds from elemental sources and should suffice for any reasonable compounds discovered in the future. Additional side chambers will be attached for fast substrate introduction through a load-lock and for high-pressure oxygen annealing if necessary. In-situ monitoring of film growth will be accomplished with reflection high-energy electron diffraction and the critical temperature of the film will be measured with a movable four-point probe. The sample will be mounted on the helium-cooled cold head so the temperature can be lowered to 20 K for these measurements.

Procurement has been made of some vacuum hardware, pumps, beam monitors, and electronics. Design of the vacuum chamber and sample transfer system is underway. We hope to have an operational system within one year.

Initial experiments will involve the study of the electronic structure of oriented thin films using the angle-resolved photoemission capabilities of the ellipsoidal mirror analyzer. As with our studies on bulk material, this information can be compared directly with band-structure calculations. Likewise, stability of the films toward atmospheric gases will be studied using controlled gas dosing. Future experiments will include studies of the growth of metal overlayers on the superconducting films which will be important for understanding the properties of interfaces and electrical contacts.

B. Studies of Oxide Surfaces, Thin-Films, and Desorption Processes Using Synchrotron Radiation

(R. L. Stockbauer, R. L. Kurtz, S. W. Robey, R. A. Demmin, D. E. Ramaker, and T. E. Madey)

The major goals of this effort are to determine the electronic structure of surfaces, thin-films, and adsorbates using variable-wavelength photoelectron spectroscopy and to identify the electronic excitations which lead to ion desorption. Synchrotron radiation provides the incident photons for both experiments with its tunability being its greatest asset. In the photoemission experiment, the tunability allows us to probe resonances which can be used to identify peaks in the valence band as well as to increase sensitivity to minority states on the surface. In the ion yield measurements, the tunability allows us to obtain ion yield data (ion intensity as a function of photon energy) which are correlated with photoemission results to identify the excitations which initiate the ion desorption process. This work has been supported in part by the Office of Naval Research.

1. Water Adsorption on Defective and Nearly-Perfect $TiO_2(110)$.
(R. L. Kurtz, R. L. Stockbauer, and T. E. Madey)

Our long-term interest in the electronic structure and chemistry of oxide surfaces continues with a synchrotron radiation photoemission study of the interaction H_2O with defective and nearly-perfect $TiO_2(110)$ surfaces at temperatures between 160 and 300 K. This work was performed as part of a co-operative agreement between the United States and Spain and involves a collaboration with Dr. E. Roman and Prof. J. L. de Segovia of the Instituto Ciencia de Materiales, CSIC, Madrid. Defect sites have been implicated in the adsorption process and, by tuning the photon energy to 47 eV, we find that a resonant process gives an enhanced photoemission sensitivity to these Ti^{3+} 3d defect states. Defects are produced on $TiO_2(110)$ by annealing to 1000 K in ultra high vacuum; subsequent exposure to 10^4 Langmuirs O_2 produces nearly perfect surfaces, as judged by the suppressed Ti 3d emission.

Both nearly perfect and defective surfaces give rise to dissociative adsorption of H_2O at 300 K but the defective surface has a saturation coverage that is nearly an order of magnitude less than that of nearly perfect $TiO_2(110)$. The enhanced sensitivity to the Ti^{3+} defect states has allowed the observation of a surprising effect: the dissociative adsorption results in increased defect-state intensity on both the nearly perfect and the defective surfaces. This apparent charge-transfer to the substrate implies that a new mode for the dissociation process is needed. At 160 K, H_2O adsorbs molecularly on both the nearly-perfect and the defective surfaces. Subsequent annealing experiments allow estimates of the interaction energies involved in the dissociation process.

This work will continue with an investigation of ammonia adsorption on the defective and nearly-perfect $TiO_2(110)$. In addition, other surfaces of TiO_2 will be studied along with MgO and oxidized Mg metal. This latter study is important in understanding the role of surface geometry in the ion desorption process.

2. Calculations of Surface Dynamics in the Ion Desorption Process
(R. L. Kurtz)

In a collaboration with Dr. R. E. Walkup of IBM, a computer program has been written to calculate classical trajectories of ions desorbed from a surface. The dynamics of the surface atoms in the neighborhood of the desorbing ion are calculated in addition to the motion of the ion itself.

This allows for the investigation of the reaction of the neighboring atoms to forces induced by the desorbing ion. Pair-wise potentials are used to calculate the potential energy surface governing the ion and neighboring atom motion.

O^+ desorption from TiO_2 was calculated since it is the prototype system used by Knotek and Feibelman to explain positive ion desorption from ionic insulators. The calculations established the time scale for desorption, and predicted the ion kinetic energy and angular distributions which can be directly compared with our experimental results. The calculations provide qualitative insight into the effects of lattice recoil and the origin of site-dependent desorption probabilities. Better agreement between the results of the calculations and the experimental data is anticipated when the effects of complications such as steps and defects are considered.

One system we propose to calculate is O^+ from MgO. This is a very ionic material and therefore, in the Knotek-Feibelman model, should have a high O^+ desorption probability. Our experiments have shown otherwise and we suspect that since the Mg in the lattice is relatively light, it can move fast enough to absorb the recoil energy from the desorbing O^+ such that the ion never leaves the surface. The calculations on the dynamics of this system should show clearly whether or not this is the case.

3. Photoemission Study of Ba and BaO Films on W(100)

(R. L. Kurtz, R. L. Stockbauer, and T. E. Madey)

As part of a collaboration with Drs. D. R. Mueller and A. Shih of the Naval Research Laboratory and with Dr. E. Roman and Prof. J. L. de Segovia of the Instituto Ciencia de Materiales, CSIC, Madrid to study the surface chemistry of dispenser cathodes, a study was made of the interaction of O_2, CO_2, and H_2O with bulk BaO and with BaO adsorbed on W(100). Using photoemission to identify the reaction products in the adsorbed layer, it was found that H_2O reacts with bulk BaO to form $Ba(OH)_2$, while CO_2 forms a surface layer of $BaCO_3$. The water reaction is unique in that a thick $Ba(OH)_2$ layer is formed; this result indicates water is able to penetrate the hydroxide layer. Water and carbon dioxide also react with a BaO monolayer adsorbed on W(100) to produce adsorbed OH and CO_3 species bound to the tungsten substrate. The presence of a BaO monolayer appears to enhance the interaction of O_2 with the tungsten substrate.

This work has been extended to include photoemission, ion desorption, and chemisorption studies of BaO overlayers on W(110) and of Ba on Ir(100).

4. Photoemission Studies of Pt Overlayers on W(110)

(R. A. Demmin, R. L. Kurtz, R. L. Stockbauer, and T. E. Madey)

A new class of experiments was initiated to investigate the electronic states and surface chemistry of metal-on-metal systems in collaboration with Drs. D. R. Mueller and A. Shih of the Naval Research Laboratory. Such systems are important in thin-film semiconductor devices and metal catalyst systems. The first measurements were made for Pt overlayers 0-6 monolayers thick on W(110) and for CO adsorbed on these surfaces. Valence band spectra of the films and shifts in the positions of the 4σ and $5\sigma/1\pi$ peaks for adsorbed CO were related to thermal desorption results of CO on these films. The first layer of Pt yielded a valence-band photoemission spectrum that was unlike those of subsequent layers; i.e., the intensity 1-2 eV below the Fermi level was greatly reduced, similar to the electronic structure of a noble metal. Moreover, the adsorption of CO on a Pt monolayer was weaker than on W or Pt alone. However, this surface adsorbed CO more strongly than did noble metals and ultraviolet photoelectron spectra from CO adsorbed on Pt/W(110) did not show features characteristic of CO adsorbed on a noble metal.

Other results were interpreted in structural terms. Tungsten core levels shifted with the addition of Pt, consistent with the suppression of surface-shifted core levels, and did not indicate alloy formation. Work function measurements and spectra for adsorbed CO suggested that Pt adatoms in sub-monolayer coverages do not form 2-dimensional islands unless the surface is annealed. Other related studies of the surface chemistry of thin-films of Pt on W(110) are described in section 3.H.

The ability to customize valence electronic states by suitable choices of substrate and overlayer metals makes the metal-on-metals field intriguing. The multi-source evaporation chamber being constructed for the thin-film high-temperature superconductor effort will be extremely useful for preparing well-characterized films for these studies.

5. Implementation of Helium-Cooled Cold Stage
(R. L. Stockbauer, R. L. Kurtz, and S. W. Robey)

We have recently purchased a helium-cooled cold head and movable stage. We plan to use these items in electron attenuation-length experiments (see section 2.A.2(b)) to condense molecules that cannot be condensed at liquid nitrogen temperatures, for instance, the rare gases, and diatomic molecules such as N_2, O_2, and CO. This facility will also be critical in our work on thin-film high temperature superconductors. We plan to determine the critical temperature of thin-films by making resistance-versus-temperature measurements *in situ*. The closed-cycle helium refrigerator will allow these measurements to be made down to 20 K.

The cold stage will also be useful for photon-stimulated desorption measurements on small diatomics as well as small organic molecules such as methane. The use of simpler molecular systems for these studies should encourage more detailed calculation of the phenomena influencing the ion desorption probability.

6. Ellipsoidal Mirror Analyzer
(R. L. Stockbauer, R. L. Kurtz, and T. E. Madey)

The construction and initial testing of the ellipsoidal mirror analyzer has been completed and the instrument is in the process of being installed on beamline 1 at SURF-II. The capabilities of this instrument are outlined in section 4.B.2. We expect this instrument to play a pivotal role in most of our photoemission projects. For instance, in the thin-film high-temperature superconductor program, the analyzer will provide angle-resolved photoemission data from oriented films of the material. Comparisons of such data to band structure calculations provide a valuable test for theory and computational methods. It is becoming clear that simple, one-electron models do not adequately describe these systems since electron-electron correlations are important. More sophisticated, multi-electron cluster calculations will be needed to better describe the electronic states of these materials.

The analyzer will also be used extensively in the ion desorption program to investigate the details of desorption dynamics. Its ability to measure ion kinetic energy as a function of desorption angle will provide, for instance, a test of the reneutralization probability as a function of takeoff angle and energy. Likewise, since it is able to distinguish the masses of the desorbed ions in the angle-resolved patterns, we will be able to better correlate the two-dimensional ion patterns with the surface geometry.

7. Second Surface Science Beamline Instrumented at SURF-II
(R. L. Stockbauer, R. L. Kurtz, and S. W. Robey)

With the installation of the ellipsoidal mirror analyzer on beamline 1 at SURF, it was necessary to find a new home for the instrument which had served us so well over the past 10 years, the double-pass cylindrical-mirror analyzer. It was decided to outfit the instrument with a new computer and updated programs and reinstall it on beamline 8. The computer system and some of the electronics that replaced those that had to stay with the ellipsoidal mirror analyzer on beamline 1 were provided by the Radiation Physics Division.

With the new beamline 8 facility, we hope to be able to devote more experimental time to the electron attenuation-length and ion-desorption measurements from condensed molecular systems. This will leave the ellipsoidal mirror analyzer on beamline 1 free to investigate the high-temperature superconductors and angle-resolved photon-stimulated desorption.

8. X-ray Beamline at Brookhaven National Laboratory
(R. L. Stockbauer, R. L. Kurtz, and T. E. Madey)

Our collaboration with Drs. J. Rife, W. R. Hunter, and M. Kabler of the Naval Research Laboratory to instrument a beamline at the Brookhaven National Synchrotron Light Source has not been active over the past two years due to the extended shutdown of the x-ray ring. During this time the NRL group has extensively tested and modified the monochromator, optics, computer control to render the instrument more usable.

Our primary use of this beamline will be for those experiments needing the higher energy photons (currently up to 600 eV). For instance, the electron attenuation length measurements on condensed molecular solids will benefit greatly from the higher photon energy which will extend the electron kinetic energy range. We also anticipate investigating the effect of core-level excitations on ions desorbed from condensed molecular layers. The extended range of the monochromator will allow these studies to be done at the C, N, and O core levels of the condensed molecules and organic compounds which we have studied previously.

9. Theory of Stimulated Desorption
(D. E. Ramaker)

During the last two years, our work has addressed the important issue of secondary electrons and the role it plays in photon-stimulated desorption (PSD). This investigation has shown that, in cases for which the direct Auger-stimulated-desorption process is active, the indirect x-ray-induced electron-stimulated-desorption (ESD) contribution (i.e. that contribution arising from secondary electrons) is generally on the order of 40% or less. On the other hand, when the direct Auger-stimulated desorption process is suppressed by some mechanism, the indirect process can dominate. For chemisorbed systems, the indirect process is essentially always negligible.

During this past year, we have initiated a study of the mechanisms for ESD of negative ions from surfaces. In simple diatomic molecules, negative ions are known to be produced by dissociative desorption (i.e. resulting from a transient negative molecular ion) and by dipolar dissociation (through an excited neutral molecular species). The dominant mechanism of ESD ion angular distributions (ESDIAD) of negative ions from polyatomic molecules adsorbed on metallic surfaces is, however, much more complicated and therefore not at all clear. Furthermore, it is not even clear that the desorption angle of the negative ions directly reflects the bond angles on the surface, as was found for the positive ions. However, recent NIST experimental work (see section 3.J) has shown that the ESDIAD of F- ions from NF_3/Ru(0001) does complement the F+ ESDIAD. Currently we are designing experiments which we hope will reveal the active mechanisms, and which will determine whether negative-ion ESDIAD can lead to direct bond-angle information. Detailed comparison of the experimental results with gas-phase dissociation data and with theoretical results is contemplated.

C. Dynamical Effects Associated with Core-Level Ionization
(T. Jach)

The NIST synchrotron beamline X-24A at the Brookhaven National Synchrotron Light Source has been utilized to obtain detailed information on the radiative excitation of deep core levels in atoms and molecules. Our present experimental apparatus allows for the irradiation of a gas sample with highly monochromatic, polarized x-rays in the energy range 2- 7 keV, with analysis of the energy and polarization of the resulting x-ray fluorescence. The combination of high incident photon flux, excellent energy resolution, and polarization detection, any one of which by itself would have opened up a new region of the physics of dynamical atomic processes, has produced a considerable body of experimental data that we are starting to understand. The results are producing a gratifying response in the theoretical community. An understanding of the experimental and theoretical problems involved in the gas-phase results has been invaluable in anticipation of similar studies we plan to perform on atoms and molecules on surfaces. Several areas of progress are listed here. This work has been conducted in collaboration with Drs. D. W. Lindle and P. L. Cowan of the NIST Quantum Metrology Division.

1. Polarization Dependence of Molecular X-Ray Fluorescence

The fluorescent x-rays observed on exciting a Cl K electron in the molecule methyl chloride (CH_3Cl) exhibits an unexpected degree of polarization. The initially polarized synchrotron beam selectively excites molecules aligned for a maximum dipole moment into an antibonding state which is selected by the incident energy. Because the time scale of core relaxation is short compared to molecular motion, the x-ray fluorescence which results from radiative decay is highly polarized as well. By means of the polarization and energy analysis capability of our spectrometer, we are able to determine the exact molecular orbitals which participate in excitation and decay of this molecule as a function of incident energy. This work is performed also in collaboration with Drs. R. E. LaVilla and R. D. Deslattes of the NIST Quantum Metrology Division and with Drs. J. A. Sheehy, T. Gil, and P. W. Langhoff of Indiana University.

2. Perturbation Effects of Excitonic States in Chlorine-Containing Molecules

The x-ray absorption spectrum of Cl in $CFCl_3$ shows a strong "white line" just below the K-edge. This line corresponds to a transition in Cl from 1s to the lowest unoccupied molecular orbital, $6a_1$. By varying the incident x-ray energy, we are able to selectively excite transitions to this orbital, to higher lying orbitals, and into the ionization continuum. The $K\beta$ emission spectrum of Cl in the excited neutral molecule shifts by 1 eV when compared to the emission spectrum from the molecule with ionized Cl. Additionally, an emission line can be identified as the de-excitation of the excitonic state. The energy shift allows one to estimate the perturbation of the exciton on the core level. This work is performed also in collaboration with Dr. R. C. C. Perera of the Lawrence Berkeley Laboratory.

D. X-Ray Diffraction Applied to Surface and Interface Research

(T. Jach)

A program has been initiated to use grazing angle diffraction (GAD) from semiconductor surfaces to study the registration of atomic overlayers. Highly collimated x-rays from a synchrotron light source are diffracted through a large angle while incident on the surface of a semiconductor at a grazing angle. The interference between the incident, specularly reflected, and reflected-diffracted beams sets up an x-ray standing wave (XSW) electric field at the surface. The x-ray fluorescence from adatoms illuminated by the XSW can be used to determine their position to a high degree of accuracy (about 0.01 Å laterally). The diffraction studies are conducted using x-rays in the 6-12 keV energy range in the B-cave at the Cornell High Energy Synchrotron Source. The configuration of this source makes it very favorable for investigations using highly collimated beams in this energy range. The program has yielded results in two quite different areas of physics: the registration of adatoms on highly regular crystal surfaces, and the microscopic behavior of x-rays at realistic interfaces. This work has been conducted in collaboration with Drs. M. Bedzyk and Q. Shen at Cornell University.

1. Dynamical Diffraction of X-Rays at Grazing Angles of Incidence

The grazing angle diffraction geometry was selected because it produces XSWs which can be translated parallel to the crystal surface. The behavior of the various x-ray beams which result is complex and non-intuitive when treated by the theory of dynamical diffraction. We have carried out the first extensive experimental studies of the phase space of this diffraction at several energies from 6 to 12 keV using a highly polished single crystal of Ge as the specimen. The results indicate generally excellent agreement with the theory although there are some slight discrepancies. We have also determined which regions of phase space yield experimental conditions which most closely approximate the theory for the purpose of producing accurate XSW results. This work is performed also in collaboration with Dr. P. L. Cowan of the NIST Quantum Metrology Division.

2. Direct Observation of Surface-Trapped Diffracted Waves

The theory of GAD predicts the existence of a diffracted wave which is trapped in a layer as little as tens of angstroms thick at the surface of the crystal. We have observed this wave directly for the first time by means of GAD from a Ge crystal whose surface was specially prepared by photolithography and etching. Our interest in the behavior of this diffracted wave is twofold. First, the trapped wave excites only atoms which are either at or near the surface. Second, the trapped wave is able to escape only by means of deviations from a rigorously smooth crystal surface. Observation of the intensity of any escaping diffracted beam gives a measure of surface roughness which can be followed down to an atomic scale since there is no background signal. Our data on the escape of the trapped beam from our prepared surface indicates an unusual and unexpected relationship between the intensity of the escaping diffracted beam and its wavevector. The investigation of these results has yielded some insight into the deficiencies of theories commonly used to determine roughness of surfaces by x-ray scattering or reflection high-energy electron diffraction. Future measurements will involve etching a 1 μm grating into the surface of a Ge diffraction crystal to obtain a quantitative relationship between the periodicity and height of the roughness and its effect on surface diffraction. This work is conducted also in collaboration with Dr. D. Novotny of the NIST Semiconductor Electronics Division.

3. X-ray Standing Wave Determination of Adsorbate Positions on Germanium

The GAD technique has been applied to observe the registration of halogen atoms deposited by chemical preparation of a polished Ge single-crystal surface. In this geometry, the XSWs are modulated parallel to the crystal surface giving atomic position information parallel to the surface. In x-ray fluorescence detection of L x-ray emission from submonolayers of Cl and I on Ge, taken during GAD at energies of 6, 8, and 12 keV, we are able to determine that the halogen atoms occupy approximately the same on-top sites that they are observed to occupy in ultra-high vacuum (UHV) conditions. The "real world" measurement which was made here is, of course, impossible to make using surface science techniques which depend on ultra-high vacuum. The grazing angle XSW method is one of the few ways in which experimental data obtained in UHV can be compared to chemical processes at atmospheric pressure. The program is developing in several parallel directions. We are analyzing existing data to obtain atomic positions to as high as accuracy as the fluorescence signal permits. We are investigating the feasibility of GAD at a buried interface of a semiconductor and another semiconductor or metal film. Finally, we are constructing a vacuum chamber containing a precision goniometer for XSW studies under UHV conditions. The chamber will permit the detection of electrons emitted from atoms excited by XSW, allowing for the separation of elements which produce overlapping emission lines in our low-resolution x-ray fluorescence spectra.

E. Development of Silicon Diode X-Ray Detectors for Synchrotron Radiation Research

(T. Jach)

The explosion of scientific activity which employs radiation from synchrotron light sources has been paralled by the development of sophisticated instrumentation. Requirements exist now for x-ray detectors which cannot be satisfied by traditional detectors such as ion chambers or scintillation crystals. The wide dynamic range of x-ray intensity (10 orders of magnitude or more) to which a detector may be subjected is compounded by other complications such as the requirement to operate in ultra-high vacuum. More sophisticated detectors are being developed to meet the needs of present experiments in a collaboration with Drs. J. Geist, G. Carver, and D. Novotny of the NIST Semiconductor Electronics Division.

Our most recent development has been a monochromatizing crystal which incorporates the detection of x-ray diffraction by means of an integrated photodiode. Most x-ray monochromators use sequential diffraction from two semiconductor crystals to obtain energy resolution in the synchrotron beam. By integrating a planar photodiode detector into the surface of the second silicon crystal, we are able to observe radiation from the first crystal. On correctly aligning the second crystal to the Bragg condition, the change which occurs in the extinction depth for the radiation in the crystal is detected by the embedded photodiode. A particular application of this device is the detector in the feedback loop necessary to maintain alignment of the crystals under conditions of extended operation.

The incorporation of a detector into a crystal without distorting it as a diffracting device proved to be a challenging problem. We believe this invention will have widespread application as synchrotron beamlines and x-ray monochromators become accepted tools in applications such as x-ray lithography and medical angiography. The Department of Commerce is proceeding to apply for a patent on this device.

F. Studies of Surface Reactions Using Synchrotron Radiation
(J. A. Yarmoff and S. A. Joyce)

Investigations have been made of several different surface reactions using the techniques of photoelectron spectroscopy and photon-stimulated desorption with synchrotron radiation.

1. Mechanistic Studies of the Selective Chemical Vapor Deposition of Tungsten on Silicon and SiO_2 via WF_6
(J. A. Yarmoff)

The chemical vapor deposition (CVD) of tungsten on silicon via WF_6 is technologically important because of the ability to deposit these films selectively. That is, W will deposit onto regions of bare Si while, under the same conditions, it will not deposit onto SiO_2. This selectivity makes W CVD useful as a process for forming interconnects in an electronic device. The usefulness of the technique is limited, however, due to problems encountered when trying to make very small structures. It is thus of importance to understand the detailed chemical mechanisms operative in this process in order to utilize it, and other selective CVD processes, to a finer degree. This work is a collaboration with Dr. F. R. McFeely of the IBM Watson Research Laboratory and has been performed at the Brookhaven National Synchrotron Light Source.

The experiments are performed using a system with which films can be grown in an ultra-high vacuum (UHV) dosing chamber, and then transferred under vacuum into the spectrometer. The samples are then measured with soft x-ray core-level photoemission. The initial experiments were performed to study the mechanism for deposition on clean silicon. It was found that WF_6 completely dissociates upon interaction with Si but that at room temperature, the deposition process is self-poisoning. This is because the fluorine liberated from WF_6 ties up dangling Si bonds which are necessary to induce the dissociation. At elevated temperatures (~450°C), the reactions proceeds because silicon can be etched one monolayer at a time at these temperatures.

The recent results involve the study of the mechanisms responsible for the selectivity. It has been found that absolutely no growth will occur on a thin layer of thermal oxide at any temperature below the desorption temperature of oxygen itself. However, small defects can be introduced into the oxide layer by Ar ion bombardment. If this is done, tungsten is then deposited by exposure to WF_6. However, the tungsten is not in the zero-valent oxidation state, as it is after deposition on clean Si. Tungsten deposited on a damaged oxide is itself oxidized. Further experiments are planned in order to more completely understand the mechanisms for selectivity of CVD reactions.

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

Reactions of fluorine with silicon provide a good model for fundamental chemical reactions involved in the etching of semiconductors. Because of the ionic nature of fluorine bonds, it is also an ideal system for the study of the physics of the photon-stimulated desorption (PSD) process. PSD of F+ has been performed at the National Synchrotron Light Source at Brookhaven National Laboratory. Surfaces were prepared by exposure of clean Si to XeF_2. Surfaces covered by a various mixtures of SiF, SiF_2 and SiF_3 species can be prepared with coverages ranging from approximately one monolayer to several monolayers. The latter situation results from steady-state etching of silicon. The chemical shift associated with each Si oxidation state can be readily ascertained with core-level photoemission, and is approximately 1 eV per attached fluorine atom.

When measuring the PSD yield in the vicinity of the Si 2p edge, it has been found that the position of the edge for any given oxidation state correlates with the transition from the bonding 2p atom to the conduction band minimum (CBM). For surfaces covered with monolayer amounts of fluorine, it has been shown from measurements of the angular dependence of the PSD yield that F+ desorbs from monofluoride units adsorbed on Si (111) along the normal direction from the sample, while F+ coming from trifluorides desorbs along a more grazing angle. This allows for the separation of the PSD yield curves for the two oxidation states. In addition to showing an edge 2 eV higher than the monofluoride edge, the yield curve for F+ desorbing from SiF_3 shows structure due to the existence of localized Rydberg-like final states (3s and 3p) which is absent from the monofluoride yield curves. Recent measurements have shown that the ion kinetic energies associated with transitions to these final states are higher than the ion kinetic energies for transitions directly to the CBM. Thus, the ions desorbed via transitions to these final states have followed a different PSD mechanism.

Additional studies have concentrated on the F 1s edge, at which the polarization dependence of the PSD yield was measured for samples covered solely with monofluoride units. In this case, the results showed a strong polarization dependence which was virtually identical to that obtained by measuring the absorption at the F 1s edge. This dependence showed a sharp feature just above threshold whose intensity was parallel to the F-Si bond. It turned out that a measurement of this type was very sensitive to the condition of the sample; small amounts of contamination reduced the sharpness of the polarization dependence of the absorption without affecting the PSD. Thus, a comparison of the absorption yield to the PSD yield is a very sensitive method for determining sample purity.

Further work is planned to study the effects of long exposures to monochromatic light. Preliminary results have indicated that fluorine desorption can be enhanced from particular oxidation states by tuning the photon energy to a transition from the Si 2p level associated with that oxidation states to the CBM. While this is certainly the case for ion desorption, it may not be true for the total yield of desorbed products. Thus, samples will be measured with photoemission before and after long exposures to the light.

3. Photoemission and Photon Stimulated Desorption Studies of PF_3 Adsorbed on Ru(0001)

(J. A. Yarmoff, S. A. Joyce and T. E. Madey)

Electron Stimulated Desorption Ion Angular Distributions (ESDIAD) collected for PF_3 adsorbed on Ru (0001) have shown a multitude of patterns which have been interpreted as due to F^+ coming from adsorbed PF_3, PF_2 and PF units. Initially, the surfaces were covered with undissociated PF_3 and the electron beam damage during the ESDIAD measurements resulted in the dissociation of the PF_3. This model has been tested by performing photoemission and PSD measurements at the Brookhaven National Synchrotron Light Source. The photoemission date showed clearly formation of PF_2, PF and P from a surface initially covered solely by PF_3 and subjected to beam damage. Additionally PSD measurements at the P 2p edge have been correlated with the oxidation state of the adsorbed phosphorus. It is planned to measure the PSD of F- ions since these have also been shown to possess unique ESDIAD patterns.

4. Studies of MoS_2 Surface Chemistry

(J. A. Yarmoff)

MoS_2 exists in a layered structure which gives it excellent properties as a solid lubricant. Single crystals of MoS_2 occur naturally and can be cleaved to give clean, well-ordered surfaces in ultra-high vacuum. These surfaces have the property that the traditional cleaning method of ion-bombardment followed by annealing is unsuccessful, since the ion-bombardment causes preferential loss of S. In the layered-crystal structure, S atoms cannot diffuse perpendicular to the layers in order to refill the empty lattice sites. This effect has been studied at the Brookhaven National Synchrotron Light Source in a collaboration with Dr. J. R. Lince of the Aerospace Corporation.

The effect of 1 keV Ne+ ion bombardment on the clean, ordered MoS_2 (0001) surface was studied using high-resolution photoelectron spectroscopy. For low ion fluences, S-vacancy-defect formation occurred in the MoS_2 lattice with the concurrent formation of a small amount (<10%) of dispersed Mo(0). For fluences greater than $\tilde{}1\times10^{16}$ Ne+/cm^2, the Mo(0) was the predominant species in the surface region, while the remaining species consisted of amorphous MoS_{2-x} and a polysulfide species. Annealing the sample to temperatures up to 1000 K resulted in the formation of metallic Mo coexisting, in approximately equal amounts, with reformed MoS_2 in a surface with no long-range order. A qualitative depth distribution of the chemical species present after Ne^+ bombardment was determined by varying the photon energies employed for core-level spectroscopy. The results indicate that the preferential sputtering of sulfur over molybdenum occurred predominantly through a mechanism involving chemical-bonding effects, specifically through the preferential emission of polysulfide ions over other species in the bombarded region.

Additional work was performed on the chemical aspects of metal adsorption on MoS_2. This work has important applications in the ability to bond the lubricant to a working part. Due to the nature of the MoS_2 structure, metals in general tend to form islands with rather poor bonding to the surface. To date, both Fe and Mn adsorption have been studied. Deposition of thin films of Fe on MoS_2 basal plane surfaces resulted in only a small decomposition of the MoS_2, indicating only a limited chemical reaction. Annealing chemically reformed the MoS_2, but produced a disordered sample that included small amounts of Fe in the lattice and did not show a LEED pattern. Mn, on the other hand, had a large reaction with the MoS_2, forming MnS and Mo metal. Annealing of this did not reform the MoS_2, but did produce a sufficient order to produce a LEED pattern. Further work is planned in which metal adsorption on chemically treated substrates will be studied. Such a treatment of a substrate may lead to a more uniform coverage.

G. Impact Collision Ion Scattering Spectroscopy
(J. A. Yarmoff)

Experiments are planned to study epitaxial growth, adsorbate geometry, melting phenomena, and other geometrical aspects of surfaces using impact collision ion-scattering spectroscopy (ICISS). An instrument is currently under construction which employs a 5 keV Li ion gun and an electrostatic analyzer mounted at a 170° scattering angle. ICISS is performed by monitoring the yield of singly scattered species as a function of the angle between the ion beam and the sample. A manipulator with stepping-motor-controlled rotations is being employed for the angular control. The advantage of using ICISS compared to conventional low-energy ion scattering is that the analysis is simplified by only considering the shadowing effects of the incoming ion beam. Alkali ions are used also to simplify the data analysis by eliminating the need to consider the neutralization of the scattered ions, as is the case with noble gas ions.

H. Reaction Kinetics over Model Single-Crystal Catalysts
(R. A. Demmin, S. M. Shivaprasad and T. E. Madey)

The overall objective of this research has been to provide a molecular understanding of heterogeneous catalytic chemistry on well-characterized single crystal surfaces. Among the areas studied are the catalytic synthesis of hydrocarbons from carbon monoxide and hydrogen on metal surfaces, the mechanism of catalytic poisoning and promotion, and the reforming of alkanes over model supported Pt catalysts. The apparatus employed for these studies contains high pressure reactors contiguous to ultrahigh vacuum surface analysis chambers. This work is supported in part by the Office of Basic Energy Sciences, Department of Energy.

During the last two years, we have continued a new effort to characterize the properties of model thin-film catalysts prepared by evaporating monolayer films of a metal (Pt) onto single-crystal metal substrates (the close-packed W(110) surface and the atomically rough W(111) surface). Such catalysts serve as model systems for understanding the properties of mixed-metal catalysts: these materials have received considerable attention recently because they often exhibit superiority over single-metal substrates as practical catalysts. It is also known that mixed-metal systems can exhibit remarkably different chemisorption properties from those of either metal alone, and we have found striking evidence for this in our own work.

We are studying the growth, thermal stability and surface chemistry of Pt overlayers (sub-monolayer to multiple-layer coverages) on W(110) and W(111) by means of a variety of surface science methods, including Auger Electron Spectroscopy (AES), low-energy electron diffraction (LEED), thermal desorption spectroscopy (TDS) of a probe molecule, CO, and ultraviolet photoemission spectroscopy (UPS) using synchrotron radiation.

Based on our studies of Pt/W(110), we find evidence for a strong interaction between platinum and tungsten that causes platinum deposited on tungsten to bind more strongly to the substrate than to neighboring platinum atoms. As a result, heating multiple layers of platinum on W(110) causes all but the first layer to agglomerate into three-dimensional clusters on the surface of the tungsten. The first layer remains dispersed in a single atomic layer with the crystal structure of the underlying tungsten and requires a higher temperature for evaporation than does the excess platinum.

The effects of the interaction between platinum and tungsten is manifested in the surface chemistry of the platinum-covered surface in the presence of reactive gases such as carbon monoxide and oxygen. A platinum monolayer on W(110) adsorbs carbon monoxide more weakly than either bulk platinum or the tungsten substrate, but the surface begins to exhibit adsorption behavior more like platinum with the addition of a second layer of platinum. Likewise, platinum on the surface of tungsten can alter the adsorption of oxygen, causing it to bind in different locations on the surface and desorb at a lower temperature than it would from pure tungsten.

The unique nature of the platinum monolayer is reinforced by the results of valence-level photoelectron spectroscopy experiments performed at the NIST SURF-II synchrotron radiation facility. As noted in section 3.B.4, the layer of Pt yields a valence spectrum that is different form those of subsequent layers; i.e., the intensity 1-2 eV below the Fermi level is greatly reduced, suggesting the electronic structure of a noble metal. The fact that the electronic structure of this surface is unlike those of the individual tungsten and platinum surfaces provides a possible explanation for the altered surface chemistry towards carbon monoxide and oxygen.

Chemical shifts observed in the tungsten core levels upon the addition of Pt indicate the elimination of surface-shifted core levels. This is consistent with a model in which the Pt remains dispersed on the surface of W(110), and does not form a Pt/W alloy. Work function measurements and UPS spectra for adsorbed CO suggest that Pt adatoms in fractional monolayer coverages do not coalesce into islands until the surface is annealed.

The structure of the Pt films on W(110) and the influence of coadsorbed oxygen on the Pt structure have been examined using LEED. Fractional monolayer coverages of Pt grow pseudomorphically in registry with W(110), and remain pseudomorphic upon annealing to > 1500 K. As indicated above, multilayers of Pt break into three dimensional clusters upon annealing; the clusters display Pt(111) surfaces oriented in one of two distinct registries with W(110), depending upon the deposition and annealing conditions. Oxygen facilitates clustering of Pt on W(110), even for fractional monolayers of Pt.

Our studies of Pt on the atomically rough W(111) are somewhat preliminary, but exhibit interesting behavior. Annealing of a Pt monolayer results in the formation of microfacets on the W surface believed to have (211) orientation. Apparently, the surface energy of Pt-covered W(211) is lower than that of Pt-covered W(111), thus driving the faceting of the W surface. The faceting is reversible, and the surface relaxes to (111) after thermal desorption of the Pt. To the best of our knowledge, this is the first report of microfaceting in a metal-on-metal overlayer system. This observation has interesting implications for the microstructure of mixed-metal supported catalysts.

We have also initiated studies of CO oxidation over Pt-covered W(110) in an attempt to identify unusual catalytic activity of monolayer thin-film catalysts.

I. Studies of Adsorption and Reaction on Metal Catalysts Using Inelastic Neutron Scattering

(R. D. Kelley and J. E. Nicol)

Inelastic Incoherent Neutron Scattering (IINS) studies of adsorbates on catalyst surfaces are providing new insights into the vibrational spectroscopy of hydrogen and hydrogen-containing species absorbed at the surfaces of high-area catalysts. Neutrons are a highly penetrating form of radiation, even in a spectral energy range (< 1200 cm^{-1}) where all the samples are optically opaque.

Although IINS activities in the Surface Science Division are now being phased out, we are still continuing a novel series of IINS experiments begun previously involving the use of an isotopically pure ^{60}Ni substrate. The idea is to use pure ^{60}Ni to reduce neutron scattering by substrate phonons to a level which will make possible studies of the vibrations of surface species which do not necessarily involve hydrogen. In effect, the low IINS cross section of ^{60}Ni will "make the bulk transparent". We plan to examine low-frequency torsional modes of surface molecules (NH_3, CH_2) and to study surface diffusion of adsorbed species. A further use of the ^{60}Ni material will include an attempt to measure adsorbate ordering with high-resolution neutron diffraction. We have a sufficient quantity of ^{60}Ni metal which is being prepared as a Raney Ni catalyst for these measurements. The catalyst is being prepared in collaboration with Dr. M. Kelley of Dupont de Nemours who has developed procedures for fabricating good quality Raney Ni. This activity has been supported in part by the Office of Basic Energy Sciences, Department of Energy.

J. Studies of Molecular Structure and Reactivity on Surfaces Using ESDIAD

(S. A. Joyce, A. L. Johnson, and T. E. Madey)

A continuing challenge in surface science is to determine the structures of molecules on surfaces, particularly in the absence of long-range order. The goal of this project is to provide a direct determination of the structures of adsorbed molecules using the electron-stimulated desorption ion angular distribution (ESDIAD) method, and to correlate the results with measurements based on other surface-sensitive techniques.

The ESDIAD method was developed at NIST and is based on electronic excitation of surface molecules by a focused electron beam (20 eV to > 1000 eV). This causes desorption of atomic and molecular ions from the surface, and is the surface analog of gas-phase dissociative ionization. The ions desorb in discrete cones of emission, in directions determined by the orientation of the bonds which are ruptured by the excitation. Thus, ion desorption angles provide direct information about surface bond angles.

During the past year, we have demonstrated the first negative-ion ESDIAD experiment with results for fluorinated molecules. We have also determined bonding structures of small halogen-containing complexes on metal surfaces. This work has been supported in part by the Office of Basic Energy Sciences, Department of Energy.

1. Negative-Ion ESDIAD

The goal of the present work is to measure the electron-stimulated desorption (ESD) angular distributions of negative ions, and to attempt to answer several fundamental questions. Does negative-ion ESDIAD contain structural information about adsorbed molecular species? How do negative-ion yields and angular distributions compare to positive-ion ESDIAD? Is the information redundant to positive-ion ESDIAD, or is there new information available?

For these first studies, we have chosen three molecules (PF_3, $(CF_3)_2$-CO, NF_3) known to yield F^- ions upon electron impact in the gas phase. Adsorption is carried out on Ru(0001), a surface for which adsorption studies of these species have been reported. The essential results of these measurements are: (a) we can detect large quantities of F^- (as well as F^+) ESD ions, (b) the F^- ESDIAD patterns are different for the three molecules, as well as for different bonding modes of each molecule, and (c) the structural information contained in the F^- ESDIAD pattern is different from and complementary to the F^+ ESDIAD results.

The major technical challenge in negative-ion ESDIAD is to separate the large secondary-electron signal from the much weaker negative-ion signal (smaller by ~10^5). This is accomplished using time-of-flight techniques. The flight paths are short, ~2 cm, and the ion angular distributions are displayed on a phosphor screen after image intensification using a double microchannel plate detector. In our ultrahigh vacuum display analyzer, the electron flight time is ~30 ns and the flight time for an F^- ion is ~800 ns. Single ion detection is achieved. The typical electron bombardment energy is 200 eV, the pulsed electron beam has a width of ~800 ns, and the repetition rate is ~10^4 per second. Data accumulation times for ESDIAD are of the order of a few seconds.

Mass-resolved ESDIAD patterns (both positive and negative ions) are obtained using a data acquisition system composed of a video camera, video recorder (with time base corrector), image processor (digitizer and computer) and graphics display. The data are processed in various ways (contour plots, intensity maps, perspective plots) and can be displayed with false color.

Figure 3.1 illustrates the F^- ESDIAD observed for a saturation coverage of PF_3 on Ru(0001). The anisotropy in F^- emission observed here, when combined with low-energy electron diffraction (LEED) and thermal desorption spectroscopy (TDS) data, led us to propose the following model for adsorbed PF_3. The PF_3 is bonded via the P atom to a single Ru substrate atom. At saturation coverage, the (3 x 3)R 30° layer causes a hindering of rotational freedom, and the PF_3 is "locked in" to azimuthal registry with the Ru(0001) substrate (see Fig. 3.2). To reduce overlap of the van der Waals radii of neighboring F atoms, the PF_3 is also believed to tilt, as indicated in Fig. 3.2.

The results to date indicate that negative-ion ESDIAD is a very useful complement to positive-ion ESDIAD. The F^- ESDIAD data for PF_3 on Ru(0001) provide insights into the adsorbate structure not available in F^+ ESDIAD data. Negative-ion ESDIAD is particularly effective for studies of surface bonding geometry in fluorine-containing molecules.

2. Determination of Bonding Structures of Small Halogen-Containing Molecules

Both positive-ion and negative-ion ESDIAD have been used in conjunction with LEED and TDS to study the bonding of PF_3, $(CF_3)_3CO$ and NF_3 to Ru(0001).

Fig. 3.1. F^- ESDIAD patterns for monolayer of PF_3 adsorbed at 110 K on Ru(0001) and annealed to 273 K. Upper left: F^- ESDIAD image as it appears on phosphor screen of ESDIAD apparatus. Upper right: Perspective plot of F^- ESDIAD, obtained using digital video image processor. Bottom: Intensity contour map of F^- ESDIAD.

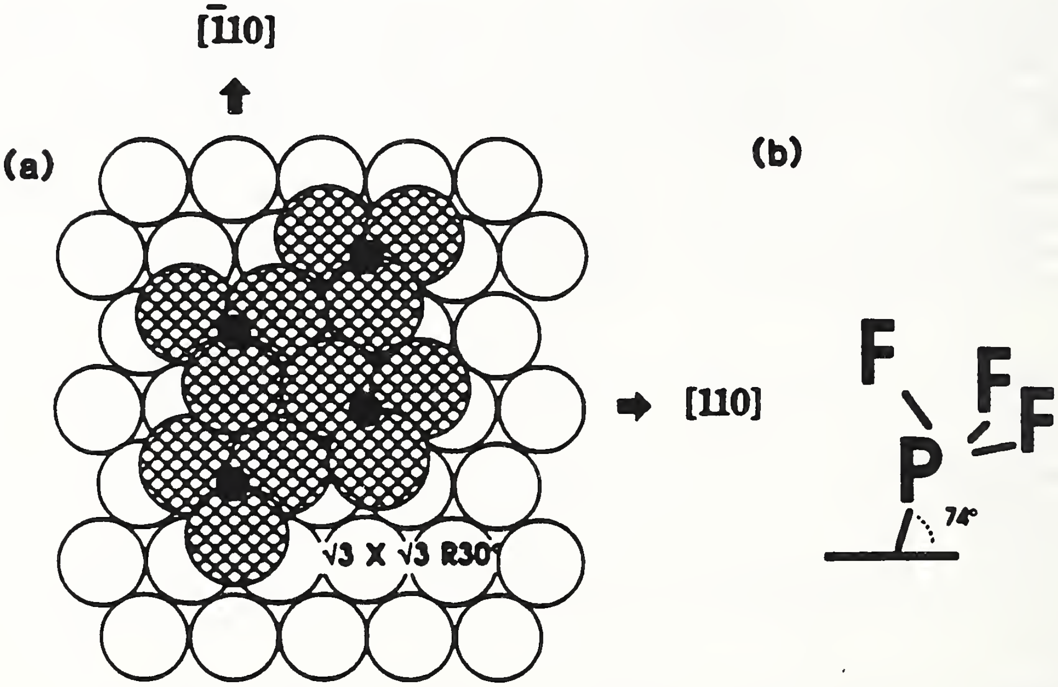

Fig. 3.2. Models of the bonding configuration of PF_3 on Ru(0001). (a) Lattice model drawn to scale, showing "interlocking" PF_3 molecules on hexagonal Ru(0001) substrate. (b) Bonding model (side view) for the proposed inclined PF_3 configuration.

For fractional monolayer coverages at 80 K, PF_3 is bonded via the P atom with the F atoms pointed away from the surface. A "halo" of F^+ emission indicated azimuthal disorder over a wide temperature range (80 to > 450 K), suggesting that the molecules are freely rotating about the Ru-P axis. As coverage increases, the "crowding" causes azimuthal ordering due to hindered rotation as indicated in Figs. 3.1 and 3.2. The adsorbed species are highly electron-beam sensitive, and PF_3 dissociates to form absorbed PF_2 and PF fragments during irradiation.

Measurements for $(CF_3)_2$ Co indicate that at least one binding state of the parent molecule is bonded in azimuthal registry with the Ru(0001) substrate. The NF_3 adsorption is predominantly dissociative, with little azimuthal ordering on planar Ru(0001).

We plan to expand the negative-ion ESDIAD to other molecules likely to produce negative-ion fragments. Suitable candidates are O- from N_2O and CO on Ru(0001) and H- from H_2O and NH_3 on Ru; all of these species yield negative ions in the gas phase. We will also initiate studies of other small halogen-containing molecules, e.g., SF_6, CF_4, C_2F_6, HF, etc. We plan to use negative-ion ESDIAD to search for molecular reorientations due to interaction between adsorbed molecules (CO, N_2O, PF_3) and impurity alkali atoms (K, Na) or impurity oxygen atoms. Finally, we will carry out studies of the surface chemistry of semiconductors; in particular, we will search for negative-ion emission for small molecules (CaF_2, PF_3, HF, H_2O) adsorbed on Si(100) and Si(111).

We plan to apply digital positive-ion ESDIAD to interesting problems involving the structure and dynamics of small molecules on metal surfaces to address question of the following type. Is CO perpendicular to the surface or "inclined" at atomic steps on Pt surfaces? Does H_2O bond to Pt(111) with the H atoms pointed toward the surface or away from the surface in the presence of adsorbed K^+? What is the bonding site of HCOO on Ag(110) and Cu(110); is the "long bridge" or the "short bridge" occupied?

K. Laser Diagnostics of Surface Dynamics
(J.D. Beckerle, S.A. Buntin, R.R. Cavanagh and L.J. Richter)

Optical spectroscopies offer several powerful advantages over other techniques when investigating molecular processes at surfaces. In particular, the spectral and temporal resolution afforded by state-of-the-art laser methods is unrivaled by any other technique.

The objective of this project is to bring modern laser-based diagnostics to bear on a variety of problems in the area of molecular dynamics at surfaces. A variety of laser based methods are used to explore divers topics including: the potential for optically driven surface reactions; the decay rates of vibrationally excited adsorbates at surfaces; and the response of surface layers to transient optical excitation. This work is conducted in close collaboration with Drs. M.P. Casassa, E.J. Heilweil, D.S. King and J.C. Stephenson of the NIST Molecular Spectroscopy Division.

1. Laser-Induced Desorption

Building on a series of experiments which had used laser-excited fluorescence to characterize the internal-state distributions of NO molecules thermally desorbed from metal surfaces, we recently began to use the same state-specific diagnostics to explore desorption induced by laser excitation of metal surfaces. This initial work was conducted on a Pt foil. Although the experiments were originally designed to utilize only the thermal heating of the surface by the incident laser, several surprising observations were made, including detection of a desorption channel whose kinetic energy exceeded the peak surface temperature by a factor of four. More remarkable, the kinetic energy in this channel increased with the rotational energy of the state, a result which suggested a desorption-laser wavelength dependence of the kinetic energy.

We have now been able to measure the laser-induced desorption of NO from Pt(111). The presence of two distinct desorption channels is confirmed, and we can now identify the slow (thermalized) channel with a weakly bound NO state ($E_a \approx 10$ kcal/mole), while the channel which displays a variety of non-equilibrium characteristics is associated with NO bound to a-top sites. These latter species desorb with non-Boltzmann rotational distributions and inverted spin-orbit populations at the three desorption wavelengths employed. The kinetic energy was characterized as a function of desorption-laser wavelength and NO state; we found a clear reduction (by 30%) at 1064 nm compared to either 532 or 355 nm. In addition, while desorbed NO in the first excited vibrational level was readily detected for 532 and 355 nm excitation, the $v = 1$ channel was effectively closed. These observations have led us to the conclusion that this desorption channel is a manifestation of NO coupling to the nascent optically excited electrons of the platinum. Inverse photoemission has identified vacant NO orbitals approximately 1-2 eV above the Fermi level, consistent with the proposed mechanism. We have further conjectured that the inverted spin orbit population may be the result of the involvement of a negative-ion resonance and its subsequent reneutralization.

In future experiments we hope to extend the wavelength range covered with the desorption pulse, reduce the duration of the desorption pulse, and investigate the importance of surface roughness and impurities on the desorption dynamics. In addition, we will extend these types of measurements to laser-induced desorption from semiconductor surfaces. A new manipulator is being fabricated which will permit a low enough temperature to be achieved to permit the study of NO adsorbed on Si(111). It will be possible to excite this system with photon energies both below and above the band gap. If desorption is driven by hot electrons in the substrate, then the wavelength dependence should be even more dramatic than that observed for platinum.

We plan to investigate the desorption dynamics of hydrogen since this represents an important prototypical system for understanding the fundamental steps in a range of surface processes, ranging from semiconductor etching, energy storage, and atom-atom recombination. We are presently developing a laser system to be used for state-specific characterization of H_2 near the LiF cut-off. Calibration and characterization of the detection efficiency is planned for the coming year.

This work is supported in part by the Department of Energy.

2. Time-Resolved Measurements of Vibrational Energy Transfer

The decay of vibrationally excited state populations at surfaces has received considerable theoretical attention, but experimental efforts in this area have been restricted to indirect measurements (lineshape measurements and collisionally induced energy transfer). Direct, time-resolved measurements of the relevant decay rates provide the central theme for this project. We have focused on the vibrational depopulation time of CO bound to metal atoms in a range of systems.

Metal carbonyls consisting of a single metal atom with six CO ligands have been measured in dilute solution. The CO ($v = 1$) lifetime is approximately 500 ps, but can range up to 1000 ps depending on solvent.

Metal carbonyls containing a single metal atom and only one carbonyl ligand are found to relax much faster than the fully carbonylated systems. The relaxation rate is found to be dependent on the vibrational modes of the other ligands bound to the metal.

Dilute solutions of metal-cluster carbonyls ($M_x(CO)_y$; $x = 2$, 4, or 6) in $CHCl_3$ have been measured to determine if the observed T_1 times show any dependence on the size of the metal cluster. While these experiments did not reveal any size dependence, several intriguing results emerged:

- Bi-exponential decays were observed for the first time. The source of these signals will require further experiments to clarify their origin, but preliminary experiments indicate that there may be rapid energy transfer between two CO stretching modes ($T_1 \approx 40$ ps) followed by a slower relaxation of the vibrational excited state ($T_1 \approx 350$ ps).

- In addition to the transient bleaching normally observed in these pump-probe experiments, conditions were found where the pump pulse leads to transient absorption. This effect has been characterized as a function of laser wavelength and power, and can be adequately accounted for in terms of contributions from CO in $v = 2$ (and higher) vibrational levels.

- The metal cluster compounds have been supported on SiO_2 and the changes in the T_1 times have been compared to the relaxation rates observed in $CHCl_3$ solutions. The T_1 times were found to be reduced by a factor of four in the presence of the SiO_2. This change in T_1 has been attributed to the participation of SiO_2 in the relaxation process. At this time, it has not been possible to identify which of several relaxation mechanisms are involved.

In an effort to probe larger metal particles, metal clusters (of ill-defined particle size and shape) have been prepared by reduction of SiO_2-supported metal salts. Transmission electron microscopy measurements indicate that mean particle diameters of about 35 Å are obtained. The infrared spectra of adsorbed CO are comparable to those in the published literature. We have observed a non-exponential decay using 2 ps infrared pulses. It is readily apparent that the CO bound to these particles have a significantly different response to vibrational excitation than any of the other supported-cluster compounds studied. Work is underway to characterize the nature of this prompt response. In addition to examining the role of laser wavelength, intensity, CO isotope, and sample preparation conditions on the observed transient, theoretical modeling is in progress to provide a measure of the nature of the low-lying electronic levels associated with metal particle of this size.

This work is supported in part by the Air Force Office of Scientific Research.

3. Single-Reflection Infrared Pump-Probe Experiment

The advantage of measuring vibrational-relaxation rates for adsorbates on well-characterized single-crystal surfaces is readily apparent. We have therefore constructed an ultra-high vacuum system in which to conduct single-reflection infrared pump-probe measurements. The system is equipped with Auger-electron spectroscopy, low-energy electron diffraction, ion-sputtering facilities, mass spectrometer, and optical ports for infrared measurements. The system is presently being used for single-reflection Fourier-transform infrared experiments in order to confirm the lineshape and line position for the samples generated in our laboratory. It is planned that this facility will be coupled to the 2 ps laser source during the coming year.

L. Theory of Dynamical Molecular Processes at Surfaces
(J. W. Gadzuk)

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

1. Chaos, Non-Linear Dynamics, and Vibrational Spectroscopy

We have initiated an in-depth study using numerical simulations and modeling of non-linear systems. In spite of progress in many other fields, the impact of the recent advances in non-linear dynamics/chaos on surface physics research has been minimal. Possible areas in the chemical physics of surfaces which could benefit from ideas out of the chaos world are being explored. Of particular emphasis are the implications of quasi-periodic versus irregular (chaotic) nuclear dynamics on: (1) vibrational spectroscopy and lineshapes of adsorbed molecules; (2) state specific vs. statistical molecular dynamics and chemical reactivity of both adsorbed molecules and molecular beams; (3) relationships between spectroscopy and scattering; and (4) iterative maps as a mathematical model for long-time surface processes.

The following specific example, drawn from our recent studies, highlights some connections between "chaology", vibrational spectroscopy, and surface dynamics. As is widely realized, many molecular systems can be characterized by a two-degrees-of-freedom model in which one degree of freedom is the subsystem of interest and the other is "everything else". With this in mind, let us suppose that vibrational spectroscopy is to be performed on an adsorbed molecule in which the potential energy function of the intra-molecular stretch vibration is a harmonically coupled to the molecule-surface bond and can be modeled in terms of a paradigm of non-linear dynamics, the Toda system and a closely related derivative, the Henon-Heiles model. The Hamiltonian for the Toda system is

$$H_{Toda} = 1/2\ (p_x^2 + P_y^2) + \frac{1}{24}\ \{\exp\ (2y + 2\sqrt{3}\ x) + \exp\ (2y - 2\sqrt{3}\ x) + \exp\ (-4y)\} - 1/8 \qquad (3.1)$$

where y is the intra-molecular stretch coordinate and x is the adsorption bond coordinate.

The potential curves implied by Eq. (3.1) and shown in Fig. 3.3(a) vary smoothly outward from the origin in both x and y, displaying a threefold symmetry. If Eq. (3.1) is expanded to cubic terms in x and y, we obtain the Henon-Heiles Hamiltonian

$$H_{HH} = 1/2(p_x^2 + p_y^2) + 1/2\ (x^2 + y^2 + 2\ x^2y - 2/3\ y^3) \qquad (3.2)$$

whose potential energy surface (PES) is shown in Fig. 3.3(b). This PES is quite similar to the Toda PES. From a dynamics point of view, these related systems are interesting because motion governed by H_{Toda} is quasi-periodic for all energies whereas complete quasi-periodic dynamics with H_{HH} occurs only for $\epsilon_{tot} < 0.1$. The onset of chaos begins at this point and increases as ϵ_{tot} is raised.

The strategy of the present study is to consider the adsorption resonance as either a Toda or a Henon-Heiles PES. Since Toda dynamics are regular whereas Henon-Heiles dynamics undergo a transition to chaos, we demonstrate the relevance (or lack of it) of chaotic behavior to surface vibrational spectroscopy and "reaction dynamics."

Using the spectral analysis technique developed by Marcus and coworkers, the vibrational lineshape associated with excitation of a mode characterized by a displacement coordinate q(t), is given by the power spectrum of q(t):

$$I(\omega) = \left(\frac{1}{2\pi}\right) \lim_{T\to\infty} \left(\frac{1}{2T}\right) <|\int_{0}^{2T} q(t)e^{i\omega t} dt|>, \qquad (3.3)$$

where q(t) is the trajectory followed by the coordinate subject to prescribed initial conditions characterizing the excitation/adsorption processes. The time evolution is obtained numerically from Hamilton's equations using either Eq. (3.1) or (3.2). Here we make an equivalence between dipole excitation of the intra-molecular stretch and initial displacement of the y coordinate (with a small non-zero x-displacement).

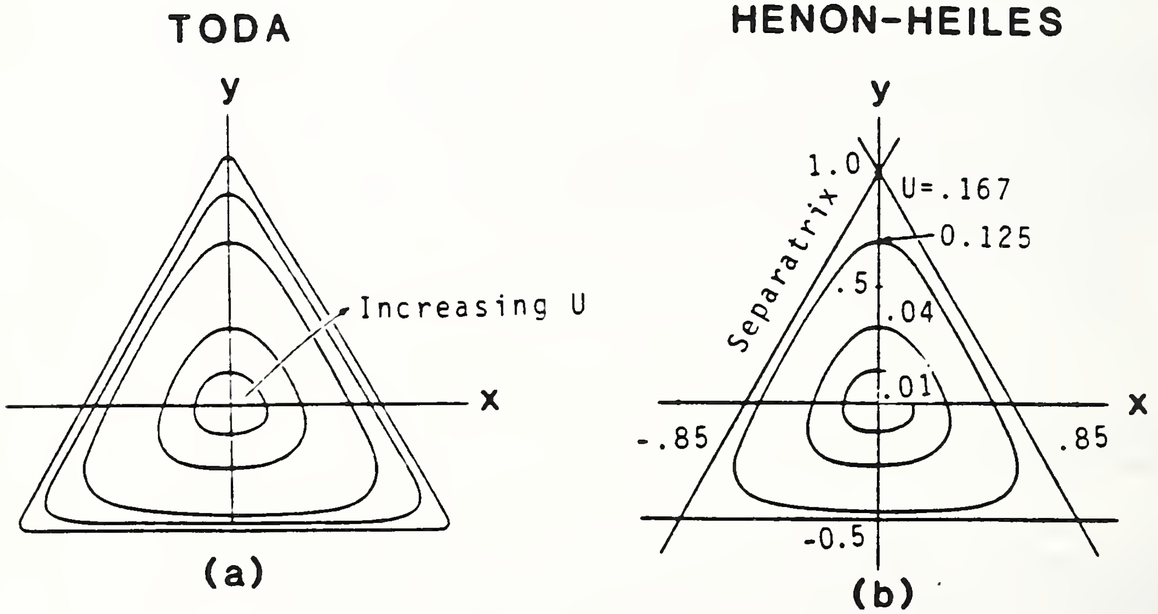

Fig. 3.3 (a) Potential well for the Toda Hamiltonian showing lines of constant potential U. (b) Potential well for the Henon-Heiles Hamiltonian showing lines of constant potential U, for closed equipotentials (U ≤ 1/6) only.

Trajectories for the Toda and Henon-Heiles potentials have been calculated and fast-Fourier transformed. The resulting lineshapes obtained from Eq. (3.3) are shown in Fig. 3.4 (a)-(d) for both potentials with the initial y displacement treated parametrically. The Toda lineshape, Fig. 3.4 (a), remains sharp for all initial conditions (and thus total energy).

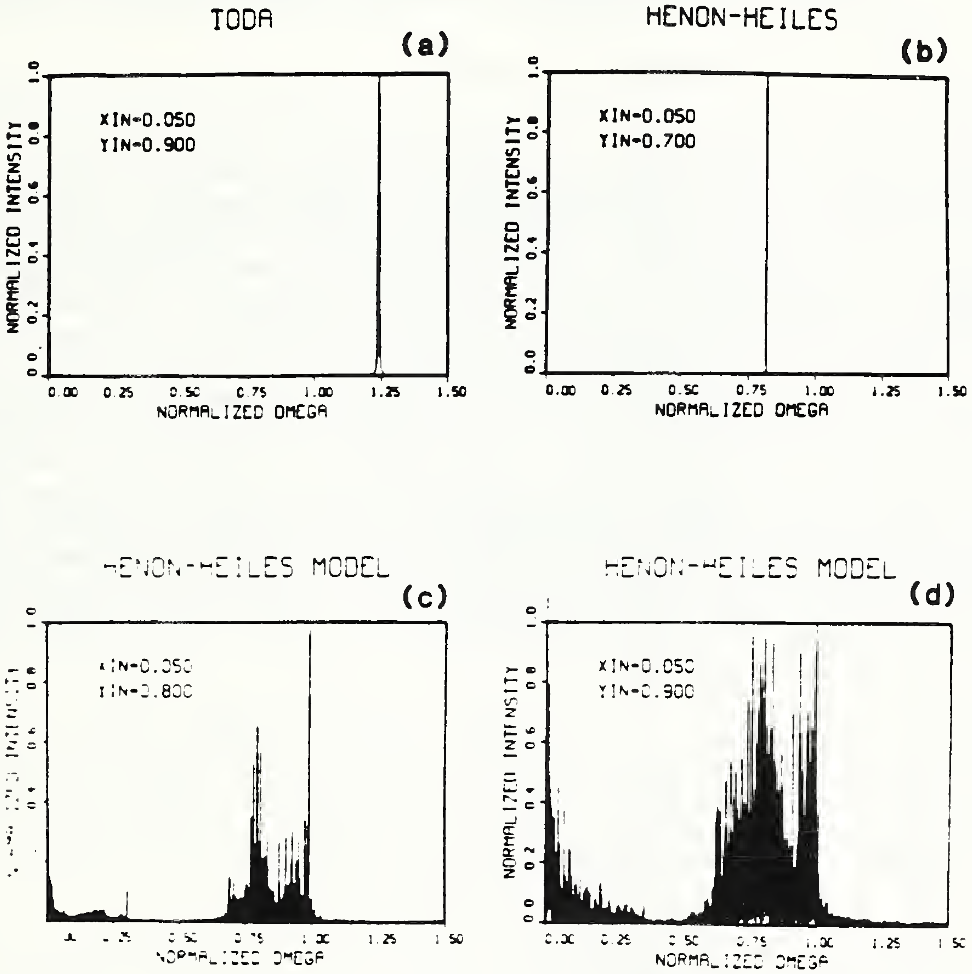

Fig. 3.4 Vibrational lineshapes for (a) Toda and (b-d) Henon-Heiles systems. The Toda lineshape (a) remains sharp for all initial displacements whereas the originally sharp (b) Henon-Heiles lineshape spreads out (c-d) for initial displacements corresponding to energies above the chaotic threshold.

This result is a characteristic of the quasi-periodic motion on the Toda PES. In contrast, the Henon-Heiles lineshape shows an evolution as the initial displacement and hence total energy increases. For small displacements in which $\epsilon_{tot} < 0.1$, the lineshape is sharp as shown in Fig. 3.4 (b).

For larger displacements in which ϵ_{tot} exceeds the chaotic threshold, the lineshape broadens and spreads throughout the spectral range, as seen in Figs. 3.4 (c) and (d). It is thus reasonable that vibrational spectroscopy exploit these characteristic signatures of quasi-periodic vs. chaotic dynamics in order to provide additional information to the scattering or reaction dynamicist on the nature of the intermediate precursor state. This is one of our ultimate goals.

2. Selectivity in Surface Dynamics

Selective control of the rate and outcome of chemical events, based on molecular-level manipulations, is a major goal in chemical physics. Laser-assisted chemistry is one area which has offered such hope. Although "surface-assisted chemistry" is certainly capable of statistically controlling rates and outcomes, it is only recently that bond selectivity has been considered within the context of surface dynamics. The physical basis for many proposed scenarios in selectivity can be summarized as follows. At some time t = 0, the molecular system is placed in an initially prepared, <u>non-stationary state</u> (say by electronic excitation) and is then allowed to time-evolve. At a later time $t = \tau_R$, the time-evolution of the initially excited state is interrupted. By choosing the time delay τ_R appropriately (depending upon system specifics), it is possible to achieve non-statistical control of the distribution of final quantum states and/or products. Amongst the different realizations of τ_R-dependent selectivity considered, currently within the context of analytically soluble models, we include: (i) the zero-energy sticking problem (ZESP); (ii) vibrational population inversions in molecule-surface scattering; and (iii) resonant electron-stimulated desorption.

Due to the relevance of the ZESP to the proposed milliKelvin trapped Na atom-surface experiments at NIST, we present here some recent advances based on the scenario stated in the above paragraph. Given an atom or molecule-surface scattering situation involving temporary non-stationary-state formation, the probability that the surrounding environment or internal degrees of freedom remain unexcited is

$$P_o\,(\tau_R) = \Big|\sum_{\tilde{m}} |\langle 0|\tilde{m}\rangle|^2 e^{-i\epsilon_{\tilde{m}}\tau_R/\hbar}\Big|^2 \qquad (3.4)$$

where $P_o(\tau_R)$ is given in terms of $|\langle 0|\tilde{m}\rangle|^2$, the "generalized Franck-Condon factors" between the ground state and $|\tilde{m}\rangle$, the ambient eigenstates associated with the temporary non-stationary state. With regards to the ZESP, the basic premise is that in the limit of a zero-kinetic-energy incident beam, any inelasticity in the molecule-target collision is sufficient to cause the molecule to stick to the target surface. Thus, within the present picture, the zero-energy sticking probability is

$$S \approx \lim_{\epsilon_p \to 0} \{1 - P_o(\tau_R(\epsilon_p))\} \qquad (3.5)$$

which demonstrates that "selectivity" in sticking can, in principle, be controlled by varying τ_R.

Within this context, the ZESP has been investigated for two analytically tractable cases. In the first case, the surrounding dissipative medium is taken to be the electron-hole pair excitations of the substrate. The exact no-loss intensity in a scattering event is then

$$P_o(\tau_R) = [1 + (\omega_c\tau_R)^2]^{-\alpha} \qquad (3.6)$$

where $\epsilon_c \equiv \hbar\omega_c$ is a cutoff energy of order the conduction bandwidth, and $\alpha \approx (\delta/\pi)^2 < 0.25$ where δ is the dominant Fermi-level electron phase shift associated with the localized potential of the incident atom or molecule. In Fig. 3.5(a), Po = 1 - S, given by Eg. (3.6), is drawn as a function of $\omega_c\tau_R$, and α is varied parametrically within a range likely to apply for real-surface scattering situations. With a not-unreasonable value of $\alpha \approx$ 0.1 for strongly interacting chemisorbed systems and ϵ_c = 10 eV, the value of τ_R for 50% elastic scattering ($P_o(\tau_R) = 0.5$) is $\tau_R \approx 2 \times 10^{-15}$ sec. For such systems, significant depletion in the no-loss line is to be expected.

The second example involves "vibrationally assisted sticking" due to the resulting intramolecular vibrational excitation in a diatomic molecule-surface collision involving charge transfer and thus temporary negative molecular-ion formation. In this case, the exact no-loss intensity has been shown to be:

$$P_o(\tau_R) = \exp[-2\beta_o(1-\cos\omega\tau_R)] \qquad (3.7)$$

where

$$\beta_o = \Delta\epsilon_r/\hbar\omega$$

and $\Delta\epsilon_r = \frac{1}{2}\kappa q_o^2$ is the relaxation energy or Franck-Condon shift associated with the harmonic potentials ($\omega = \sqrt{\kappa/\mu}$) displaced with respect to each other by q_o in the $A_2 \leftrightarrow A_2^-$ transitions. As with electron-hole pairs, the ZESP is $S = 1 - P_o$ with P_o given by Eq. (3.7).

In analogy with Fig. 3.5(a), $P_o(\tau_R)$ given by Eq. (3.7) is shown in Fig. 3.5(b) as a function of $\omega\tau_R$ taking β_o parametrically. (Note: $\beta_o \approx$ 1-3 for A_2/A_2^- displaced oscillators of C, N, O diatomics.) Unlike P_o due to the continuum of electron-hole pairs (Eq. (3.6)) which is a monotonically decreasing function of intermediate state lifetime, P_o from a localized oscillator, Eq. (3.7) is periodic. If τ_R is such that $\omega\tau_R$ is an odd (even) integral multiple of π, maximum (minimum) oscillator excitation occurs. Thus the commensurability between the oscillator frequency and the time delay between curve crossings is a crucial factor in controlled selectivity and the vibrationally assisted ZESP.

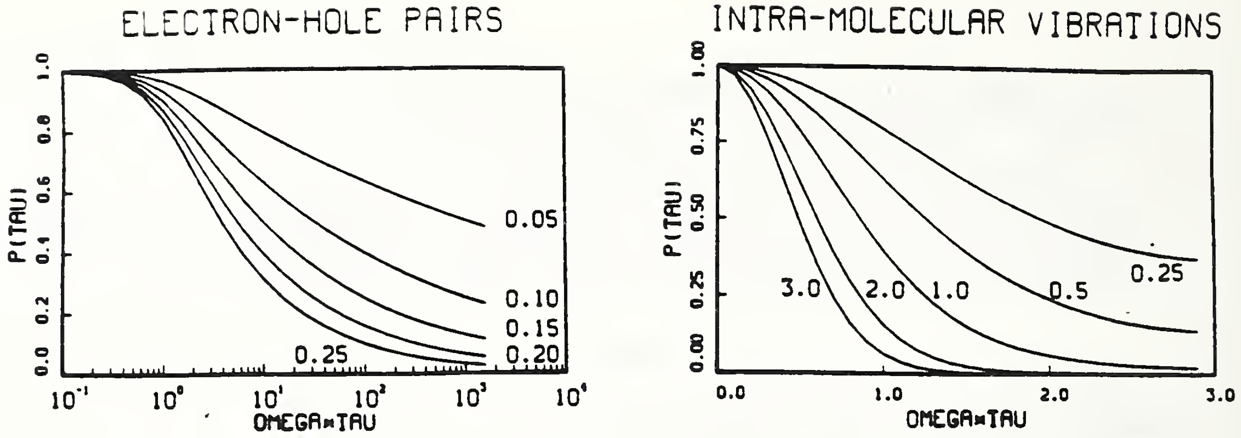

Fig. 3.5 (a) P_0 vs. $\omega_c \tau_R$, from Eq. (3.6) with α varied parametrically (left) and (b) P_0 vs. $\omega \tau_R$, from Eq. (3.7) with β_0 varied parametrically (right).

3. Semi-classical Surface Dynamics

There exists a wide range of system-independent and seemingly different molecular-level phenomena which show an aesthetically pleasing unity when considered as problems in time-dependent quantum mechanics. This belief has served as a main guiding principle in much of our work in the chemical physics of surfaces. For instance, one might ask, what do photoemission lineshapes and/or satellites, stimulated desorption energy distributions, vibrational overtone losses in electron energy-loss spectroscopy, and internal-state excitation in molecular beam scattering have in common? A new and worthwhile perspective on the physics and chemistry of such surface processes has been attained through inquiries focused on common aspects of nuclear dynamics experienced in these surface spectroscopic and molecular processes. The results have been presented in an invited review article for Annual Reviews of Physical Chemistry.

We plan to continue work in the area of surface reaction dynamics with near-term emphasis on the determination of self-consistent reaction trajectories, realistic electron-hole pair coupling constants, determination of energy-redistribution patterns amongst translational, vibrational, rotational, and electronic degrees of freedom of "reactant" molecules and electron and phonon modes of surfaces. Analyses are made for controllable dynamic and reactive conditions with synthesis of the various components of the elementary reaction theories into theories of experimentally realizable processes. Special emphasis will be placed on the phenomenon of dissociative surface processes and on the role of non-linear dynamics.

In addition, analysis will be made, whenever possible, of novel experimental results. Current interest includes laser-assisted surface processes and state-to-state analysis, high-resolution surface vibrational spectroscopy, picosecond pump-probe studies of molecular vibrational relaxation times in the presence of small metal clusters showing quantum-size effects, and other experimental probes of non-adiabatic effects.

4. SURFACE COMPETENCE PROGRAM

W. F. Egelhoff, Jr., J. Fine, S. M. Girvin, M. J. DeWeert, I. Jacob,
R. Klein, R. L. Kurtz, T. E. Madey, A. J. Melmed,
D. A. Steigerwald, P. Roncin, and R. Stockbauer

The Surface Competence Program is a part of the NIST "Competence Program." The NIST program was introduced to provide long-term support of the establishment and maintenance of areas of excellence in science and technology contributing to the NIST mission and the projected needs of the NIST clientele.

The Surface Competence Program was established in 1984 with two principal components, "Novel Two-Dimensional Materials" and "State Characterization of Energetic Species Ejected from Surfaces". The initiation of this program represents a new focus on these topics. The principal objectives of each program component are described in the following two main sections together with reports of individual projects.

A. Novel Two-Dimensional Materials

In recent years an increasing awareness has developed of the important modifications in physical properties which occur in materials as they approach the ultra-thin two-dimensional limit. Some examples of unusual behavior discovered in such systems include the enchanced catalytic properties of a gold surface with two monolayers of platinum compared to bulk platinum, superconductivity of a silver monolayer on germanium, the quantum Hall effect, the enhanced magnetism in alternating monolayers of iron and cobalt, the electrical properties of metal-semiconductor junctions (Schottky barriers), and multiple quantum-well systems for optical logic devices. These examples suggest a whole new range of scientifically and technically important chemical and physical properties waiting to be explored in the two-dimensional regime. Concepts and methods developed in surface and interface science have been particularly valuable in many areas of application, and it is believed that these concepts and methods can be further developed and extended to two-dimensional systems with component thicknesses from one to one hundred atomic layers.

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

We are performing work in two main project areas. First, we are planning to develop the techniques needed to synthesize, by alternating monolayer deposition, a new class of materials: non-equilibrium ordered alloys. The structural properties of these materials as grown and during thermal processing will be investigated by x-ray and electron diffraction. The chemical reactivity, catalytic activities, and magnetic properties of these materials will also be investigated. Second, we plan to determine the microstructure and microcomposition of candidate layered structures by atom-probe and field-ion microscopy methods with emphasis on the interface region. These techniques provide composition and structure data with near-atomic spatial resolutin. An emphasis in this area during the past year has been an investigtion of the new high-temperature superconducting materials. In a third area, now concluded, we have investigated theoretically the properties of two types of novel thin-film materials.

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

(W. F. Egelhoff, Jr., D. A. Steigerwald, K. Ong, and I. Jacob)

There are a number of techniques for determining the atomic structures of ordered and disordered surfaces, each having distinct advantages and limitations. During the past few years, we have been developing another structural technique, termed the "searchlight effect," which can be conveniently used in conjunction with two common techniques for measurement of surface composition, x-ray photoelectron spectroscopy (XPS) and Auger-electron spectroscopy (AES). It has been found in prior NIST work that XPS and AES intensities are strongly enhanced along nearest-neighbor and next-nearest-neighbor axes of a crystal. The angle-resolved spectra thus provide intensity peaks that point out what are in effect the "bond directions" in the near-surface region. The searchlight effect is a powerful probe of short-range order in the top few monolayers of a crystalline surface.

We have been continuing to develop additional understanding of the important diffraction mechanisms that give rise to the searchlight effect. In addition, we have been exploiting the technique for surface structural analysis.

We have made progress in investigations of the diffraction processes through semiclassical calculations of diffracted intensities. Semiclassical results are especially instructive for visualizing the single and multiple scattering processes involved in diffraction and can provide insights often missing in the obscurities of partial-wave expansion (full quantum) treatments. This work has led to an improved understanding of how the first few scattering events tend to form the enhanced intensity of the searchlight effect and subsequent scattering events defocus the searchlight beams so that the technique is useful as a probe of near-surface short-range order. The searchlight effect has been demonstrated to give direct insights into the thin-film microsctructure that would be difficult to obtain by other techniques.

Figures 4.1 and 4.2 show examples of experiments in which the calculations have assisted interpretations of the results. The data of Fig. 4.1 are angular profiles of the Ni CVV Auger peak from a Ni(100) specimen covered with 12 monolayers (ML) of cobalt. The cobalt film is thick enough to defocus the searchlight beams from the underlying nickel crystal. On heating the structure, however, the nickel intensity increases and the angular profiles show structure which indicate that Ni atoms are diffusing through the cobalt film and forming a random alloy. At temperatures above 900 K, the Ni atoms occupy the top 2 or 3 ML of the surface and the searchlight beams are well developed.

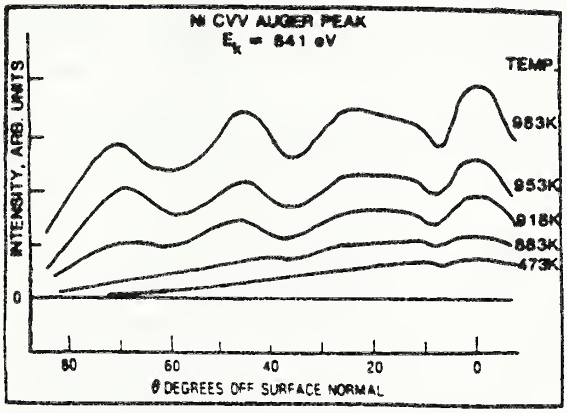

Fig. 4.1. The angular dependence of the Ni CVV Auger peak for increasing annealing temperatures for a 12 ML epitaxial film of Co on Ni(100).

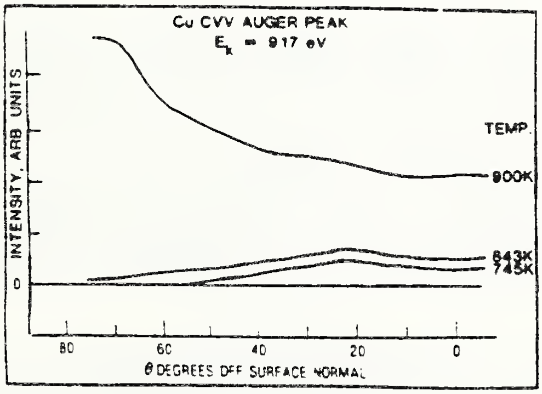

Fig. 4.2 The angular dependence of the Cu CVV Auger peak for increasing annealing temoeratures for an epitaxial sandwich structure of 17 ML Ni on 3 ML Cu on Ni(100).

Figure 4.2 shows similar data for another thin-film structure. Angular profiles are plotted for the Cu CVV Auger peak ansing from a 3 ML Cu layer on Ni(100) which has been covered by 17 ML layer of Ni to form an epitaxial sandwich. No searchlight beams are observed on heating the sandwich and it can be concluded that no near-surface alloy is formed. Instead, 1 ML of Cu segregates to the surface (a second monolayer is required to produce a searchlight beam) and the remaining Cu diffuses deeper into the Ni. A random alloy does not form upon heating in this case even when it is expected.

The searchlight effect has been applied to a variety of other surface structural problems. We have made a study of the short-range order (i.e., bonding site) around a submonolayer coverage of Ni atoms that have thermally diffused into a GaAs(110) surface to pin the Schottky barrier. We have observed and analyzed some unusual crystal structures that occur in epitaxial growth of Au film and Au-Ag sandwich structures on Ni(100). The searchlight effect has also played a key role in a major new activity begun during the past two years, the study of magnetic elements in novel crystal structures produced by epitaxy; this work is described in the following section.

We plan to continue ways of improving the power of the searchlight effect further. A new XPS system has been designed that will enable more complete and efficient measurements of the searchlight effect and other diffraction phenomena than are possible with the present eighteen-year-old XPS instrument. The new system will have a gonimometer-mounted analyzer that will be used to measure the angular distributions of photoelectrons, Auger electrons, and scattered ions. This facility will be used to characterize the structural, magnetic, and electronic properites of a variety of thin-film materials.

2. Magnetic Thin Films, Sandwiches, and Superlattices

(W. F. Egelhoff, Jr., D. A. Steigerwald, and I. Jacob)

Surface magnetism and the magnetism of ultrathin films is an area of surface science that has experienced very rapid growth in the past 3 to 5 years. This growth is motivated, in part, by the recognition that, in the near future, the advanced thin-film media used for magnetic recording will need to be of smaller dimensions then at present. Such thin films can be usefully studied by the powerful techniques of surface science. The importance of such studies is due to the size and economic significance of the magnetic recording industry and to the fact that magnetic properties are notoriously structure sensitive.

During the past two years, we have initiated a project in which the XPS searchlight effect (described in the previous section) is used as a surface-structural diagnostic of different thin-film structures we have fabricated. Specifically, we use the searchlight effect to learn how to grow magnetic thin films with improved structural integrity and in novel or unusual crystal structures. We also use other techniques such as reflection high-energy electron diffraction (RHEED), low-energy electron diffraction (LEED), XPS intensities, and XPS core-level shifts. Rapid progress has been made with this array of techniques.

The first magnetic thin-film system we have investigated consisted of Fe layers on Cu(100). The literature on this system is both voluminous and awash with controversy, with no careful structural studies having been conducted. We found that contrary to the universal assumption that Fe grows in a layer-by-layer mode, in fact such a mode is extremely difficult to achieve. Segregation of Cu and agglomeration of Fe are pronounced effects under the conditions of growth used in earlier work. Clearly, structural imperfections of diverse sorts were a major factor in the controversy.

In our work, we have developed growth methods, based on low-temperature epitaxy and subsequent gentle annealing, that produce Fe films of high quality. We have then fabricated sandwich and superlattice structures by growing Cu epitaxially on the Fe.

A typical superlattice structure is illustrated in Fig. 4.3. We have found that the Fe films grow in the face-centered cubic structure on Cu(100) rather than with the body-centered-cubic structure of bulk Fe. The superlattice structure of Fig. 4.3 consists of a set of 3 ML thick single crystals of fcc-Fe sandwiched between Cu(100) surfaces. With such a novel crystal structure, it was thought that novel magnetic properties might occur.

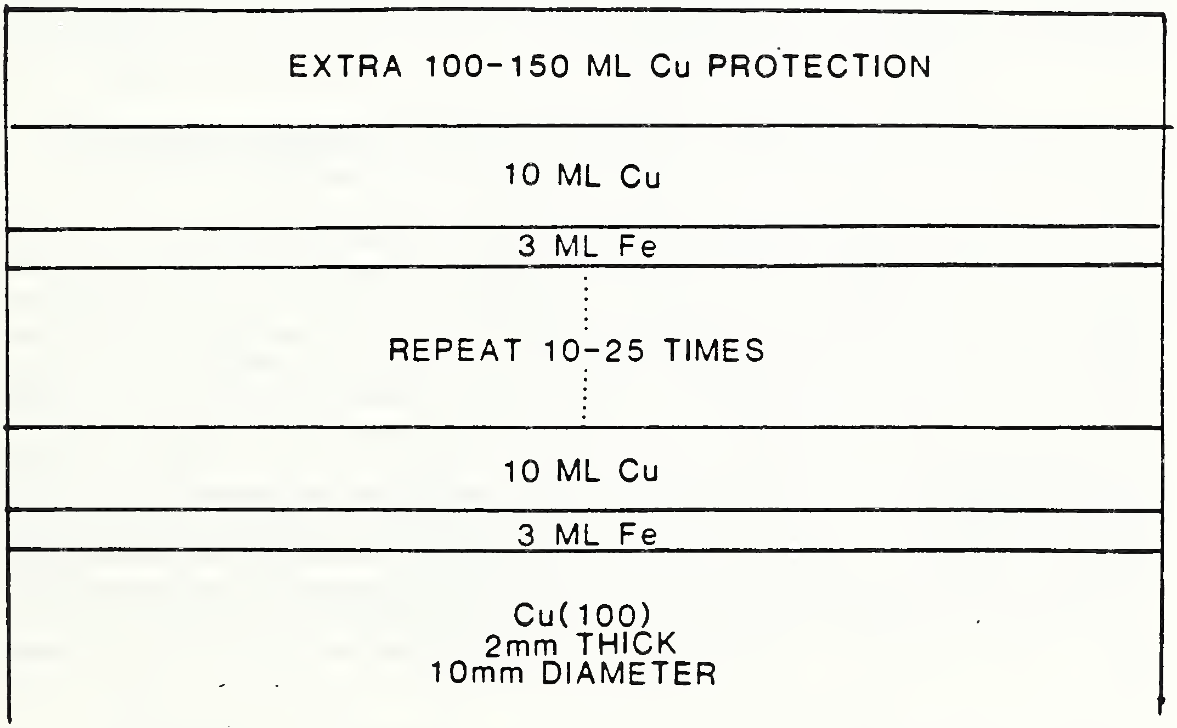

Fig. 4.3 A typical superlattice structure consisting of Cu and face-centered-cubic Fe.

In collaboration with Prof. B. Heinrich's group at Simon Fraser University in Canada, we have made Brillouin light scattering measurements and ferromagnetic resonance measurements on several sandwich and superlattice structures. We have found that our careful preparation of the Fe films has produced a major improvement in the magnetic properties of fcc-Fe films as compared to earlier work. Our films are ferromagnetic at room temperature and exhibit a strong perpendicular anisotropy holding the magnetic moment normal to the film. This anisotropy is uncommon, valuable, and a much-sought-after property for high-density magnetic recording. We have found that Fe film thicknesses of 3 ML produce the best magnetic properties.

Other groups have expressed an interest in collaborations to measure the properties of the novel and exotic crystal structures we are presently synthesizing. The group of Dr. R. F. Willis at Cambridge University in England is presently using neutron spin-flip methods to measure the absolute magnetic moment for several of our samples. We also expect to provide samples to groups at the Naval Research Laboratory (Dr. B. Jonker) and the University of Arizona (Dr. J. Dutcher) who will make measurements of other magnetic properties.

We plan to synthesize other novel or exotic crystal structures with other magnetic elements such as Co, Ni, Mn, and Cr on other non-magnetic substrates such as Ag, Au, and Pt. We believe that such structures hold considerable scientific promise and are an important source of new materials for technological applications.

3. Field-Ion Microscopy of High-Temperature Superconducting Materials

(A. J. Melmed, H. B. Elswijk, and P. P. Camus)

A major activity during the past year has been an effort to use the special analytic capabilities of field-ion microscopy (FIM) and atom-probe (AP) mass analysis to obtain information towards the understanding of the atomic structure and physical properties of the new high-transition-temperature (T_c) superconducting oxides, a subject of intense worldwide interest. These superconductors are mostly produced in the form of ceramic wafers from compacted and heated powders, occasionally as small single crystals and most recently as thin films. They have, in general, a complex microstructure and most types are easily damaged by exposure to humidity in the environment or to many liquids. The mechanism of superconductivity is not known, and there are outstanding questions concerning the relationship between atomic structure and composition, microstructure, electronic structure, and superconductivity. The roles of grain-boundaries, twin planes, other defects, and composition variations are especially interesting.

The techniques of FIM and AP applied to metals, alloys and semiconductors provide real-space determinations of surface structure and qualitative bulk atomic structure, complementary to 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. Additionally, measurements of field-ion and field-electron energy distributions and electron work function provide probes of near-surface electronic structure. However, materials as complex as the high-T_c superconducting oxides have not in the past been studied by these techniques; new experimental methods were needed to enable such studies.

We have developed a new method of specimen preparation for FIM-AP and field electron emission microscopy (FEEM) of superconducting oxides. This method has proven to be applicable to other oxides, compound semiconductors, and probably a host of other non-ductile conducting materials, as well as to all of the presently known types of superconducting oxides. A small amount of material, typically about 10 cubic millimeters, is broken into fragments from which sharply pointed pieces are selected and attached to ends of tapered metal wires using an electrically conducting epoxy. The advantages of this technique compared to conventional methods of specimen preparation are: (1) no chemical or electrochemical artifacts occur, which is especially important for grain-boundary composition studies, (2) no weakening due to ion milling damage occurs, and (3) it is very rapid and conservative of sample material. We were initially concerned about the possibility of introducitng mechanical damage by the fracture process. However, transmission electron microscopy (TEM) results show that this does not occur. Also, if small-scale damage occurred on the fracture surface, we would normally remove such damage by field evaporation which allows probing through a depth of 1000 nm or more. This new method of specimen preparation heralds the application of FIM and associated measurements to a wide range of materials hitherto not amenable to such studies.

We have been able routinely to obtain FIM images of the other La-Sr-Cu-O type superconducting oxide, the R-Ba-Cu-O so-called "1,2,3" oxides (with R=Y, Yb, Sm, Gd, Dy, Ho, Er, Pr, Eu or La), and the newer Bi-Sr-Ca-Cu-O and Tl-Ba-Ca-Cu-O types. We have, however, mostly studied the "1,2,3" superconductors because the La-Sr-Cu-O type has proven to be too sensitive to degradation by laboratory humidity, and samples of the newer types have only recently become available. The work has progressed in collaboration with the following NIST scientists: Dr. C. K. Chiang of the Cermaics Division who prepares samples and measures resistivity; Dr. R. D. Shull of the Metallurgy Division who characterizes the samples by ac magnetic susceptibility; and Dr. H. A. Fowler of the Mathematical Analysis Division who provides computer-generated FIM images based on particular models. We also have two external collaborations: (1) Dr. M. K. Miller of the Oak Ridge National Labortory who is searching for defects and grain boundaries and determining microcomposition by AP; and (2) Dr. N. Ernst at the Fritz Haber Institute in Berlin who is measuring electron work functions and field-ion and field-electron energy distributions.

Our survey of the "1,2,3" superconductors has shown that a range of FIM image features occurs and that significant changes occur over a storage period of 8-10 months. Relatively fresh specimens made from wafers which had been shown by ac magnetic susceptibility meaurements to have sharp superconducting transitions at about 90 K and which had been stored in dry atmospheres for a few weeks or less yielded specimens whose FIM images had a totally unexpected character. The images consisted mostly of orderly parallel rows of brightly imaging atoms and molecules. These rows clearly are the intersections with the surface of parallel layers. This result was established from experiments in which several surface layers were field evaporated and photographically integrating the changing FIM image. As seen in Fig. 4.4, the image superposition results in approximately parallel bright stripes. These layers are perpendicular to the orthorhombic c-axis, demonstrated by TEM, and are spaced about 1.2 nm apart, measured from the FIM micrographs. The stripes are due to a very orderly and relatively rapid field evaporation of the atoms between the stripes. We are presently pursuing the identification of the atoms between the stripes, using an AP technique which selectively images a pre-chosen atomic species. The unusual, very orderly field evaporation suggests some special property of the layers, possibly enhanced electrical conductivity compared to the inter-layer material.

In addition to the striped images, we found some specimens whose images were mostly disordered and some with intermediate type images; that is partially ordered. Samples that were several months old yielded significantly fewer specimens which gave striped or partly striped images. The gradation of FIM images from striped through various decreasing amounts of striping can possibly be understood as the result of decreasing order of some elements in the oxide that would effect the field evaporation process. The most obvious correlation is with the known continuous variations in the stoichiometry and ordering of oxygen and oxygen vacancies in the Cu-O end-planes of the orthorhombic unit cell. Interestingly, a sample of Y-Ba-Cu-O which had been heated in nitrogen to remove some oxygen and which was shown by x-ray diffraction to be tetragonal, gave specimens which had mostly disordered FIM images. Some specimens, however, had images that were partly striped. These results indicate that the well-ordered tetragonal phase of Y-Ba-Cu-O also manifests some degree of ordered preferential field evaporation. It is difficult to produce bulk wafer samples with uniform oxygen doping. If we could, this would remove some of the variations in image types which we have observed. We hope to obtain improved material in order to better understand the FIM images.

We found no first-order effect in the FIM images going through the superconducing transition temperature, although there may be a second-order effect. This result is reasonable since the material is a layered electrinical conductor above T_c.

An exciting prospect arises from the fact that the striping of the FIM images provides a well-ordered atomic pattern, interruptions of which are easily detected. Thus, we have identified, with the help of TEM, the commonly occurring twin boundaries of the orthorhombic phase, grain-boundaries and other defects as well as various small inclusions of different material. We are beginning to apply our AP to the compositional analysis of local regions in and near such irregularities which may obstruct the transport of electrical current.

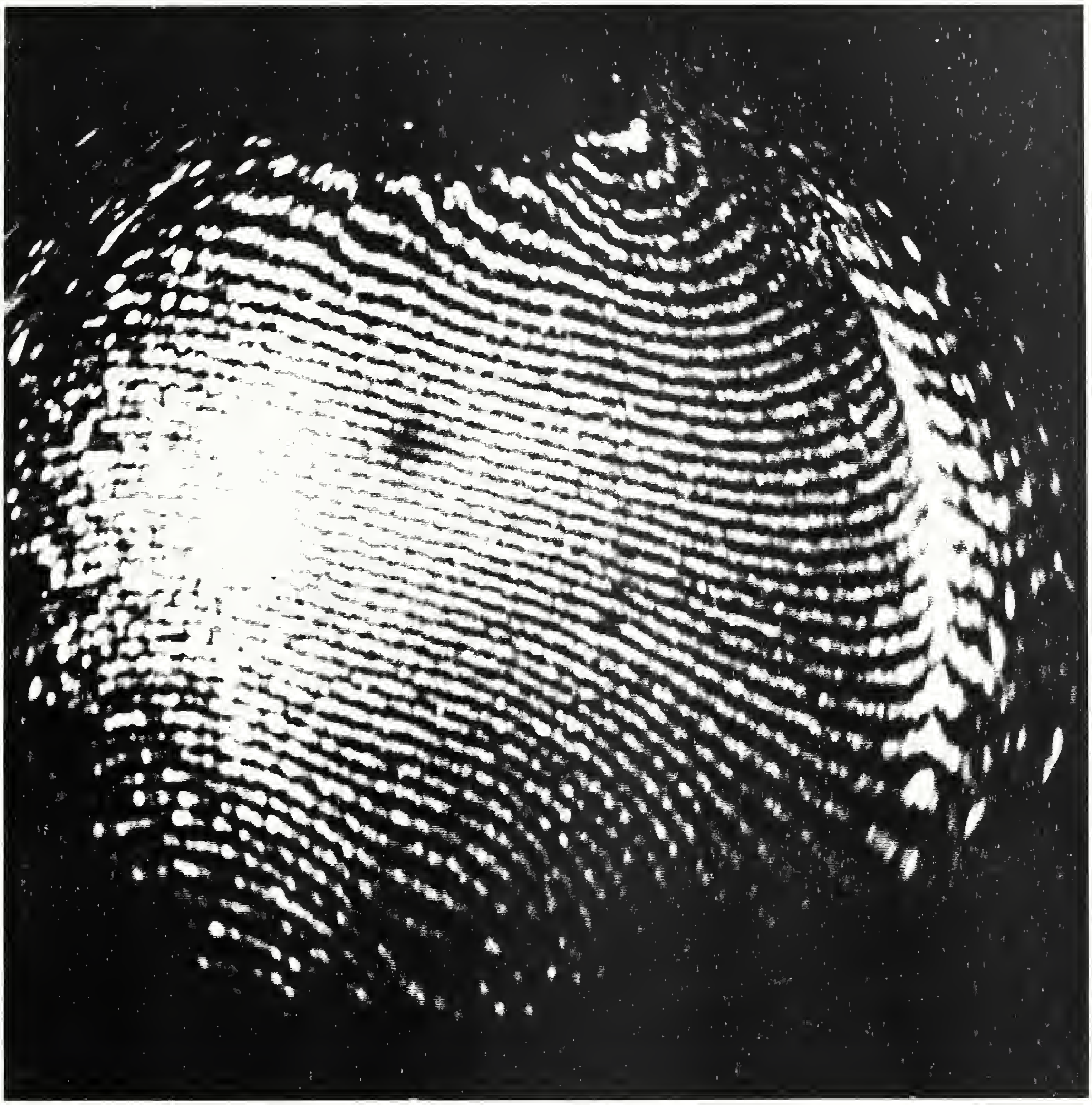

Fig. 4.4 Field-ion micrograph of the superconductor $YBa_2Cu_3O_{7-x}$ at 30 K. The orthorhomic c-axis is vertical. The separation of the layers (bright stripes) is about 1.2 nm. A twin boundary is seen on the right side as a vertical bright arc.

The problems of making good and durable electrical contacts and of applying protection overlayers for long-term storage of the superconducitng oxides are technologically important. Both problem areas involve questions of atomic diffusion between superconductors and adlayers. Therefore, we are beginning to study interdiffusion processes using our AP. We have done an experiment to learn how well our instrument could define a sharp interface. Copper was vapor-deposited onto an atomically smoothed and then air-exposed rhodium surface. Then, a composition depth-probe was made, going through the Cu and into the stepped surface adjacent to a Rh(111) plane. The results, shown in Fig. 4.5, shows two features of interst. First, the Cu/Rh(111) interface is defined within about a monolayer and second, the oxygen originally present on the Rh surface diffused several atomic layers into the Cu film. We intend to use several metals such as Ag, Rh and Al for overlayers on both clean and air-contaminated superconductors. An important advanatage of the AP compared to other composition probes for this type of study is its essentially single-atom sensitivity. This will allow us to investigate the important temperature regime between room temperature and, say, 100°C which is important in practical devices.

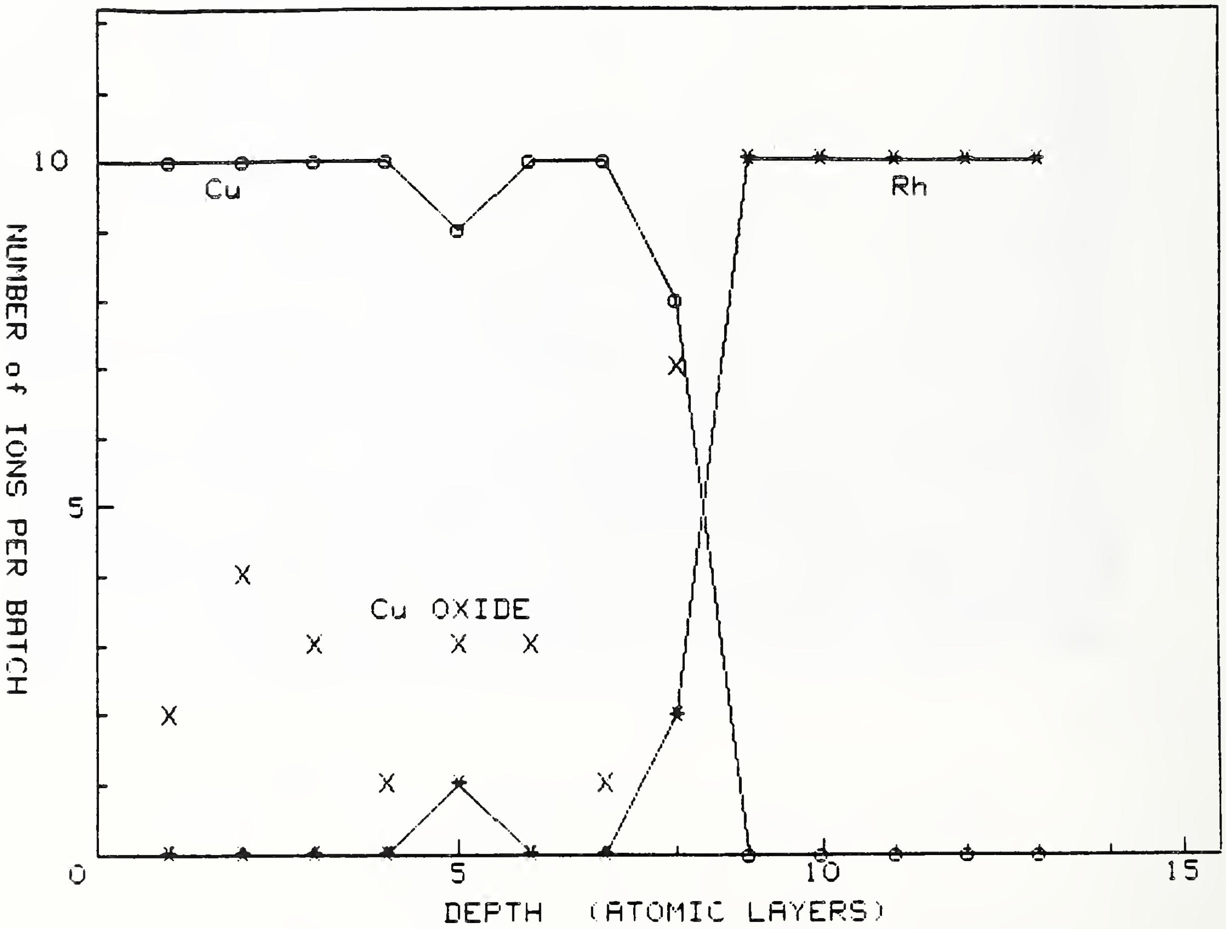

Fig. 4.5 An atom-probe depth profile for an air-exposed copper film on a Rh(111) surface showing the compositional variation of Cu(o), copper oxides (x), and rhodium (*) as a function of depth.

4. Microcomposition and Microstructure of Thin Films

(A. J. Melmed)

The nucleation and epitaxial growth of Cr crystalline overlayers were studied by vapor depositing chromium onto thermally annealed W field electron emitters. This procedure provided highly stepped substrates with low-index facets of various atomic configurations. Temperature and substrate morphology effects were identified and Cr/W epitaxial relationships were determined. In addition to the common Stranski-Krastanov (SK) nucleation mechanism (nucleation on top of a Cr overlayer) observed generally above ~ 500 K, low-temperature Cr nucleation and growth (~ 300 K) was observed on the W{110} planes. This process proceeded via either the SK or Volmer-Weber (VW) (nucleation directly on the substrate) mechanisms, depending upon the Cr deposition geometry.

Similar studies of Cr overlayer nucleation and crystal growth on Re substrates revealed that only bcc Cr (the normal structure) polycrystalline layers formed, in contrast to an earlier study of Eu/Re where both bcc and fcc structures occurred, depending on substrate crystallography. The difficulty of growing single crystals was attributed to the multiplicity of similar nucleation sites on the curved hcp substrate.

Our field-ion microscopy (FIM) studies of the Al/Mn icosahedral i-phase have agreed with transmission electron microscopy (TEM) determinations of long-range icosahedral symmetry. However, a consistent feature of the i-phase seen by FIM was short-range disorder, and this had not been reported in TEM results. In a collaboration with Dr. M. J. Kaufman, formerly of the NIST Metallurgy Division, we have conducted a careful TEM study to search for hitherto possibly overlooked evidence for structural disorder. Selected-area diffraction patterns from "off-axis" orientations showed not only sharp intensity maxima, but also a diffuse ring; overexposed diffraction patterns from axial orientations also showed the weak diffuse ring. These results were interpreted as evidence for structural disorder in the i-phase and support icosahedral cluster models with intercluster disorder. Our studies of the i-phase have been de-emphasized in favor of atom-probe FIM measurements of atomic interdiffusion across interfaces in metal/metal, metal-semiconductor, and metal/superconductor systems.

5. Theory of Novel Two-Dimensional Materials

(S. M. Girvin and M. J. DeWeert)

In this project, now concluded, we have investigated theoretically two problems concerning thin-film systems, the fractional quantum Hall effect and tunneling through a metal-insulator-metal junction.

In a collaboration with Dr. A. H. MacDonald, formerly with the Canadian National Research Council, we have investigated several aspects of the fractional quantum Hall effect (FQHE) and have demonstrated the existence of a peculiar type of off-diagonal long-range order (ODLRO) which gives rise to the FQHE.

In a superfluid, ODLRO is associated with Bose condensation. In the presence of a condensate, however, there is a non-zero amplitude that can destroy a particle in the condensate and create one far away. For the FQHE, one can show that normally the density matrix is short-ranged and hence fails to exhibit ODLRO. This result occurs for two reasons, electrons are not bosons and so cannot Bose condense and even if they could, the magnetic field would destroy the long-range phase coherence. We have found nevertheless that there is a peculiar type of ODLRO hidden in this system. If one makes a singular gauge transformation which attaches a solenoid containing m flux quanta of a fake gauge field to each particle, two useful things occur. The statistics of the particles change from fermion to boson and the effect of the external magnetic field is eliminated. To see why the statistics change, consider exchanging two of the composite objects. In addition to the usual (-1) for fermions one obtains a Bohm-Aharanov phase factor from the charge of one particle seeing the flux tube on the other. This yields another factor of $(-1)^m$ which (m is odd) cancels the fermion sign leaving a (+1) as one would have for bosons. The singular-gauge density matrix exhibits ODLRO which we have been able to compute explicitly for the case of Laughlin's variational wave function. Thus the FQHE represents a condensation, not of ordinary particles, but of composite objects consisting of a particle and a gauge flux tube. It should be emphasized that this is not a tube of physical flux but rather a fake, non-dynamical gauge field.

This result extends the already deep analogies we have previously found between the FQHE and superconductivity and superfluidity. Both systems have dissipationless transport because of a remarkably low density of excited states at low energies. The collective mode is phonon-like at long wavelengths and exhibits a 'roton' minimum at intermediate wave lengths. Both types of systems exhibit quantized vortices. The vortices in a superconducting film carry quantized magnetic flux. In the FQHE, they carry quantized (fractional) charge. We have shown that one can develop a Landau-Ginsburg theory for the FQHE which is of the 'θ-vacuum' form of current interest in high-energy physics. This means essentially that charge and flux are mixed up in such a way that the natural objects in the theory carry both charge and flux.

The theory of the FQHE is now in excellent shape. Using Laughlin's wave function and the superfluidity analogy we have quantitatively accurate predictions for the collective mode dispersion, static susceptibility and related quantities which are amenable to experimental test.

In our second project, we have investigated the problem of what happens in a metal-insulator-metal tunnel junction when the insulator is ferromagnetic. The exchange field causes a spin asymmetry in the barrier height which allows only one spin to have a significant probability for tunneling. For example, typical parameters for a EuS barrier allow approximately 85% polarization of the tunnel current. The particular questions we have studied are: How large is the polarization that can be induced in the tunnel electrodes by this effect and what happens if the electrodes are superconducting? The steady-state polarization which builds up results from a competition between the tunneling time and the spin-flip relaxation time in the electrodes. For reasonable choices of parameters, it is possible to achieve polarizations equivalent to those which could be obtained in equilibrium only by application of magnetic fields of several Tesla (fields much larger than those in the barrier for example). This polarization can affect the tunnel characteristics of the junction and can mimic the effect of field leaking out of the insulator into the electrodes.

A particularly interesting special case is that of superconducting electrodes. A polarizing barrier eliminates the possibility of Josephson tunneling for two reasons. First, only one spin member of the Cooper pair can tunnel easily. Second, the vector potential due to the ferromagnetic insulator destroys the phase coherence across the junction. This means that the tunnel characteristics are radically altered since only tunneling in the quasiparticle branch can be seen. It is then pertinent to ask how this injection of spin-polarized quasiparticles affects the superconductivity. This is a difficult non-equilibrium problem which we have chosen to attack in the following way. We assume a pseudo-equilibrium situation and seek that state which minimizes the free energy subject to the constraint that there is a given net spin polarization (so that not all electrons can be paired). This is handled by assuming a 'dead zone' in k-space in which the pair potential vanishes and the electrons are 100% polarized. The resulting modified BCS gap equation is then solved self-consistently. It turns out as expected that spin polarization weakens the superconductivity. If the polarization increases to the point that the width ν of the dead zone reaches

$$\nu = \Delta_0/2$$

where Δ_0 is the bare gap value, the superconductivity collapses and a normal Pauli spin-polarized state results. This leads to the prediction of a critical current in the tunnel junction above which superconductivity is destroyed. For lesser currents it may be possible to see the gap reduction optically (in the infrared absorption) although this may be a difficult experiment. It turns out that the dead zone produces a rather novel particle distribution which should also be detectable by spin resonance and related experiments.

B. State Characterization of Energetic Species Ejected from Surfaces

Specific state characterization of desorbed and ejected species from surfaces, whether induced by sputtering or by electron and photon bombardment, is still rare. It is now possible to address such dynamical surface interactions using laser techniques to determine the energy state, velocity, and angular distributions of <u>all</u> the ejected species--especially the neutrals which are the most abundant. Such studies can provide detailed microscopic information concerning energy transfer in these excitation-interaction processes.

The objective in this component of the program is to understand the excitation dynamics by which atoms and molecules are desorbed from surfaces in ion-sputtering processes as well as in electron- and photon-stimulated processes. Detailed characterization of the internal energy, kinetic energy, and desorption thresholds of desorbed species will provide a microscopic understanding of the nature of the electronic excitations leading to desorption due to collisions with electrons, photons, and ions. Angular distributions will provide direct structural information concerning the surface geometry, as well as information concerning energy transfer during the collisional interaction.

We are performing work in two project areas. First, we are conducting an experiment in which laser-spectroscopic techniques will be used to determine the energy states of neutral atoms and molecules sputtered from surfaces by ion bombardment. Second, we are constructing a new type of display analyzer to measure angular and energy distributions of charged species desorbed from surfaces by electrons or photons to obtain surface-geometry information and to test theories of ejection mechanisms. Close contact is made with the related experimental and theoretical projects in the Division described in sections 3.A, 3.B, 3.J, 3.K, and 3.L.

1. Energy States of Neutral Species Sputtered from Surfaces

(J. Fine, P. Roncin, R. Klein, M. H. Mintz, and M. H. Shapiro)

Energetic ion-surface collisions generate extensive near-surface collision cascades in a solid. The energy transfer and atomic excitations that take place as a result of such collisions are not well understood in part because, until rather recently, the primary method for monitoring these collision phenomena was to measure macroscopic effects such as the total sputtering yield. The collision cascade causes the ejection of atoms, ions, electrons, and photons from the surface but it has only been in the past few years that measurements of the ejected particles or radiation have been utilized to obtain detailed information on specific atomic collisions that take place in condensed materials.

In recent experiments in which aluminum or silicon targets were bombarded by argon ions, we have shown that the Auger decay of collisionally excited Al or Si atoms can take place outside the solid depending on the distance from the surface (within the material) at which the excitation occurred, the atom's velocity, and the lifetime of the atomic excitation. As a result of our Monte-Carlo calculation to analyze these experiments, we expect that such sputtered atoms will have rather high kinetic energies - extending up to hundreds of electron volts. Collisions capable of transferring this much energy and creating inner-shell (2p) excitation can generate sputtered atoms (ions) which are in highly excited states. Such energy-transfer and excitation mechanisms are basic to our enhanced understanding of collisional processes in condensed materials. Information is required of those atomic processes which lead to electron promotion, excitation and ionization, and particle ejection. It is now possible to obtain this type of information by: (1) probing specific ejected (sputtered) atoms via resonant, multiphoton laser techniques; (2) monitoring the Auger-electron de-excitation of ejected atoms as well as those which decay inside the solid; and (3) computer calculations of the ion-solid collision cascade. Progress in each of these areas is described below.

(a) Laser Spectroscopy of Sputtered Atoms and Ions

(J. Fine, P. Roncin, R. Klein, and M. H. Mintz)

In collaboration with Dr. J. D. Fassett of the NIST Inorganic Analytical Research Division, a new series of experiments has been designed to determine the kinetic energy distributions of specific sputtered atoms (ions) and their states of excitations. Measurements have been planned of: (1) the kinetic energy distributions of all the sputtered ions as a function of charge state, (2) the kinetic energy distributions of emitted electrons, (3) the collisional excitation of Rydberg states, (4) excited-state decay by photon emission, and (5) the kinetic energy distributions of sputtered atoms in specific excited states. Resonance multiphoton laser-ionization schemes have been developed to detect sputtered atoms in specific excited states.

During the past two years, a new instrument was constructed which consists of a sample manipulator, rapidly pulsed (50 ns) ion gun, pulsed time-of-flight (TOF) ion-extraction optics and detector, and windows for two laser beams. This instrument is now operational. Measurements have begun on the kinetic energy distributions of sputtered ions using the TOF spectrometer in an impulse-extraction mode together with pulsed ion-beam bombardment. Timing characteristics of the entire TOF impulse-mode extraction optics have been carefully analyzed. Timing of the ion pulse from ion gun to target has been established and observed flight times for sputtered ions have been found to be consistent with calculated flight times based on our analyzer geometry and potentials. TOF measurements were made as a function of the target potential and compared to calculations in order to establish an accurate kinetic energy scale for our energy distribution data. This turned out to be a non-trivial excercise and has resulted in an energy scale calibration which is probably accurate to < 3 eV.

Since it is critical that the impuse acceleration be applied just after all of the pulsed beam ions strike the target, we experimentally established optimum impulse extraction timing for various ion beam energies. This timing was verified by our calculations of flight times and trajectories for our high-collection-efficiency, large-aperture TOF analyzer. The transmission of this analyzer depends on both the emitted ion energy and the ion angle of emission for a given set of accelerting potentials. By varying these potentials, we can change the acceptance angle of our analyzer and so obtain information on the energy and angular distributions of collisionally ejected ions. Calculation of these critical ejection angles as a function of ion ejection energy for various TOF potentrals has been done and gives us a way of unfolding our ion kinetic energy distributions to obtain such energy/angle distributions.

Measurements have been made of the kinetic energy distributions of collisionally ejected ions from both polycrystalline Mg and Al due to the impact of 1.5 to 4 keV argon ions. The ions were incident on the target at 75°. Figure 4.6 shows the ion energy distributions obtained on polycrystalline aluminum as a function of bombarding ion energy; it is interesting to note the high abundance of ejected aluminum ions at energies greater

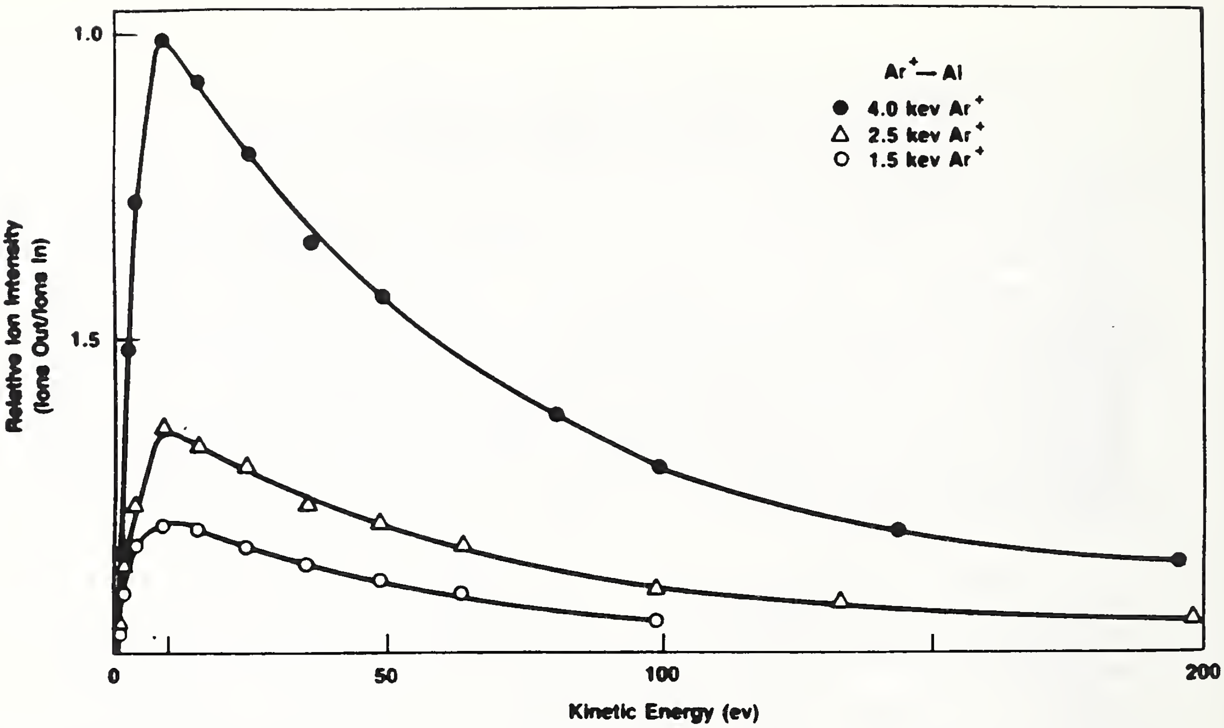

Fig. 4.6 Kinetic energy distributions of aluminum ions sputtered from an aluminum surface by argons ions of three different energies at an angle of incidence of 75°. These data have not been corrected for the enegy-dependence of the analyzer transmission function; the falloff in the distributions with increasing kinetic energy is less than that shown.

than 50 eV which is probably associated with collisional excitation and ionization mechanisms. Such measurements have also been made as a function of the TOF accelerating potentials; the data have been analyzed to obtain approximate emitted angular distributions for ions of 4, 9, 50, and 100 eV energy. Our results indicate that at higher energies, the emitted ions are strongly peaked toward the specular direction; at 4 eV the ions are emitted more uniformly but still peak near 50°. These results are consistent with computer calculations (such as those described below) which predict that collisionally excited, sputtered ions have high kinetic energy (~ 100 eV), are more probable for greater angles of incidence of the impacting ion beam, and are ejected with an angular distribution strongly peaked toward the specular direction. All of these angular/energy distribution results make it possible for us to proceed to the next phase of our research--to probe the charge and excitation state of collisionally excited ions and atoms using multiphoton resonance-ionization techniques.

We are currently measuring energy and angular distributions of sputtered ions from silicon and magnesium. We expect that a correlation of our results for Mg, Al, and Si with Auger-electron emission data for atomic-like collisional excitation should lead to a better understanding of the emission of singly and doubly charged, high-energy ions. We are also currently procuring a new high-current, pulsed ion gun and a tunable dye laser with frequency doubler.

(b) Auger-Electron De-Excitation of Sputtered Atoms
(J. Fine)

In collaboration with Drs. C. Le Gressus, J. P. Duraud, and D. Celier (Centre d'Etudes Nucleaires de Saclay, France), a series of measurements has been performed to investigate the Auger-electron emission from ion-bombarded single-crystal aluminum surfaces. Aluminum (100) and (111) surfaces were bombarded with argon ions and the dependence of atomic-like and band-like Auger-electron emission was monitored as the crystals were rotated about an axis normal to the surface. Our results indicate a very marked change in the total Auger-electrom emission intensity as a function of azimuthal angle. Intensity minima correspond to geometrical conditions where the incident ion beam is aligned with a string of atoms (i.e., there is a shadowing or underlying atoms by the outermost surface atom of a given string).

Similar measurements have now been obtained with incident xenon ions. Analysis of the data for both argon and xenon ions strongly suggests that collisional excitation and ejection of excited target atoms occur as a result of primary, asymmetric collisions (inert gas ion with target atom) and not because of secondary symmetric collisions (target atom with target atom) as previously suggested in the literature. This asymmetric model, developed in conjunction with Dr. G. Blaise (Orsay, France) is based on atom-atom scattering calculations and indicates that excited atoms are ejected from the outermost layer of surface atoms. Such excited atoms can be scattered directly (and ejected) or may be reflected by the second layer of atoms (and subsequently ejected) if the geometry of these second-layer atoms is appropriate.

(c) Simulation of Ion-Surfce Collisions
(M. H. Shapiro and J. Fine)

Multiple-interaction calculations have been performed to simulate the ion-surface collisions occurring for typical sputtered conditions and to investigate the dynamical phenomena occurring in the resulting collision cascades. Preliminary results for argon ions bombarding an aluminum target indicate that asymmetric collisions are responsible for aluminum excitation and suggest that second-layer reflection is often important for ejection. Further analysis of the calculations should help to establish collisional-excitation mechanisms and trajectories and their dependence on atom geometry in the target.

2. Measurement of Angular, Energy and Mass Distributions of Desorbed Ionic Species
(R. L. Stockbauer, R. L. Kurtz, and T. E. Madey)

Several years ago we embarked on a program to design and construct a unique charged-particle energy analyzer which would have the capability of simultaneously measuring the energy, angular distribution, and mass of ions desorbed from surfaces. The design was based on an ellipsoidal mirror analyzer developed by Dr. D. E. Eastman of IBM. The construction of the analyzer is now complete and it will be installed on beamline 1 at SURF-II this autumn. This analyzer will play a key role in two areas of research, ion-desorption dynamics and angle-resolved photoemission.

We plan several experiments to elucidate the mechanisms of photon-stimulated desorption. One of the key questions which remains concerns the role of surfce geometry in the desorption process. With the new analyzer we will be able to tackle this problem. For instance, calculations of image-charge and reneutralization effects predict that the kinetic energy distributions of desorbed ions depend on the desorption angle. Since the new analyzer is capable of measuring kinetic energy as a function of angle, we will be able to assess the importance of these phenomena.

Likewise, the mass of the ions which make up the spots in the two-dimensional desorption pattern is also an important piece of information which has not been available to date. Hydrogen has a very large desorption probability and is present on most surfaces. Since it is the main background gas in an ultrahigh vacuum chamber, it is detected in almost all ion desorption studies. In our studies of O^+ desorption from different cyrstal faces of TiO_2, for example, almost as much H^+ was detected as was O^+. Without mass analysis, it was not possible to determine which spots or portions of spots in the pattern were due to H^+ and which to O^+. The new analyzer with its simultaneous mass and angle-resolving capabilities will be able to distinguish between the two ions and give separate patterns for each ion.

The analyzer will also play an important role in our photoemission studies of high-temperature superconductors (section 3.A). With its simultaneous energy and angle-resolving capability, we will be able to obtain angle-resolved photoelectron data on oriented thin films. This information can be compared directly to band-structure calculations which should lead to an understanding of the electronic interactions responsible for the superconductivity.

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Ciszewski, A. and Melmed, A. J., "Epitaxy of Metals on Metal Substrates: The Contributions of Field Emission Microscopy," Appl. Surf. Sci. (in press).

Cowan, P. L., Brennan, S., Jach, T., Lindle, D. W., and Karlin, B. A., "Performance of a High Energy Resolution, Tender X-Ray Synchrotron Radiation Beamline," Review Scientific Instr. (submitted)

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

Demmin, R. A. and Madey, T. E., "Interaction of Oxygen and Platinum on W(110)," J. Vac. Sci. Tech. (submitted).

Demmmin, R. A., Shivaprasad, S. M., and Madey, T. E., "Adsorption Properties of Pt Films on W(110) Surface," Langmuir (in press).

Egelhoff, Jr., W. F., "The Role of Adsorbed Gases in Metal on Metal Epitaxy," J. Vac. Sci. Tech. (submitted).

Egelhoff, Jr., W. F., "XPS Forward Scattering Studies of Surface Segregation and Interdiffusion in Epitaxial Ni-Cu/Ni(100) Overlayers and Sandwich Structures," J. Vac. Sci. Tech. (submitted).

Elwsijk, H. B., Melmed, A. J., and Fowler, H. A., "On the Interpretation of Field Ion Microscopy (FIM) Images of Asymmetrical Specimens of "1,2,3"-Type High-T_c Superconductors," J. de Physique (in press).

Ernst, N., Bozdech, G., and Melmed, A. J., "Combined Field Ion and Field Emission Microscopy of $YBa_2Cu_3O_{7-x}$," J. de Physique (in press).

Gadzuk, J. W., "The Semiclassical Way to Molecular Dynamics at Surfaces," Ann. Rev. Phys. Chem. (in press).

Gadzuk, J. W., "Soluble Models in Surface Collision Dynamics," Proc. Solvay Conference on Surface Science (in press).

Grant, J. T., Williams, P., Fine, J., and Powell, C. J., "The Status of Reference Data, Reference Materials, and Reference Procedures in Surface Analysis," Surf. & Interface Anal. (in press).

Heilweil, E. J., Cavanagh, R. R., and Stephenson, J. C., "Picosecond Study of the Population Lifetimes of CO(v=1) Chemisorbed on SiO_2-Supported Rhodium Particles," J. Chem. Phys. (in press).

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Jach, T., Cowan, P. L., Shen, Q., and Bedzyk, M. J., "Dynamical Diffraction of X-Rays at Glancing Incidence," Phys. Rev. B (in press).

Jach, T., Novotny, D. B., Bedzyk, M. J., and Shen, Q., "Direct Observation of Surface-Trapped Diffracted Waves," Phys. Rev. Lett. (submitted).

Johnson, A. L., Joyce, S. A., and Madey, T. E., "Electron Stimulated Desorption Ion Angular Distributions (ESDIAD) of Negative Ions," Phys. Rev. Lett. (submitted).

Joyce, S. A., Johnson, A. L., and Madey, T. E., "The Methodology of ESDIAD of Negative Ions," J. Vac. Sci. Tech. (submitted).

King, D. S. and Cavanagh, R. R., "Molecular Desorption from Solid Surfaces: Laser Diagnostics and Chemical Dynamics," Adv. in Chem. Phys. (in press).

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Marton, D. and Fine, J., "Sputtering Induced Surface Roughness of Metallic Thin Films," Thin Solid Films (submitted).

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Polak, M. and Madey, T. E., "The Structure of Molecular and Dissociated H_2O Adsorbed on Cu(110)," Surface Sci. (in press).

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(c) Recent Publications of New Staff Members Resulting From Previous Positions (Buntin, Camus, Joyce, Richter, Robey, Stiles, and Yarmoff)

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Himpsel, F. J., Karlsson, U. O., Morar, J. F., Rieger, D., and Yarmoff, J. A., "Microscopic Model for the Epitaxy of CaF_2 on Si(111)," Proc. of 1987 Spring Materials Research Society Meeting, Anaheim, CA.

Himpsel, F. J., Karlsson, U. O., McFeely, F. R., Morar, J. F., Rieger, D., Taleb-Ibrahimi, A., and Yarmoff, J. A., "Dielectrics on Semiconductors," Materials Science and Engineering B 1, 9 (1988).

Himpsel, F. J., Meyerson, B. S., McFeely, F. R., Morar, J. F., Taleb-Ibrahimi, A., and Yarmoff, J. A., "Core Level Spectroscopy at Silicon Surfaces and Interfaces," Proceedings of the Enrico Fermi School on "Photoemission and Absorption Spectroscopy of Solids and Interfaces with Synchrotron Radiation," Varenna, Italy, 1988 (North Holland, 1989).

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6. TALKS

Buntin, S. A., "The Wavelength Dependence of NO/Pt(111) Laser-Induced Desorption: Evidence for the Role of Hot Electrons," Physical Electronics Conference, Brookhaven National Laboratory, Upton, NY, June 6, 1988.

Buntin, S. A., "Wavelength Dependent Dynamics in Laser Driven Surface Reactions: Photogenerated-Electron Induced Desorption of NO from Pt(111)," Gordon Research Conference, Plymouth, NH, August 2, 1988.

Cavanagh, R. R., "Molecular Desorption from Surfaces: Thermal and Non Thermal Processes," Department of Chemistry, Catholic University, Washington, D.C., October 2, 1987.

Cavanagh, R. R., "Laser-Induced Desorption: The Role of Photons, Phonons, and Electrons," Greater Washington Surface Science Seminar, National Institute of Standards and Technology, Gaithersburg, MD, May 20, 1988.

Cavanagh, R. R., "Time Resolved Measurements of Vibrational Relaxation: Comparison of CO ($v=1$) in Metal Carbonyls and on Supported Metal Clusters," American Chemical Society Meeting, Toronto, Canada, June 9, 1988.

Demmin, R. A., "Structure and Chemical Properties of Pt Films on W(110)," Greater Washington Surface Science Seminar, National Institute of Standards and Technology, Gaithersburg, MD, May 20, 1988.

Demmin, R. A., "Structure and Adsorption Properties of Tungsten-Supported Platinum Films," Exxon Research and Engineering Company, Linden, NJ, June 9, 1988.

Demmin, R. A., "Characterization and Surface Chemistry on Thin Pt Films on W(110)," American Chemical Society Colloid and Surface Science Symposium, State College, PA, June 22, 1988.

Demmin, R. A., "Structure and Adsorption Properties of Tungsten-Supported Platinum Films," W. R. Grace & Co., Columbia, MD, June 27, 1988.

Demmin, R. A., "Structure and Adsorption Properties of Tungsten-Supported Platinum Films," Air Products and Chemicals, Inc., Allentown, PA, July 7, 1988.

Demmin, R. A., "CO Adsorption on Platinum Overlayers on a W(110) Substrate: Photoemission Studies," American Chemical Society Meeting, Los Angeles, CA, September 26, 1988.

Egelhoff, Jr., W. F., "Short Range Order in Submonolayer Ni on GaAs(110) by XPS Forward Scattering," American Vacuum Society Meeting, Anaheim, CA, November 4, 1987.

Egelhoff, Jr., W. F., "Epitaxial Overlayers and Sandwich Structures of Au and Ag on Ni(100)," American Vacuum Society Meeting, Anaheim, CA, November 4, 1987.

Egelhoff, Jr., W. F., "Ultrathin Fe Films on Cu(100): Mechanism, Morphology, and Stability," American Vacuum Society Meeting, Anaheim, CA, November 4, 1987.

Egelhoff, Jr., W. F., "XPS Forward Scattering Studies of Epitaxial Growth," University of Colorado, Boulder, CO, November 13, 1987.

Egelhoff, Jr., W. F., "XPS and Auger Forward Scattering: A Structural Tool for Studying Ultrathin Films, Epitaxial Growth, Surface Segregation, and Interdiffusion," Fritz-Haber-Institut, Berlin, W. Germany, December 7, 1987.

Egelhoff, Jr., W. F., "XPS and Auger Forward Scattering: A Structural Tool for Studying Ultrathin Films, Epitaxial Growth, Surface Segregation, and Interdiffusion," Physics Institute, Clausthal University, Clausthal, W. Germany, December 9, 1987.

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Egelhoff, Jr., W. F., "XPS and Auger Forward Scattering: A Structural Tool for Studying Ultrathin Films, Epitaxial Growth, Surface Segregation, and Interdiffusion," Cambridge, University, Cambridge, England, December 14, 1987.

Egelhoff, Jr., W. F., "XPS and Auger Forward Scattering: A Structural Tool for Studying Ultrathin Films, Epitaxial Growth, Surface Segregation, and Interdiffusion," Warwick University, Warwick, England, December 15, 1987.

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Egelhoff, Jr. W. F., "XPS and Auger Forward Scattering: A Structural Tool for Studying Ultrathin Films, Epitaxial Growth, Surface Segregation and Interdiffusion," Department of Materials Sciences, University of Florida, Gainesville, FL, January 19, 1988.

Egelhoff, Jr., W. F., "Surface Segregation and Interdiffusion in Epitaxial Cu-Ni Sandwich Structures on Ni(100) and Cu(100)," American Physical Society Meeting, New Orleans, LA, March 23, 1988.

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Fine, J., "State Characterization of Collisionally Ejected Atoms from Surfaces," Division of Physical Chemistry, CEN-Saclay, France, October 10, 1987.

Fine, J., "Radiation Enhanced Diffusion (RED) in a Sputtered Ag/Ni Layered System," Second Topical Conference on Quantitative Surface Analysis, Monterey, CA, October 30, 1987.

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Fine, J., "In-Situ Surface Roughness Measurement During Sputter Depth Profiling," Symposium on the Physics of Ionized Gases, Sarajevo, Yugoslavia, August 16, 1988.

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Gadzuk, J. W., "Molecular Aspects of Surface Chemical Dynamics," Workshop/Symposium on Chemistry at Interfaces, Battelle Pacific Northwest Laboratories, Richland, WA, October 8, 1987.

Gadzuk, J. W., "Elementary Molecular Dynamics at Surfaces," Joint Institute of Laboratory Astrophysics Colloquium, University of Boulder, Boulder, CO, October 27, 1987.

Gadzuk, J. W., "Charge Transfer and Molecular Processes at Surfaces," Chemical Dynamics Seminar, Naval Research Laboratory, Washington, D.C., November 12, 1987.

Gadzuk, J. W., "Soluble Models in Surface Collision Dynamics," International Solvay Conference on Surface Science, University of Texas, Austin, TX, December 14, 1987.

Gadzuk, J. W., "Elementary Molecular Dynamics at Surfaces, Surface Science Seminar, University of Pittsburgh, Pittsburgh, PA, March 4, 1988.

Gadzuk, J. W., "Vibrational Relaxation at Surfaces," American Physical Society Meeting, New Orleans, LA, March 25, 1988.

Gadzuk, J. W., "Chaos in Surface Physics," Department of Physics Colloquium, Rice University University, Houston, TX, April 13, 1988.

Gadzuk, J. W., "Dynamics and Charge Transfer Processes at Surfaces," 173rd Meeting of the Electrochemical Society, Atlanta, GA, May 18, 1988.

Gadzuk, J. W., "Chaos in Surface Physics," Surface Physics, Physical Chemistry, and Theoretical Physics Departments, Fritz-Haber-Institut, Berlin, W. Germany, June 28, 1988.

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Jach, T., "Developments in X-Ray Standing Waves," Cornell Synchrotron Users Conference, Cornell University, Ithaca, NY, June 14, 1988.

Jacob, I., "Epitaxy of Fe on Cu(100)," American Physical Society Meeting, New Orleans, LA, March 21, 1988.

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Joyce, S., "Determination of Molecular Adsorbate Structures Using Electron Stimulated Desorption Ion Angular Distributions (ESDIAD)," Greater Washington Surface Science Seminar, National Institute of Standards and Technology, Gaithersburg, May 20, 1988.

Kurtz, R. L., "Photoemission Studies of High T_c Superconductors," American Vacuum Society Meeting, Anaheim, CA, November 4, 1987.

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Kurtz, R. L., "Photoemission Studies of the Electronic Structures of High-T_c Superconductors," Yale University, New Haven, CT, April 8, 1988.

Kurtz, R. L., "Synchrotron Radiation Studies of High-T_c Superconductors," Greater Washington Surface Science Seminar, National Institute of Standards and Technology, Gaithersburg, MD, May 20, 1988.

Kurtz, R. L., "Surface Structure and Mechanisms in Ion Desorption from Oxide Surfaces," CSIC, Madrid, Spain, September 20, 1988.

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Madey, T. E., "The Interaction of Water with Surfaces," Rutgers University, Brunswick, NJ, October 29, 1987.

Madey, T. E., "Electron and Photon Stimulated Desorption as Probes of Structure and Bonding at Surfaces," Department of Materials Science, University of Virginia, Charlottesville, Virginia, November 16,1987.

Madey, T. E., "Electron and Photon Stimulated Desorption as Probes of Structure and Bonding at Surfaces," 7th International Conference on Thin Films, New Delhi, India, December 10, 1987.

Madey, T. E., "Interaction of H_2O with Surfaces," Solar Energy Research Institute, Golden, CO, January 14, 1988.

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Madey, T. E., "Structure and Reactivity of Chemisorbed Species," Engelhard Corp., Newark, NJ, March 8, 1988.

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Madey, T. E., "Characterization of Ultrathin Pt Overlayers Deposited on a W(110) Surface," American Physical Society Meeting, New Orleans, LA, March 23, 1988.

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Madey, T. E., "Radiation Damage in Auger Electron Spectroscopy and X-Ray Photoelectron Spectroscopy," 10th Symposium on Applied Surface Analysis, Topical Conference of the American Vacuum Society, Lakewood, CO, April 29, 1988.

Madey, T. E., "Electron and Photon Stimulated Desorption as Probes of Structure and Bonding at Surfaces," Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA, May 10, 1988.

Madey, T. E., Series of 5 lectures on "Electron and Photon Stimulated Desorption as Probes on Structure and Bonding at Surfaces," International Center for Theoretical Physics, Trieste, Italy, May 30-June 3, 1988.

Madey, T. E., "The Adsorption of Water on Surfaces: Basic Aspects," International Conference on the Chemistry and Physics of Electrified Surfaces, Bologna, Italy, August 30, 1988.

Madey, T. E., "The Adsorption of Water on Surfaces: Basic Aspects," Fourth Joint Vacuum Conference, Portoroz, Yugoslavia, September 23, 1988.

Madey, T. E., "IUVSTA - Past, Present, and Future," Swedish Academy of Engineering Sciences, Stockholm, Sweden, September 27, 1988.

Madey, T. E., "Direct Determination of the Structure of Surface Molecules," Swedish Academy of Engineering Sciences, Stockholm, Sweden, September 27, 1988.

Marton, D., "Ion-Bombardment Induced Surface Roughness of Thin Metallic Layers," Fourth International Conference on Metrology and Properties of Engineering Surfaces, National Institute of Standards and Technology, Gaithersburg, MD, April 14, 1988.

Melmed, A. J., "The Atomic Fingerprint of High-T_c Superconductors Observed by FIM," Physics Department Seminar, Michigan State University, Lansing, MI, January 26, 1988.

Melmed, A. J., "The Atomic Fingerprint of High-T_c Superconductors Observed by FIM," American Physical Society Meeting, New Orleans, LA, March 22, 1988.

Melmed, A. J., "A Method of FIM-FEEM Specimen Preparation Suitable for Superconducting and Other Oxides," International Field Emission Symposium, Oak Ridge National Laboratory, Oak Ridge, TN, July 18, 1988.

Melmed, A. J., "Progress in FIM Imaging of High-T_c Superconducting Oxides: La-Sr-Cu-O, Y-Ba-Cu-O Type, Bi-Sr-Ca-Cu-O and Tl-Ca-Ba-Cu-O," International Field Emission Symposium, Oak Ridge National Laboratory, Oak Ridge, TN, July 19, 1988.

Powell, C. J., "Dependence of Inelastic Electron Mean Free Paths on Electron Energy and Material," European Conference on Applications of Surface and Interface Analysis, Schwabenlandhalle, Fellbach, W. Germany, October 19, 1987.

Powell, C. J., "Observation of Recoil Energy Losses in Elastic Scattering of Electrons from Surfaces," European Conference on Applications of Surface and Interface Analysis, Schwabenlandhalle, Fellbach, W. Germany, October 20, 1987.

Powell, C. J., "Surface Chemical Analysis: Report on the VAMAS Project," European Conference on Applications of Surface and Interface Analysis," Schwabenlandhalle, Fellbach, W. Germany, October 22, 1987.

Powell, C. J., "High-Accuracy Measurements of XPS Binding Energies for Copper, Silver, and Gold," Topical Conference on Quantitative Surface Analysis, Monterey, CA, October 30, 1987.

Powell, C. J., "The International Development of Standards for Surface Analysis," Topical Conference on Quantitative Surface Analysis, Monterey, CA, October 31, 1987.

Powell, C. J., "Dependence of Inelastic Electron Mean Free Paths on Electron Energy and Material," American Vacuum Society Meeting, Anaheim, CA, November 3, 1987.

Powell, C. J., "Observation of Recoil Energy Losses in Elastic Scattering of Electrons From Surfaces," American Vacuum Society Meeting, Anaheim, CA, November 4, 1987.

Powell, C. J., "Accomplishments of the VAMAS Surface Chemical Analysis Working Party," Versailles Project on Advanced Materials and Standards (VAMAS) International Steering Committee, Brussels, Belgium, February 17, 1988.

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," Physics Institute, University of Odense, Odense, Denmark, February 18, 1988.

Powell, C. J., "Cross Sections for Inelastic Electron Scattering in Solids," U.S.-French Workshop on Electron Beam Induced Spectroscopies at Very High Spatial Resolution, Aussois, France, February 29, 1988.

Powell, C. J., "Appearance Potential Spectroscopy of Solids and Comparisons of L_3-Shell Binding Energies of Ti-Ni as Measured by APS, EELS, and XPS," Workshop on Electron-Beam Induced Spectroscopies at Very High Spatial Resolution, Aussois, France, March 1, 1988.

Powell, C. J., "Comparison of L_3-Shell Binding Energies of Six 3d Metals by X-ray Photoelectron Spectroscopy, Appearance-Potential Spectroscopy, and Electron Energy-Loss Spectroscopy," University of Liverpool, Liverpool, England, April 14, 1988.

Powell, C. J., "Recent Developments in Applied Surface Science," Research Highlights Seminar of the International Union of Vacuum Science, Technique and Applications, University of Salford, Manchester, England, April 15, 1988.

Powell, C. J., "Calculations of Electron Inelastic Mean Free Paths for 31 Materials," Greater Washington Surface Science Seminar, National Institute of Standards and Technology, Gaithersburg, MD, May 20, 1988.

Powell, C. J., "Calculations of Electron Inelastic Mean Free Paths for 31 Materials," Gordon Research Conference, Wolfeboro, NH, July 18, 1988.

Richter, L. J., "Laser Induced Desorption of NO from Pt(111): Dynamics of Excitation and Desorption," Application of Lasers in Surface Science Conference, Trieste, Italy, August 25, 1987.

Richter, L. J., "The Importance of Dispersion in Overtone Spectra: Two Phonon Bound States in the Vibrational Spectra of H/Rh(100)," Physical Electronics Conference, Brookhaven National Laboratory, Upton, NY, June 7, 1988.

Stockbauer, R., "Electronic Structure and the Surface Chemistry of High T_c Superconductors and Related Compounds," An International Symposium on the Uses of Synchrotron Radiation in Chemistry, Upton, NY, November 6, 1987.

Stockbauer, R., "Surface Chemistry of High T_c Superconductors," NIST Gaithersburg-Boulder Superconductivity Meeting, December 7, 1987.

Stockbauer, R., "The Surface Chemistry of High-T_c Superconductors," American Physical Society Meeting, New Orleans, LA, March 23, 1988.

Stockbauer, R., "Recent Photoemission Results on High-T_c Superconductors," NIST Boulder-Gaithersburg Superconductivity Meeting, Boulder, CO, July 14, 1988.

Stockbauer, R., "Photoemission Studies of High Temperature Superconductors," Department of Physics, Louisiana State University, Baton Rouge, LA, September 29, 1988.

Yarmoff, J. A. , "Chemical Vapor Deposition of Tungsten on Silicon Studied with Soft X-Ray Photoemission," American Vacuum Society Meeting, Anaheim, CA, November 4, 1987.

Yarmoff, J. A., "The Interaction of Fluorine with Silicon Surfaces," Gordon Research Conference on the Chemistry of Electronic Materials, Ventura, CA, March 8, 1988.

Yarmoff, J., "Angle-Resolved Stimulated Desorption of Fluorine From Silicon," American Physical Society Meeting, New Orleans, LA, March 23, 1988.

Yarmoff, J. A., "Synchrotron Radiation Studies of the Fluorine-Silicon Interaction," Xerox Webster Research Center, Rochester, NY, June 10, 1988.

7. SURFACE SCIENCE DIVISION SEMINARS

Amirav, A., Tel Aviv University, Tel Aviv, Israel, "Molecular Ionization and Dissociative Ionization in Hyperthermal Molecular Surface Scattering," September 21, 1988.

Ballentine, C., University of Texas, Austin, TX, "Magnetic Properties of Epitaxial Fe, V, and Ni Films on Ag(100)," June 10, 1988.

Bloch, J. M., Argonne National Laboratory, Chicago, IL, "Studies of Interfaces and Thin Films Using X-Ray Grazing Incidence Techniques," February 25, 1988.

Camus, P. P., Oak Ridge National Laboratory, Oak Ridge, TN, "Atom Probe Field Ion Microscopy of Fe-Cr-Co Alloys," March 18, 1988.

Doren, D., AT&T Bell Labortories, Murray Hill, NJ, "Precursors to Chemisorption: What Difference Do They Make?" December 4, 1987.

Dutcher, J., Simon Fraser University, Vancouver, Canada, "Brillouin Light Scattering of Magnetic Surface Anisotropy," June 3, 1988.

Heinrich, B., Simon Fraser University, Burnaby, Canada, "MBE Studies and Magnetic Properties of Ultrathin Films and Sandwiches of bcc Ni(001) and bcc Fe(001) Epitaxially Grown on fcc Ag(001)," Joint seminar with Electron Physics Group, March 17, 1988.

Henrich, V. E., Yale University, New Haven, CT, "Bulk and Surface Electronic Structure of Rock Salt Transition-Metal Monoxides," November 24, 1987.

Holloway, S., Liverpool University, Liverpool, England, "Time-Dependent Quantum Approach to Gas-Surface Dynamics and Rust-Busting," April 19, 1988.

Kevan, S. D., University of Oregon, Eugene, OR, "Intuition and Surface Electronic Structure," October 8, 1987.

Kiskinova, M., University of Pittsburgh, Pittsburgh, PA, "CO and NO Adsorption on Pt(111) and Modified Pt(111) Surfaces," August 12, 1988.

McFeely, F. R., IBM T. J. Watson Research Center, Yorktown Heights, NY, "Photoemission Studies of Selective Tungsten CVD on Silicon and SiO_2," September 6, 1988.

Mundschau, M., University of Clausthal, Clausthal, Germany, "Low-Energy Electron Microscopy," January 19, 1988.

Paul, J., Royal Institute of Technology, Sweden, "Adsorption on Aluminum," November 18, 1987.

Richmond, G. L., University of Oregon, Eugene, OR, "Non-Linear Optics as a Probe of Interfacial Structure and Dynamics," October 13, 1987.

Robey, S. W., IBM Watson Research Center, Yorktown Heights, NY, "Photoemission Studies of Plasma Etched Surfaces," March 15, 1988.

Ross, P., Department of Energy, Germantown, MD, "Structure Determination at Liquid-Solid Interfaces Using Grazing Incidence X-Ray Scattering," February 3, 1987.

Sault, A., Sandia National Laboratories, Albuquerque, NM, "Dissociation of Alkanes on Ni(100)," January 11, 1988.

Shapiro, M. H., National Science Foundation, Washington, DC, "Molecular Dynamics Simulations of Ion/Surface Collisional Excitation," June 15, 1988.

Stiles, M., AT&T Bell Laboratories, Murray Hill, NJ, "Ballistic Electron Transmission Through Interfaces," May 26, 1988.

Stuve, E., University of Washington, Seattle, WA, "The Adsorption of Solvent and Ionic Species on Metal Surfaces," November 20, 1987.

Tatar, R. C., General Electric R&D Center, Schenectady, NY, "Electron Correlation and Valence Bonds in Metals and Intermetallic Compounds," September 21, 1987.

Whitman, L. J., Cornell University, Ithaca, NY, "Kinetics and Mechanisms of K-Promoted Surface Reactions," March 30, 1988.

8. CONFERENCES ORGANIZED OR HOSTED

Workshop on Quantitative Surface Analysis, NIST, October 24, 1986 (cosponsored by the Applied Surface Science Division of the American Vacuum Society, ASTM Committee E-42 on Surface Analysis, and the Surface Chemical Analysis Working Party of the Versailles Project on Advanced Materials and Standards).

Meeting of ASTM Committee E-42 on Surface Analysis, Gaithersburg, MD, October 25, 1986.

10th International Vacuum Congress/6th International Conference on Solid Surfaces/33rd National Symposium of the American Vacuum Society, Baltimore, MD, October 27-31, 1986.

Symposium on Surface Analysis, 22nd Annual Meeting of the Microbeam Analysis Society, Kona, HI, July 13-17, 1987.

6th Department of Energy, Catalysis and Surface Chemistry Research Conferences, NIST, October 14-16, 1987.

2nd Topical Conference on Quantitative Surface Analysis, Monterey, CA, October 30-31, 1987 (cosponsored by the Applied Surface Science Division of the American Vacuum Society, ASTM Committee E-42 on Surface Analysis, and the Surface Chemical Analysis Working Party of the Versailles Project on Advanced Materials and Standards).

Greater Washington Surface Science Seminar, NIST, May 20, 1988.

9. TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Cavanagh, R. R.

Treasurer, General Committee of the Physical Electronics Conference

Local Co-Chairman, Physical Electronics Conference in 1990

Member (1987) and Chairman (1988) of the NIST Research Advisory Committee

Egelhoff, Jr., W. F.

NIST Representative to SEMATECH Planning Workshop on Physical Vapor Deposition, San Francisco, CA, September 21-22, 1987.

Erickson, N. E.

Member, ASTM Committee E-42 on Surface Analysis

Fine, J.

Chairman, Subcommittee E-42.09 on Standard Reference Materials of ASTM Committee E-42 on Surface Analysis

Gadzuk, J. W.,

Member, Editorial Advisory Board, "Progress in Surface Science"

Member, International Steering Committee, 5th International Conference on Vibrations at Surfaces, Garmisch-Partenkirschen, FRG, September, 1987

Member, Organizing Committee, 6th International Conference on Vibrations at Surfaces, 1990

Madey, T. E.

Member, American Institute of Physics Subcommittee on Intellectual Property Rights

Program Chairman, 10th International Vacuum Congress/6th International Conference on Solids Surfaces/33rd National Symposium of the American Vacuum Society, Baltimore, MD, October, 1986

Secretary General, International Union for Vacuum Science, Technique and Applications

Member, Program Advisory Committee for the Synchrotron Radiation Center of the University of Wisconsin, Madison, Wisconsin

Member, International Advisory Committee, Beijing Laboratory of Vacuum Physics, Peoples Republic of China

Member, Advisory Committee for Laboratory of Surface Science and Technology at the University of Maine, Orono, ME

Member, Policy Board for High Resolution Electron Microscope Facility, Arizona State University

Member, International Advisory Committee, Second International Conference on the Structure of Surfaces, Amsterdam, The Netherlands, June, 1987.

Member, International Advisory Committee, Workshop on Desorption Induced by Electronic Transitions, DIET-III, Long Island, NY, May, 1987 and DIET-IV, Austria, October, 1989

Member, ASTM Committee E-42 on Surface Analysis

Member, Editorial Board, "Methods of Surface Characterization"; co-editor of two volumes in series

Melmed, A. J.

President (7/86 through 7/87), International Field Emission Society

Division Safety Officer (2/86 through 1/88)

Chairman, Organizing Committee, International Field Emission Symposium, 1990

Powell, C. J.

Member, Executive Committee, and International Liaison, ASTM Committee E-42 on Surface Analysis

Chairman (through 10/87) and Vice-Chairman (from 11/87), Surface Chemical Analysis Working Party, Versailles Project on Advanced Materials and Standards

Member, Board of Trustees, Gordon Research Conferences

Member (from 1/88), Board of Directors, American Vacuum Society

Member (through 11/87), Ad Hoc Committee on Topical Conferences, American Vacuum Society

Chairman, Applied Surface Science Division Steering Committee, International Union of Vacuum Science, Technique, and Applications

Chairman, Applied Surface Science Program Committee for the 11th International Vacuum Congress and 7th International Conference on Solid Surfaces, Cologne, FRG, September 25-29, 1989

National Representative, Commission I.6 on Colloid and Surface Chemistry including Catalysis, International Union of Pure and Applied Chemistry

Co-Opted Member, Subcommittee on Surface Analysis of Commission V.2 on Microchemical Techniques and Trace Analysis, International Union of Pure and Applied Chemistry

Chairman, Organizing Committee, Workshop on Quantitative Surface Analysis, NIST, October 24, 1986

Co-Chairman, Symposium on Surface Analysis, Microbeam Analysis Society, Kona, HI, July 13-17, 1987.

Chairman, Organizing Committee, 2nd Topical Conference on Quantitative Surface Analysis, Monterey, CA, October 30-31, 1987

Member, Editorial Board, "Applications of Surface Science"

Member, Editorial Board, "Surface and Interface Analysis"

Member, Editorial Board, "Methods of Surface Characterization"; co-editor of one volume in series

NIST Representative, SEMATECH Workshop on DoE National Laboratories and the US Semiconductor Industry, Albuquerque, NM, May 26-28, 1987

Stockbauer, R.

Assistant Program Chairman, 10th International Vacuum Congress/6th International Conference on Solid Surface/33rd National Symposium of the American Vacuum Society, Baltimore, MD, October, 1986

Member, Office Automation Committee, American Vacuum Society

Division Safety Officer (from 2/88)

10. PROFESSIONAL INTERACTIONS, CONSULTING AND ADVISORY SERVICES

Cavanagh, R. R.

Collaborating with Drs. J. J. Rush, T. J. Udovic and J. M. Nicol of the NIST Reactor Radiation Division on measurements of vibrational, torsional, and re-orientational dynamics of molecular species in and on high-surface-area materials.

Collaborating with Drs. J. C. Stephenson, T. E. Heilweil and M. P. Casassa of the NIST Molecular Spectroscopy Division on time-resolved measurements of vibrational relaxation of molecules bound to surfaces.

Collaborating with Dr. D. S. King of the NIST Molecular Spectroscopy Division on the dynamics of molecular desorption from surfaces.

Collaborating with Dr. J. B. Beckerle, contractor, on the electronic density of states of small metal particles and the importance of these states on the vibrational relaxation properties of adsorbates.

Demmin, R. A.

Collaborated with Dr. N. H. Turner of the Naval Research Laboratory in scanning Auger microprobe experiments on thin films.

Collaborated (with R. L. Kurtz and R. L. Stockbauer) with Drs. D. R. Mueller and A. Shih of the Naval Research Laboratory in a photoemission study of thin films.

Egelhoff, Jr., W. F.

Collaborating with Dr. J. E. Rowe of AT&T Bell Laboratories in investigations of the diffusion of nickel into GaAs(110) using the XPS searchlight effect.

Collaborating with Dr. B. Heinrich of Simon Fraser University, Canada to measure magnetic properties of novel crystal structures.

Collaborating with Dr. R. F. Willis of Cambridge University, England to make neutron spin-flip measurements of novel crystal structures.

Collaborated with Prof. S. Bauer of Cornell University to make synchrotron x-ray diffraction measurements of the structural quality of superlattices fabricated at NIST.

Fine, J.

Collaborating with Dr. I. Terzic of the Boris Kidric Institute, Belgrade, Yugoslavia on electronic excitation and electron emission for ion-bombarded surfaces. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Drs. L. and N. Tanovic of the University of Sarajevo, Yugoslavia on characterizing surface topography changes that result from ion bombardment. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Dr. T. Nenadovic of the Boris Kidric Institute, Belgrade, Yugoslavia on the surface topography effect of both particle and laser-beam interactions with thin solid films. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Dr. J. D. Fassett of the NIST Inorganic Analytical Research Division on the use of laser multiphoton-ionization techniques to identify sputtered atoms and to determine their kinetic energies.

Collaborating with Dr. W. Kirchhoff of the Department of Energy on a data analysis procedure for sputter-depth-profile interface characterization.

Collaborating with Drs. C. Le Gressus and J. P. Duraud of the Centre d'Etudes Nucleaires, Saclay, France on the collisional excitation and electron decay of atoms at single-crystal surfaces.

Collaborating with Dr. P. Roncin of the Université Paris, CNRS/Orsay, France on the use of laser multiphon-ionization techniques to identify sputtered atoms and to determine their kinetic energies.

Collaborating with Dr. G. Blaise of the Université Paris, CNRS/Orsay, France on the collisional excitation and sputtering of atoms at surfaces.

Collaborating with Dr. M. H. Shapiro of the California State University at Fullerton on multiple-interaction calculations of collisional atomic excitation and ejection at single-crystal surfaces.

Collaborating with Dr. G. P. Chambers of the Naval Research Laboratory, Washington, D.C. on the compilation and evaluation of absolute sputtering yield data.

Collaborating with Dr. M. Szymonski of the Jagellonian University, Krakow, Poland on energy distributions of collisionally excited and ejected atoms at surfaces.

Gadzuk, J. W.

Collaborating with Prof. M. Sunjic of the Ruder Boskovic Institute and the University of Zagreb, Yugoslavia on theories of electron spectroscopies and dynamics of molecular processes at surfaces. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Dr. S. Holloway, University of Liverpool, England on theories of molecular processes at surfaces. This collaboration is assisted by a grant from the NATO Scientific Affairs Division.

Collaborating with Dr. N. Sathyamurthy, Indian Institute of Technology, Kanpur, India, and serving as monitor for a project "Chemical Dynamics and Laser Spectroscopy", under the auspices of the India-U.S. Materials Science Program funded via the provisions of PL-480.

Mini-course on "Chemical Dynamics at Surfaces," presented at Workshop on Fast Chemical Processes organized by Tata Institute of Fundamental Research, Bombay, India.

Consulted for Battelle Pacific Northwest Laboratory Symposium on New Frontiers in Surface Science.

Invited participant in the First Joint Physics and Chemistry Solvay Conference: Surface Science.

Collaborating with Prof. J. T. Yates, Jr., University of Pittsburgh on problem of resonant electron-stimulated desorption.

Collaborating with Dr. C. W. Clark of the NIST Radiation Physics Division on atomic physics aspects of oxygen chemisorption related to resonant electron-stimulated desorption.

Collaborated with NIST Center for Applied Mathematics in presentation of a Mini-Course on Chaos.

Consulted with Dr. J. Harris and other members of the Solid State Theory Group, KFA (Nuclear Research Organization) Julich, W. Germany on problems associated with molecular dynamics at surfaces.

Jach. T.

Collaborating with Drs. R. D. Deslattes, P. L. Cowan, D. Lindle, R. Lavilla and J. Cooper of the NIST Quantum Metrology Division on gas-phase x-ray fluorescence experiments at the Brookhaven National Synchrotron Light Source.

Collaborating with Dr. R. C. C. Perera, Lawrence Berekely Laboratory on the measurements and interpretation of the x-ray spectra of chlorinated molecules.

Consulting with Drs. M. B. Bedzyk and Q. Shen of Cornell University to investigate superficial waves in surface dynamical x-ray diffraction.

Collaborated with Drs. J. Geist, G. Carver, and D. Novotny, of the NIST Semiconductor Electronics Division on the design and fabrication of silicon x-ray detectors.

Consulted by Drs. W. R. Ott, D. L. Ederer, and R. Canfield of the NIST Radiation Physics Division on the extension of silicon photodiode calibrated into the far ultraviolet and soft x-ray region.

Consulted by Dr. J. Comas of the NIST Semiconductor Electronics Division on incorporating silicon x-ray detector development into the program for the silicon process line.

Consulted by the NIST Research Advisory Committee on the procurement of unified computer-aided design (CAD) software for personal computers and organized, under the auspices of the Center for Applied Mathematics, a meeting to determine the need for such procurement.

Collaborated with Drs. J. P. Kirkland and R. A. Neiser of the Naval Research Laboratory on the characterization of commercial silicon photodiodes as x-ray detectors.

Collaborated with Dr. R. Spal of the NIST Ceramics Division on characterization of the x-ray monochromator crystal with integrated detector.

Joyce, S. A.

Collaborating (with J. Yarmoff) with Dr. F. R. McFeely of the IBM Watson Research Center on measurements of electron attenuation lengths in SiO_2.

Kurtz, R. L.

Collaborating (with R. L. Stockbauer and T. E. Madey) with Drs. A. Shih, D. R. Mueller, L. Toth, M. Osofsy, and S. Wolf of the Naval Research Laboratory on studies of high T_c superconductors.

Collaborating (with R. L. Stockbauer and T. E. Madey) with Drs. A. Shih and D. R. Mueller of the Naval Research Laboratory in photoemission and ion desorption studies of Ba and BaO on W and Ir as models for high-emission dispenser cathodes.

Collaborating (with R. L. Stockbauer and T. E. Madey) with Prof. J. L. de Segovia and Dr. E. Roman of the Instituto Ciencia de Materiales, CSCIC, Madrid on a study of the electronic structure and molecular adsorption of H_2O at low temperatures on transition-metal oxide surfaces.

Collaborating (with R. L. Stockbauer) with Drs. J. Rife, W. Hunter, and M. Kabler of the Naval Research Laboratory to instrument a surface science beamline at the Brookhaven National Synchrotron Light Source to extend the photon energy range of experiments beyond what is available at SURF-II.

Collaborating with Prof. V. E. Henrich, Yale University on investigations of the interaction of molecules of catalytic interest with $Fe_2O_3(0001)$.

Collaborating with Dr. R. Walkup of IBM in studies of ion desorption using molecular dynamics calculations to predict surface reconstructions, stability of various defect structures, and ion-desorption trajectories.

Madey, T. E.

Collaborating with Drs. I. Terzić, J. Vukanić and Z. Misković of the Boris Kidrić Institute, Belgrade, under the auspices of the U.S.-Yugoslav Agreement for Cooperation in Science and Technology, on theoretical and experimental studies of electron-stimulated desorption and scattering of alkali ions from surfaces.

Collaborated with Dr. C. Benndorf of the University of Hamburg, under the auspices of a NATO grant, on studies of the influence of surface additives on local molecular structure.

Collaborated with Prof. P. A. Thiel of Iowa State University in writing a comprehensive review article on the interaction of water with solid surfaces.

Collaborating (with R. L. Kurtz and R. L. Stockbauer) with Dr. J. L. de Segovia of the Instituto de Fisica de Materiales, Madrid, Spain, under the auspices of the U.S.-Spain Joint Committee for Technical Cooperation, on experimental studies of adsorption on metals and oxides using electron-stimulated desorption and synchrotron radiation methods.

Collaborating (with C. J. Powell) with Drs. J. K. N. Sharma and S. M. Shivaprasad of the Indian National Physical Laboratory, under the auspices of the U.S.-Indo Cooperative Program, on experimental studies of metal-semiconductor interfaces.

Collaborating (with A. J. Melmed) with Prof. R. Meclewski and Drs. A. Cizewski and R. Blasczyszyn of the University of Wroclaw, Poland on problems concerning ultrathin films of metals on metals, and the adsorption on water on these films. This work is conducted under the auspices of the Maria Sklodowska Curie Foundation.

Melmed, A. J.

Collaborating with Dr. C. K. Chiang of the NIST Ceramics Division who has provided samples of high-T_c superconducting materials for field-ion microscopy.

Collaborating with Dr. R. D. Shull of the NIST Metallurgy Division on magnetic susceptibility and x-ray diffraction measurements of high-T_c superconducting materials used for field-ion microscopy.

Collaborating with Dr. H. A. Fowler of the NIST Mathematical Analysis Division on simulations of images by field-ion microscopy.

Collaborating with Dr. M. K. Miller of the Oak Ridge National Laboratory on field-ion microscopy and atom-probe micro-composition measurements of high-T_c superconducting materials.

Collaborating with Dr. N. Ernst of the Fritz Haber Institute, West Berlin, FRG on field-ion and field-electron energy-distribution measurements of high-T_c superconducting materials.

Powell, C. J.

Collaborating (with T. E. Madey) with Drs. J. K. N. Sharma and S. M. Shivaprasad of the Indian National Physical Laboratory, under the auspices of the U.S.-Indo Cooperative Program, on experimental studies of metal-semiconductor interfaces.

Collaborating with Dr. D. R. Penn of the NIST Electron Physics Group and Dr. S. Tanuma of the Nippon Mining Company, Japan on calculations of the inelastic mean free paths of low-energy electrons in solids.

Collaborating with Dr. M. P. Seah of the UK National Physical Laboratory on an analysis of the factors affecting the accuracy and precision of quantitative surface analyses by Auger-electron spectroscopy and x-ray photoelectron spectroscopy.

Collaborating with Dr. M. P. Seah of the UK National Physical Laboratory on the development of plans and programs for the Surface Chemical Analysis Working Party of the Versailles Project on Advanced Materials and Standards.

Adjudicator for the Science Prize of the UK ESCA and Auger Users Group.

External examiner for a Doctor of Science candidate, Odense University, Denmark.

Consulted with the Office of Naval Research on a review of selected FY90 Basic Research Options.

Consulted with the Canadian National Sciences and Engineering Research Council on a site visit to the Surface Science Western Laboratory of the University of Western Ontario.

Stockbauer, R. L.

Collaborating (with R. L. Kurtz and T. E. Madey) with Drs. A. Shih, D. R. Mueller, L. Toth, M. Osofsky, and S. Wolf of the Naval Research Laboratory on studies of high-T_c superconductors.

Collaborating (wtih R. L. Kurtz and T. E. Madey) with Drs. A. Shih and D. R. Mueller of the Naval Research Laboratory in photoemission and ion-desorption studies of Ba and BaO on W foil and W(100) as models for high-emission dispenser cathodes.

Collaborating (with R. L. Kurtz and T. E. Madey) with Prof. J. L. de Segovia and Dr. E. Roman of the Instituto Ciencia de Materiales, CSIC, Madrid, on a study of the electronic structure and molecular adsorption of H_2O at low temperatures on transition-metal oxide surfaces.

Collaborating (with R. L. Kurtz) with Drs. J. Rife, W. Hunter, and M. Kabler of the Naval Research Laboratory to instrument a surface science beamline at the Brookhaen National Synchrotron Light Source to extend the photon energy range of experiments beyond what is available at SURF-II.

Consulted with the staff of the American Vacuum Society and the program chairman for the National Symposia on the data base of meeting abstracts and related software.

Yarmoff, J. A.

Collaborating with Dr. J. W. Hudgens of the NIST Chemical Kinetics Division on reactive scattering of molecular and free-radical beams with semiconductor surfaces using multiphoton ionization for detection.

Collaborating with Dr. J. Stroscio of the NIST Radiation Physics Division on electron energy-loss spectroscopy studies of Cs adsorbed on GaAs (110).

Collaborating with Dr. F. R. McFeely of the IBM Watson Research Center on mechanistic studies of the selective chemical vapor deposition of tungsten on silicon and SiO_2 via WF_6 and measurements of the attenuation lengths of very low energy electrons in silicon oxide, and of the relative Si 2p photoemission cross sections at the SiO_2/Si interface as a function of oxidation state and final-state energy.

Collaborating with Dr. J. R. Lince of The Aerospace Corporation on studies of the surface chemistry of MoS_2.

11. VISITING SCIENTISTS

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

Blaisten-Barojas, E., Professor of Physics at the National University of Mexico, is working at NIST during 1987-88 for four months beginning in September, 1988 on theoretical studies of coupled electronic and vibrational excited states of molecule/cluster systems.

Chambers, G. P., a graduate student at the University of Maryland, has worked at NIST for most of the past two years under a cooperative agreement. He has been involved in the development of a data base system for the compilation of evaluated sputtering yield data.

Chen, C.-K., of the Precision Instrument Development Center, Taiwan, worked for one year at NIST during 1987-88 writing a data acquisition software package for the ellipsoidal mirror analyzer.

Drachsel, W., of the Fritz Haber Institute in West Berlin worked at NIST for six weeks during the summer of 1988 on developing a simplified energy-correcting lens for improving the mass resolution of atom-probe field-ion microscopes and on the production of energetic neutral hydrogen atoms in the field ionization of hydrogen.

Elswijk, H. B., of the University of Groningen, The Netherlands is working at NIST for ten months beginning in June, 1988 on studies of the microcomposition and microstructure of high-T_c superconducting materials.

Jacob, I., of the Ben Gurion University of the Negev, Israel has worked at at NIST for one year beginning September, 1987 on the growth of novel epitaxial crystal structures.

Kelley, R. D., of the Department of Energy has collaborated on the design of neutron scattering experiments involving the use of ^{60}Ni in a Raney nickel catalyst.

Larsson, C. U. D., of the Royal Institute of Technology, Stockholm, Sweden has worked at NIST on an occasional basis on ESDIAD experiments to investigate the interaction of water with silicon surfaces.

Marton, D., of the Technical University of Budapest, Hungary has worked at NIST over most of the past two years to determine the interface-width dependence in the depth profiling of thin films on topographic changes during sputtering, to determine effects of radiation-enhanced diffusion on depth profiles, and to characterize thin-film systems as standard reference materials

Mintz, M., of the Ben Gurion University of the Negev, Israel is spending one year at NIST beginning August, 1988 performing experiments to measure kinetic energy distributions of sputtered neutrals and ions and their states of excitation.

Mueller, D. R., of the Naval Research Laboratory has worked at NIST during the past two years on photoemission studies of high-T_c superconducting materials and dispenser cathode materials using the SURF-II synchrotron light source.

Nicol, J. M., of the University of Maryland has worked at NIST from the fall of 1986 to the fall of 1987 on neutron-scattering experiments to characterize adsorption on surfaces of high-area metallic and zeolite catalysts.

Ong, C. K., a Professor of Physics at the National University of Singapore, worked at NIST for six months beginning in October, 1987 on the development of a semiclassical theory of x-ray photoelectron diffraction.

Polak, M., of the Ben Gurion University of the Negev, Israel spent one year at NIST beginning in the summer of 1986 performing studies of the structure and reactivity of water on Cu(110).

Roman, E., of the Instituto Ciencia de Materiales, CSIC, Madrid worked at NIST for five months in 1987 on photoemission studies of the effects of defects on chemisorption on TiO_2 surfaces using synchrotron radiation from the NIST SURF-II facility.

Roncin, P., of the Universite Paris, Orsay, France worked at NIST for seven months in 1987 on an experiment to determine the kinetic energy distribution of sputtered atoms.

Shapiro, M. H., a Professor of Physics at the California State University at Fullerton, has worked at NIST on an occasional basis during the year beginning September, 1987 on multiple-interaction calculations of ion-surface collisions.

Shih, A., of the Naval Research Laboratory has worked at NIST during the past two years on photoemission experiments to characterize high-T_c superconducting materials and dispenser cathode materials using the SURF-II synchrotron light source.

Shivaprasad, S. M., of the National Physical Laboratory, New Delhi, India worked at NIST for six months beginning in May, 1987 studying the surface chemistry and physics of ultrathin films of platinum on tungsten.

Tanuma, S., of the Nippon Mining Company, Saitama, Japan, worked at NIST on a two-year assignment beginning in August, 1985. He made calculations of inelastic mean free paths of low-energy electrons in solids and analyzed algorithms for locating peak maxima in x-ray photoelectron spectroscopy.

Thurgate, S. M., of Murdoch University, Perth, Western Australia worked at NIST for eight months beginning March, 1988 on experiments to study the oxidation of indium phosphide and on the design and construction of an experiment to measure the shifts of core-level binding energies for surface atoms by grazing-angle photoemission.

Walczak, M. M., a graduate student at Iowa State University, spent five months at NIST in early 1987 studying the structure and bonding of fluorinated molecules on surfaces using ESDIAD.

Wang, Q., Fudan University, Shanghai, Peoples Republic of China has worked at NIST for 1 1/2 years beginning June, 1987 on experiments to measure electron attenuation lengths in condensed molecular solids.

12. SURFACE SCIENCE DIVISION STAFF

As of September 30, 1988 the Surface Science Division was staffed as follows:

C. J. Powell, Chief
L. M. Johnson, Secretary
T. E. Madey

Surface Dynamical Processes Group

R. R. Cavanagh, Group Leader
P. M. Connelly[#]
S. A. Buntin[*]
R. A. Demmin[*]
J. W. Gadzuk
S. A. Joyce[*]
R. L. King[+]
R. L. Kurtz
E. O. Neitzel[#]
D. E. Ramaker[@]
L. J. Richter[*]
S. A. Robey
R. L. Stockbauer
J. A. Yarmoff

Thin Films and Interfaces Group

W. F. Egelhoff, Jr., Group Leader
P. P. Camus
T. J. Jach
A. J. Melmed
M. D. Stiles

Surface Spectroscopies and Standards Group

C. J. Powell, Group Leader
N. E. Erickson
J. Fine

[*] NIST-NRC Postdoctoral Research Associate

[@] Faculty Appointment, Part-Time

[#] Engineering Technician

[+] Electronics Technician

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This report summarizes technical activities of the NIST Surface Science Division during Fiscal Years 1987 and 1988. These activities include surface-standards work, experimental and theoretical research in surface science, the development of improved measurement methods, and applications to important scientific and national problems. A listing is given of publications, talks, professional committee participation, and professional interactions by the Division staff.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

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