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Technical Activities 1984
Surface Science Division

C.J. Powell, Chief

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
National Measurement Laboratory
Center for Chemical Physics
Surface Science Division
Gaithersburg, MD 20899

November 1984

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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

ABSTRACT

This report summarizes technical activities of the NBS Surface Science Division during Fiscal Year 1984. 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 NBS Surface Science Division for the period October 1, 1983 to September 30, 1984. The report was prepared as part of the Annual Report of the Center for Chemical Physics within the National Measurement Laboratory of NBS. Much of the writing was done in June and July of 1984 and the report contains details of work completed since the preparation of the 1983 report a year earlier.

The technical work of the Division is separated formally into a task for the Development of Measurement Methods for Surface Properties and a Surface Science Competence task, as outlined briefly in the Introduction. The former task has two principal activities, a Surface Standards Program and a Surface Measurements Program. Work performed for these two programs is reported in Sections 2 and 3, respectively, of the report while work performed for the competence task is reported in Section 4. There are a number of separate technical projects for each activity. Information is given on project objectives, results obtained during the past year, 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 NBS are given in Section 7. The involvement of Division staff on professional committees is shown in Section 8 while internal and external scientific collaborations are described in Section 9. Visiting scientists who have worked in the Division during the year are identified in Section 10 and the Division staff is listed in Section 11.

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 Bureau of Standards, Gaithersburg, MD 20899 (telephone, 301-921-2188).

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SURFACE SCIENCE DIVISION

C. J. Powell, Chief

SUMMARY OF ACTIVITIES

Fiscal Year 1984

1. INTRODUCTION

A. Background

Over the last ten years, there has been a dramatic growth of surface science and its applications. At the national and local meetings of many professional societies, there are typically multiple sessions of papers concerned with the physical and chemical properties of surfaces. Similarly, many current professional journals and books are devoted in whole or in part to similar reports of recent advances in this field. These advances result from investigations of basic surface properties (such as composition, atomic structure, electronic structure) of surfaces and the dependence of many complex surface processes (such as molecular sticking, dissociation, diffusion, reaction, and desorption) on the basic properties and other variables relevant to catalysis, corrosion, thin-film systems, microelectronics, computer elements, and communications applications. Investigations of this type range from fundamental studies, at an atomic and molecular level, on clean single-crystal surfaces to similar studies on appropriately modified surfaces or structures and lead not only to the development of surface science but also to new materials, devices, and processes. Similar investigations, principally measurements of surface composition and of other needed properties, are frequently made of a large variety of materials (e.g., metals, polymers, semiconductors, oxides, glasses, etc.) after fabrication and at various time during their service life for quality control, process optimization, and failure analysis.

A large number of techniques are utilized for surface characterization. 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). 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 very 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.

The techniques utilized in surface science have generally been applied to characterize surfaces in an ultrahigh vacuum environment. The solution of many scientific and technical problems often requires removal of liquid- or gas-phase material prior to surface examination and/or the removal of solid-phase material to expose a region of interest. While this approach has often been successful, artifacts of many different types can arise during the removal of one or more phases. There is therefore a growing need for improved measurement methods that can be used for the *in situ* characterization of solid-solid, solid-liquid and solid-gas interfaces with the sensitivity, elemental specificity, and spatial resolution comparable to those attained with the current surface-characterization methods.

B. Goal, Objectives and Division Program

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 standard procedures, calibration data, and reference materials in cooperation with national and international standards organizations; and

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

Objectives (1) through (3) are met organizationally through an NBS task titled "Development of Measurement Methods for Surface Properties" (Task 15502). The Division's program for this task is divided into two principal activities, a Surface Standards Program and a Surface Measurements Program. Work performed during the year in these two areas is reported in Sections 2 and 3, respectively. This work is supported by NBS resources (including some funds transferred through the Office of Standard Reference Data) and by contracts with three Federal agencies (Office of Naval Research, Department of Energy, and National Aeronautics and Space Administration).

Objective (4) is met as a result of the NBS Competence Program through a task titled "Surface Science" (Task 26103). Some objectives of this task are also supported by contracts with other agencies (Office of Naval Research, Department of Energy). A separate report on these activities is given in Section 4.

C. Technical Output and Professional Interactions

Sections 5 and 6 of this report contain listings of the publications and talks, respectively, for the past year by Surface Science Division staff and for projects supported by the Division. These listings were prepared before the end of the fiscal year and include publications and talks for the latter part of FY 83 not given in the previous Division report.

Many members of the Division staff hold leadership positions in professional societies and groups, as listed in Section 8. These interactions not only reflect the professional esteem in which these staff members are held but provide useful mechanisms for both disseminating the results of NBS work and for learning of significant measurement problems being faced by those using surface-characterization equipment.

Interest in surface science and surface characterization at NBS continues to grow. The Division has had an active Seminar program, as indicated in Section 7, and these seminars have been attended by other NBS staff. The Division staff also participates in an informal weekly lunch meeting, attended by scientists from a number of NBS organizational units, at which developments in surface science are discussed. Members of the Division staff are frequently consulted on a wide range of NBS problems.

Much of the Division's work is carried out in collaboration with other scientists within NBS, within the U.S.A., and internationally. The nature of these collaborations is shown in Section 9. These collaborations are considered important because they enable a relatively small Division staff to work synergistically with other experts, they enable us to have access to unique facilities or expertise, and they enable our expertise to be extended to a larger range of important scientific and technical problems.

The Division has been fortunate in having eleven visiting scientists work at NBS for varying periods during the past year, as indicated in Section 10. These scientists enrich our staff and our projects. A further enrichment of our programs comes from Postdoctoral Research Associates who hold 1- to 2-year appointments; six Postdoctoral Research Associates worked in the Division during FY 1984.

2. SURFACE STANDARDS PROGRAM

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 standard practices, 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.

A. Reference Data

We describe here results of projects in which needed reference data are being generated. Section 2.C includes recent review articles that summarize and evaluate data required in a number of surface spectroscopies.

1. Measurement of Absolute Ion Sputtering Yields
(J. Fine)

The principal aim of this work is to obtain absolute sputtering yields of 1-5 keV ions on well-characterized elemental samples in order to improve the accuracy of depth-profiling measurements by current surface-methods. The accuracy of depth-profiling measurements is at present limited by the unavailability of accurate, reliable, sputtering-yield data and by the lack of knowledge of the topographical and morphological effects produced by ion bombardment.

The use of quartz-oscillator techniques to measure mass loss due to ion bombardment can result in very accurate determinations of ion-sputtering yields. In addition to the third-harmonic oscillator method developed at NBS, another system (operating in the fundamental mode) has been developed at the J. Stefan Institute in Ljubljana, Yugoslavia as part of a joint US/Yugoslavia program and is presently in operation.

Measurements have been made using the quartz oscillator facilities in Ljubljana to determine sputtering yields of Ni/Cr multilayered thin-film materials of structure and morphology similar to those of the NBS Ni/Cr SRMs (Section 2.B). Similar measurements have been initiated at NBS using the third-harmonic method. Quartz crystal of our own design, having highly polished surfaces, were used as substrates during the actual production-run deposition of our SRM structures. These same SRM materials will be used for mass-loss sputtering-yield determinations; such data will then permit our Ni/Cr SRMs to be useful in the calibration of depth scales for other materials whose sputtering yields are known.

Similar measurements are planned on a variety of in-situ prepared elemental targets to obtain ion-dose dependent sputtering yields.

2. 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 therefore will prepare 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 NBS 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. We will initially prepare such compilations of sputtering yields for elemental targets only. We anticipate making use of the HP1000 Data System in the Center for Chemical Physics.

This project was initiated in June, 1984. Progress to date and plans are:

a. A system designed to compile sputtering yield data is being developed and is to be implemented on the HP1000 System.

b. A bibliography of sputtering yield data is being assembled and reprints are being collected.

In the coming year we intend to abstract, evaluate, and compile sputtering-yield data of interest to the surface-analysis and sputter-depth-profiling community on elemental targets.

3. Measurement of Core-Level Binding Energies
(C. J. Powell and N. E. Erickson)

Accurate reference values of the binding energies of core-level electrons are needed for the commonly used technique of x-ray photoelectron spectroscopy (XPS) and for other surface-characterization methods. These values are needed for the calibration of instrumental energy scales. For this application, data are required for a limited number of pure materials that adequately cover the range of common measurements.

We have previously made high-accuracy measurements of the principal core-level binding energies of Ni, Cu, Ag, and Au by XPS. These values compare favorably with similar high-accuracy values measured independently in other laboratories by other methods. We have similarly made high-accuracy measurements of the kinetic energies of Auger electrons from Ni, Cu, Ag, and Au.

At the time that these measurements were being made, we noticed that literature values of XPS binding energies appeared to be systematically higher, by about 1 eV, than those measured by appearance-potential spectroscopy (APS). As systematic errors can occur and remain undetected in binding-energy measurements by any one technique, we have measured binding energies by XPS, APS, and core-level electron energy-loss spectroscopy (EELS) with the same samples and the same reference power supplies to eliminate the more obvious sources of possible error in comparisons of measurements made in different laboratories.

We have determined the L_3 binding energies for Ti, V, Cr, Fe, Co, and Ni by XPS, APS, and EELS. XPS measurements were made from the energy positions of the photoelectron peaks and the EELS measurements were made of the minimum energy loss for a particular core excitation. The latter measurements were made as a function of incident electron energy, from about 50 eV above the threshold for L_3-shell excitation to 1500 eV; in general, the measured EELS binding energies varied slightly with incident energy. The determination of an APS binding energy requires comparison of the measured spectrum with a calculated spectrum. The latter is based on a one-electron model in which the core-electron and the scattered electron both reach final states above the Fermi level. If agreement of the calculated and measured APS data is obtained, it is then possible to identify the electron energy on the experimental spectrum that corresponds to a final state with two electrons at the Fermi level.

Table 1 summarizes our numerical results. For Ti and V, there was significant disagreement in the calculated and measured APS spectra so the indicated APS binding energies must be regarded only as estimates. For Cr, Fe, Co, and Ni, the differences between XPS and APS binding energies range between 0.6 and 1.5 eV, a result similar (for Fe, Co, and Ni) though different in detail to that found in the literature. In general, the EELS energies do not interpolate between the APS and XPS binding energies, the limits expected for adiabatic and sudden excitation, respectively.

Our principal conclusions are as follows: (1) There is a breakdown of the simple one-electron model to describe the APS data for Ti and V. (2) There may be different final states for each type of excitation. We do, in fact, observe changes in EELS lineshapes for Ti, V, and Cr, as the incident energy is varied. (3) There appears to be a varying screening response of the solid for each type of excitation. (4) Our results indicate that conventionally measured binding energies obtained by different methods may differ. A more detailed knowledge of the applicable final states and selection rules is needed to transfer binding energies from one spectroscopy to another.

We plan to compare our present method of calibrating electron energies using a thermionic electron source with a field-emission electron source. The latter method may be more accurate since no work-function correction is required. We also plan to use an existing x-ray monochromator as the detection device in a bremsstrahlung isochromat spectrometer. Core-level binding-energy measurements by this technique will complement the current measurements with XPS, APS, and EELS.

Table 1. Summary of L_3-shell binding-energy data for 3d elements obtained by APS, EELS, and XPS. The EELS binding energies were found to depend on incident electron energy; the lowest and highest measured EELS binding energies are shown here and correspond to the lowest and highest incident energies, respectively, used for each element. The uncertainty of each measurement is estimated to be ±0.2 eV. The APS data for Ti and V are questionable as there was inadequate agreement of measured and calculated spectra.

Element	Binding energy (eV) APS	EELS	XPS
Ti	455.1(?)	453.5-454.0	454.1
V	510.9(?)	512.0-512.4	512.6
Cr	573.9	573.7-574.5	574.6
Fe	705.8	706.7-707.0	707.3
Co	777.7	777.7-777.9	778.7
Ni	852.2	851.6-851.8	852.8

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

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

A project was initiated in FY 82 with funding by the NBS Office of Standard Reference Data 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 Dr. C. D. Wagner, a contractor to NBS, and the Surface Science Division is providing technical review. Dr. Wagner has currently generated over 8000 "lines" of data in his data files. It is expected that a report will be prepared for the Journal of Physical and Chemical Reference Data.

5. Inelastic Mean Free Paths and Attenuation Lengths of Electrons in Solids

(C. J. Powell)

The inelastic mean free path (IMFP) of low-energy electrons in solids is a key parameter in quantitative surface analysis by Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS). For electrons of energy between 100 and 2000 eV, the range of practical interest for AES and XPS, the IMFP is typically between 3 and about 30Å. Experimental measurements of the related quantity, the attenuation length (AL), are difficult and most published AL values are believed to have substantial uncertainties. (The IMFP is the average distance between successive inelastic collisions while the AL results from measurements analyzed with a model in which elastic electron scattering is assumed to be insignificant.) Theoretical IMFP calculations may also be in error on account of approximations and assumptions made in the analysis. It has therefore been difficult to reconcile available IMFP calculations and AL measurements and, in particular, to establish how IMFP and AL values vary with material and electron energy.

IMFP calculations have been made for eight materials (C, Mg, Aℓ, $A\ell_2O_3$, Cu, Ag, Au, and Bi) from tabulations of dielectric data. The dielectric data, from the infrared to the x-ray region, satisfies various sum rules. As assumption needs to be made concerning the momentum-transfer dependence of the complex dielectric constant but this choice does not affect the conclusions appreciably.

Previous authors have fitted values of IMFP, λ, to a relation of the form $\lambda \propto E^n$, where E is the electron energy. A widely-used empirical formula based on AL data suggests that $n = 0.5$ while simple theory indicates $n \approx 0.75$. The present calculations show that $n \approx 0.75$ for the "free-electron-like" solids (e.g., Mg, Aℓ, Bi) but that $n \approx 0.6$ for the noble metals. These differences, which are in accord with trends of the available AL data, can be explained by different spectral distributions in the dielectric data. Differences in the absolute values of IMFP from one material to another (for a constant electron energy) appear to be greater than expected from the empirical formula. These results indicate that additional IMFP calculations and more AL data are needed in order to perform quantitative surface analyses by AES and XPS with the desired accuracy.

6. Electron Attenuation Lengths in Condensed Molecular Films
(R. L. Kurtz, R. Stockbauer, N. Usuki, T. E. Madey)

Measurements of the electron attenuation length, λ, in condensed molecular layers have been made for electron energies from 18-70 eV at the NBS SURF-II synchrotron radiation facility. The molecules (H_2O, CH_3OH, and C_6H_{12}) were condensed with unit sticking probability at 90 K on clean Cu(100) by dosing with the known flux of a calibrated micro-capillary array doser. The drop in photoelectron emission intensity from the Cu 3d band was measured as a function of increasing layer thickness. By varying the incident photon energy, the resultant photoelectron kinetic energy was varied. Semi-logarithmic plots of the emission intensity versus the molecular dose yield straight lines whose inverse slopes give the attenuation length directly. Plots of λ vs. electron energy for each molecule exhibit weak energy dependences, with broad minima in the range 30-40 eV. The mean minimum values of λ for each film are: C_6H_6, (6.1 ± 1.5) Å; CH_3OH, (7.3 ± 1.8) Å; H_2O, (9.0 ± 2.2) Å. These are the first such measurements for these molecules in this energy range, and have important implications for the theory of electron transport in solids, as well as radiation damage processes in biomaterials.

7. Angular-Anisotropy Effect in Measurements of Electron Attenuation Lengths in Crystalline Films

(W. F. Egelhoff)

Attenuation lengths of low-energy electrons in solids, important for quantitative surface analysis by Auger-electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS), have been frequently measured from the characteristic decay or growth of an AES and XPS signal as a film of increasing thickness is deposited on a substrate (see section 2.1(f)). We have recently found evidence for a serious source of error that may arise in such measurements when the overlayer film is ordered.

Figure 1 shows a striking example of the observed effect. The lower curve shows XPS data for the nickel $2p_{3/2}$ photoelectron peak measured after 0.3 monolayers of nickel had been deposited on a Cu(100) substrate. The top curve shows similar data, recorded under the same measurement conditions, after the nickel film had been covered by 1.5 monolayers of copper. Instead of the expected decrease in the Ni signal due to electron attenuation in the Cu overlayer, there is a sharp increase if, for this case, the photoelectrons are collected at a polar angle of 45° in the <100> surface azimuth. For these conditions, the overlayer film acts to increase rather than attenuate the Ni signal.

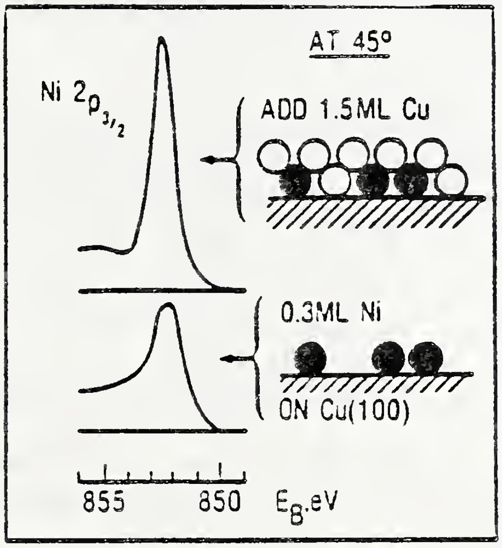

Fig. 1. X-ray photoelectron spectrum from 0.3 monolayers of nickel on a Cu(100) substrate (bottom) and following the addition of 1.5 monolayers of copper (top).

The basis of this new phenomenon is the forward-scattering enhancement of photoelectron intensities along internuclear axes that is described in Section 4.B.5. The overlying Cu atoms redirect the Ni core-level intensity from being nearly isotropic to being peaked at the 45° polar angle. At other polar angles, the Ni XPS signal decreases as expected.

These measurements indicate that conventional attenuation-length measurements by the overlayer-film method may have substantial errors. These errors will depend on the particular measurement geometries and the degree of crystalline order in the overlayer film. Work is in progress to determine the magnitude of the forward-scattering effect in other systems and to examine its impact in more detail on attenuation-length measurements.

8. Background Estimation in X-Ray Photoelectron Spectroscopy and Auger-Electron Spectroscopy

(W. F. Egelhoff)

A difficult problem that arises when x-ray photoelectron spectroscopy (XPS) and Auger-electron spectroscopy (AES) are used for quantitative surface analysis is the estimation and subtraction of the "background" intensity under the peaks of interest. No rigorous experimental or theoretical method has as yet been devised for making separations of the XPS and AES signals from the often large and sloping background of secondary and scattered electrons. Common practice now consists of making arbitrary (but reasonable) estimates of this background guided by inelastic electron scattering data.

A new approach to the background-estimation problem has been discovered based on the forward-scattering phenomena described in section 4.B.5. Figure 2 shows XPS data for Ni(100) that has been decomposed into two parts, XPS intensity which exhibits enhancement at a polar angle of 45° and XPS background intensity (shaded) which does not. The basis of the decomposition is the observation that the primary photoelectron intensity is enhanced along internuclear axes whereas background electrons are emitted isotropically. Although this method of background estimation can be accomplished only with single-crystal materials, the background shape can be compared with results from electron transport calculations.

9. Theory of the Quantum Hall Effect: Application to Measurement of the Fine-Structure Constant and to Realization of a New Resistance Standard

(S. M. Girvin)

Theoretical investigations of the quantum Hall effect have been undertaken in support of the NBS Electricity Division's quantized Hall resistance project. The quantization of the Hall resistance is being used to measure the fine structure constant to very high accuracy and to realize a universal standard of electrical resistance based solely on

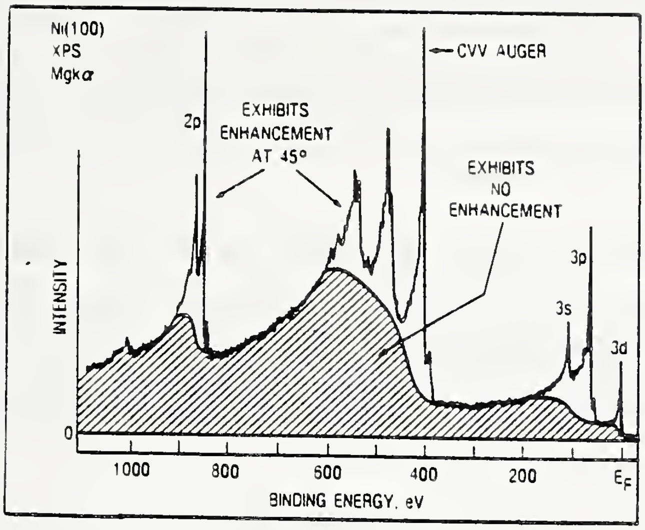

Fig. 2. X-ray photoelectron spectrum of Ni(100). The shaded (background) region indicates the intensity that does not show enhancement at a polar angle of 45°.

fundamental constants of nature. We have addressed both fundamental physics questions (see section 4.2 (g) as well as practical problems concerning possible sources of experimental error in the extremely high accuracy measurements being made. Recent topics of investigation in the latter category include thermoelectric effects and the role of finite temperatures and disorder. Another important area has been the successful interpretation of the sudden, extremely non-linear onset of dissipative breakdown at high current densities. This phenomenon occurs when the carrier drift speed exceeds the speed of sound resulting in a phonon lasing effect.

10. Needs for Reference Data

The growth of surface science and its applications has led to needs for expanded reference data. These needs can be summarized in the following three categories.

a. Surface Analysis

Four techniques are now in common use for surface analysis: Auger-electron spectroscopy (AES), x-ray photoelectron spectroscopy (XPS) or electron spectroscopy for chemical and analysis (ESCA), secondary-ion mass spectroscopy (SIMS), and ion-scattering spectroscopy (ISS). With each technique, there is need for the following reference data:

- evaluation of spectra from pure elements for common conditions of measurement

- evaluation of chemical or matrix effects on spectra

- benchmark data for the calibration of the energy and intensity scales of instruments

- reference data on line positions in compounds

- reference data for key parameters in quantitative analysis (e.g., ionization cross sections (AES, XPS), ion scattering cross sections (ISS), electron inelastic mean free paths and attenuation lengths (AES, XPS), electron backscattering (AES), ion neutralization cross sections (SIMS, ISS), and multiple ionization (SIMS)

- algorithms for data analysis (e.g., determination of background due to multiple scattering (AES, XPS, ISS) and fragments (SIMS, ISS), deconvolution to obtain source lineshape (AES, XPS, ISS), inelastic scattering (AES, XPS), and double scattering (ISS))

- data for ion sputtering yields in elements, alloys, and compounds as a function of ion type, ion energy, and bombardment geometry

- data for radiation damage rates during analysis, including cross sections for desorption from surfaces and decomposition of surface layers.

b. Surface Science

Many techniques are in common use for the determination of surface properties and processes. Data are needed in the following areas:

- reference data on vibrational energies and intensities for molecular species on surfaces (as measured by electron energy-loss spectroscopy, infrared spectroscopy, Raman scattering, neutron inelastic scattering)

- reference data for determination of surface structures by low-energy electron diffraction and other techniques (e.g., library of basic data, algorithms to compute surface structure)

- reference data for absolute determination of surface coverages (atoms/cm^2) on surfaces of different structure and atomic composition

- reference data for surface processes (kinetic data for catalytic and surface reactions, desorption, diffusion, segregation)

- Ion-surface interactions are of importance in sputtering and ion scattering spectroscopy. Reference data are needed to characterize the electron and photon spectroscopy of scattered and sputtered ions, as well as of excited neutral species leaving the surface.

c. Interface Science

There is rapid development now of techniques that can be used for the *in situ* characterization of solid-solid, solid-gas, and solid-liquid interfaces. A variety of techniques (e.g., Rutherford backscattering spectroscopy, infrared spectroscopy, Raman spectroscopy, extended x-ray absorption fine structure, neutron inelastic scattering, particle-induced x-ray emission) are being utilized and reference data and algorithms will be required for their effective application.

The Division plans to establish priorities for these data needs in collaboration with the interested groups including the NBS Office of Standard Reference Data, the recently formed Standard Reference Data Subcommittee of ASTM Committee E-42 on Surface Analysis, and the Surface Chemical Analysis Project of the Versailles Agreement on Materials and Standards (section 2.D.2). A plan for generation of high-priority data will then be prepared.

B. Reference Materials

1. Development and Production of Standard Reference Materials (J. Fine)

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 densities 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.

Prototype thin-film structures were initially fabricated in order to evaluate their usefulness as depth profiling SRM's and to develop appropriate characterization techniques. These structures were made by sputter deposition as part of a joint US/Yugoslavia program between NBS and Dr. B. Navinsek at the J. Stefan Institute in Ljubljana. Analyses of these prototype materials at NBS and by members of ASTM Committee E-42 on Surface Analysis were done using Auger-electron spectroscopy, x-ray fluorescence, secondary-ion mass spectroscopy, Rutherford backscattering spectroscopy, and proton-induced x-ray emission. The results were satisfactory and a stock of similar thin-film SRM's were fabricated in 1982 using the sputter deposition facility at the J. Stefan Institute in Ljubljana.

The analyses obtained on our nickel-chromium multilayered thin-film structures indicate that this material should be of considerable benefit as a depth-profiling SRM. Work on its characterization and calibration is now completed. We have determined the uniformity and periodicity of the thin-film layers, absolute film thicknesses, sputtered interface depth resolution, and structural stability. Measurement methods used to characterize this Ni/Cr SRM include N(E) Auger sputter profiling, Rutherford backscattering spectroscopy (RBS), and neutron activation analysis (NAA).

Previous results of absolute film thicknesses and uniformity obtained by RBS indicate that samples taken from the same production batch, as well as from 3 separate batches are all uniform to ±3 percent for a given layer material. These values now have been further verified with NAA techniques by Dr. R. Fleming of the NBS Inorganic Analytical Research Division. This method analyzes the total Ni and Cu content of the multilayered films by using a gravimetrically calibrated reference; the resulting accuracy is better than 1 percent. NAA results obtained on the Ni layers indicate that the average Ni layer thickness (areal density) determined from three batches is $58.3 \mu g/cm^2$ (±2 percent). The uncertainty in the film thickness variation in samples of a given batch is ±1 percent. The average Ni layer thickness as determined by NAA is 4 percent greater than the RBS value. This difference is probably due to the uncertainty in the stepping power data used in the RBS analysis; this uncertainty is generally recognized to be between 5 and 10 percent. Statistical analysis of our characterization results and calibration data is being completed. This Ni/Cr structure will be issued as NBS Standard Reference Material 2135 once the certificate has been written.

Future work includes characterization and calibration of a "marker" layer-type sputter depth profile SRM which we have recently fabricated in production quantities. This material also was fabricated in Dr. Navinsek's laboratory and consists of eight Cr layers (~ 40 nm each) separated by about 2 monolayers of Cr_2O_3.

2. Quantitative Sputter Depth Profiling of Interfaces
(J. Fine)

Determination of composition-versus-depth at virgin solid/solid interfaces is at present difficult to achieve with sputter-depth-profiling techniques. This is due, to a large extent, to a lack of understanding of the dependence of the sputtered-interface depth resolution on ion bombardment conditions (i.e., ion beam energy, species, angle of incidence, current density, and on sputtered depth). A careful evaluation of such factors which affect interface resolution is not available for any given interface system. A consistent set of such measurements obtained for various ion beam parameters, all done on the same material, would significantly enhance our ability to assess the abruptness of interfaces before sputter-profile analysis took place and would be of value in determining optimum sputter-profile conditions.

Our development of Ni/Cr multilayered SRMs with known layer thickness and periodicity makes it both possible and practical to systematically examine the dependence of interface resolution on ion beam parameters. Use of the computer-controlled, sequential-mode N(E) Auger data system which has been previously developed allows us to obtain reliable and accurate measurements of the interface depth resolution for the Ni/Cr material.

We have made the following measurements during the past year:

a. Sputtered interface depth data has been obtained for 1 and 2 keV argon ion bombardment at various ion current densities at 50° angle of incidence as a function of sputtered depth. We have demonstrated that measured interface depths (using the 10 to 90 percent intensity-change criterion) as narrow as 5.0 nm can be obtained with these SRMs.

b. In collaboration with Dr. B. Navinsek and his group at the J. Stefan Institute in Ljubljana we have made use of quartz crystal microbalance techniques to monitor the rate of mass-loss during sputter profiling. This method allows us to observe interface depths as evidenced by the change in sputtering rate due to the differences in the sputtering yields of Ni and Cr at an interface. Our results indicate that interface depths as narrow as 3.5 nm can be observed on our Ni/Cr SRMs during sputtering with 8 keV argon ions.

c. We also are collaborating with Dr. P. Lindfors of the Perkin-Elmer Corporation - Physical Electronics Division and Dr. D. Mitchell of the National Research Council of Canada, Ottawa to document interface depth resolution dependence on ion beam angle of incidence and on current density. Due to the outstanding structural composition of our SRMs, we have been able to collect a large set of data, and we will be able to define interface "shapes" as well as interface depths. This data should be adequate to warrant calculations of the collision cascade broadening effect at sputtered interfaces.

3. Needs for Reference Materials

The following needs for additional reference materials have been identified.

a. Depth-Profiling SRMs

Surface analysis is frequently combined with ion sputtering to measure composition versus depth and to investigate solid-solid interfaces. It is believed that sputter-depth-profiling applications will continue to grow and, with the development of new techniques for deposition of materials (e.g., molecular-beam epitaxy), the development of better depth-profiling techniques, and demands for better accuracy, use of new materials, and desire for sharper interfaces, there will be an increased demand for suitable SRMs to ensure the reliability of the relevant measurement system.

NBS has recently developed a multi-layer periodically-modulated SRM consisting of alternate layers of Ni and Cr (section 2.2 (a)). Similar structures consisting of Ni/Ag and Cr/Cr_2O_3 have been fabricated but remain to be characterized. We have also fabricated films of Ta_2O_5 on Ta and these also have to be characterized.

There are needs for similar SRMs involving other types of materials in high-technology industries, for example, SiO_2 on Si, epitaxial modulated-thickness films of GaAs/GaAℓAS, thin layers of metals on semiconductors (Schottky barriers), and polymer films on metal substrates.

b. Calibration of Surface Analysis Instruments

There is a growing need for the characterization and calibration of surface-analysis instrumentation, particularly since the newer computer-controlled instruments require greater system stability and reproducibility than before. Until recently, most surface analyses have been qualitative but there is increasing demand for quantitative analyses of defined accuracy. These developments require SRMs for instrument calibration (e.g., of the instrument transmission functions for Auger-electron spectrometers (AES) and x-ray photoelectron spectrometers (XPS) and for the determination of instrument performance (e.g., the detection of trace constituents).

Pure elemental and multicomponent materials can be utilized for calibration of the energy and intensity scales (and instrument transmission functions) of AES and XPS instruments. A suite of pure elements (e.g., Cu, Ag, and Au) could be used for both purposes. Liquid alloys (e.g., Ga-Sn or Ga-In) can be cleaned readily to generate two-component surfaces of known composition for checks of instruments and algorithms for analyses. Multicomponent materials with known quantities of trace elements are needed for determining the ability of an instrument to detect trace species. Suitable materials could include ion-implanted impurities in silicon (with a specified depth distribution and maximum concentration) and multi-component liquid alloys (with homogeneous compositions or with segregation of trace species at the surface).

c. Surface Science

There is a need for SRMs that would lead, with the user following a prescription, to surfaces of known composition (e.g., to known coverage of a chemisorbed layer of molecules on a metal substrate or to a monatomic layer of a metal on a substrate). A single crystal SRM (e.g., Ni) could be cleaned and exposed to different gases (e.g., O_2, N_2, H_2, CO, H_2S) to establish known surface coverages of such gases. Such an SRM would enable calibration of AES and XPS equipment now used for measurements of surface coverages. Another use of the SRM could be through the deposition of several monolayers of a metal (e.g., Ag), again after cleaning, with appropriate thermal treatment to remove all but a monolayer of the deposit. This process could also be used for the calibration of AES and XPS equipment used for investigations of novel properties of ultrathin metal films.

The Division intends to establish priorities for new SRMs in collaboration with the NBS Office of Standard Reference Materials and the Standard Reference Materials Subcommittee of ASTM Committee E-42 on Surface Analysis. Plans for producing additional SRMs will also depend on sales of the recently developed Ni/Cr SRM 2135 (section 2.2 (a)) that will be announced shortly.

C. Review Articles and Books

1. Review Articles

The Division staff authors many review articles and book chapters that provide information on measurement methods, relevant reference data, reference materials, and theories of the measurement process for many surface spectroscopies.

Division staff members have authored 24 review article recently. The titles and abstracts of review articles published since 1983 are listed below:

a. "Adsorption on Metal Surfaces: Some Key Issues," J. W. Gadzuk, in Atomistics of Fracture, eds: R. M. Latanision and J. R. Pickens (Plenum Press, NY), 391-418 (1983).

The physical picture and basic philosophy of the principal techniques for performing theoretical calculations of the electronic structure of adsorbates on metal surfaces are presented. A discussion of spectroscopic probes and non-adiabatic effects is given. These ideas are illustrated via specific case studies.

b. "Fundamental Excitations in Solids Pertinent to Desorption Induced by Electronic Transitions," J. W. Gadzuk, in Desorption Induced by Electronic Transitions DIET-I, eds: N. H. Tolk, M. M. Traum, J. C. Tully and T. E. Madey (Springer-Verlag, NY), 4-25 (1983).

Various aspects of the importance of treating the initial electronic excitation and subsequent atomic, ionic, or molecular nuclear motion as a coherent single process is emphasized. Theoretical modeling is carried out in terms of Franck-Condon factors for both translational degrees of freedom as well as intrinsic substrate excitations. Several desorption scenarios are discussed and model desorbate energy distributions which follow from the theory outlined here are presented.

c. "The Determination of Molecular Structure at Surfaces using Angle Resolved Electron and Photon Stimulated Desorption," T. E. Madey, F. P. Netzer, J. E. Houston, D. M. Hanson, and R. L. Stockbauer, in Desorption Induced by Electronic Transitions DIET-I, eds: N. H. Tolk, M. M. Traum, J. C. Tully, and T. E. Madey (Springer-Verlag, NY), 120-138 (1983).

We review recent data and theoretical models related to the use of angle-resolved electron and photon stimulated desorption in determining the structures of molecules at surfaces. Examples include a variety of structural assignments based on ESDIAD (electron stimulated desorption ion angular distributions), the observation of short-range local ordering effects induced in adsorbed molecules by surface impurities, the influence of electron-beam damage on surface structure, and a direct comparison of ESD and PSD ion yields for the same system.

d. "The Quantum Hall Effect I," M. E. Cage and S. M. Girvin, Comments on Solid State Physics, 11, 1 (1983).

The recent surprising observation of a quantization of the Hall resistance in units of h/e^2 in quasi-two-dimensional conductors presents the possibility of obtaining an improved value of the fine structure constant and development of a quantum standard of resistance using a solid state device.

e. "The Quantum Hall Effect II," S. M. Girvin and M. E. Cage, Comments on Solid State Physics 11, 47 (1983).

The recent surprising observation of a quantization of the Hall resistance in units of h/e^2 in quasi-two-dimensional conductors has necessitated a major rethinking of our theoretical picture of transport in these systems. The central problem is understanding why ideal behaviour persists even in the presence of strong disorder.

f. "Thin Film Reference Materials for Sputter Depth Profile Calibration," J. Fine and B. Navinsek, in Proc. of Invited Lectures and Progress Reports, Symposium on the Physics of Ionized Gases, ed: G. Pichler, Institute of Physics of the University (Zagreb, Yugoslavia), 223 (1983).

Standard reference materials for calibrating depth-of-erosion scales in ion beam sputtering are presently being developed jointly by the National Bureau of Standards, the Josef Stefan Institute, and ASTM Committee E-42 on Surface Analysis. Four separate types of thin film structures have been selected and produced in order to satisfy various needs in depth profile analysis using surface spectroscopies. Advantages of these specific structures as well as details of their fabrication will be discussed. Preliminary results on the characterization and compositional analysis of these prototype materials have been obtained regarding uniformity and periodicity of multilayered films, interface widths, absolute film thickness, film stoichiometry, and film stability and diffusion. The measurement methods used to characterize these thin-film structures include compositional sputter depth profiling using Auger spectroscopy as well as x-ray fluorescence, Rutherford backscattering spectroscopy, chemical analysis, weight-loss measurements due to sputter erosion using quartz oscillator techniques, and proton induced x-ray emission. The results of these analyses indicate that such materials may be well suited for use in sputter depth profile calibration.

g. "Electron and Photon Stimulated Desorption: Benefits and Pitfalls," T. E. Madey, D. L. Doering, E. Bertel, and R. Stockbauer, Ultramicroscopy 11, 187 (1983).

Electron beam irradiation of solids often results in damage-producing events along with information-producing events. In the present paper we explore mechanisms of beam damage in solids, as well as examples of the benefits of electron (and photon) stimulated processes to study molecules at surfaces. Information about the geometrical structure of adsorbed species can be obtained from measurements of the angular distribution of ions released by electron or photon stimulated desorption. The directions of ion emission are directly related to the orientations of the surface bonds which are ruptured by the excitation. The method of Electron Stimulated Desorption Ion Angular Distributions (ESDIAD) has proven particularly useful in characterizing local molecular structure at surfaces in the absence of long range order; recent measurements of bonding configurations stabilized by impurities or by lateral interactions are discussed. Photon stimulated desorption (PSD) studies using synchrotron radiation are providing new insights into fundamental electronic excitation processes at surfaces. Mechanisms for the excitation and desorption of ions are examined (valence, shallow core level and deep-core-level excitations), and examples include ion desorption from adsorbed monolayers, as well as ion formation and desorption processes in condensed molecular films.

h. "An Overview of Research at NBS using Synchrotron Radiation at SURF-II," D. L. Ederer, R. P. Madden, A. C. Parr, E. B. Saloman, G. Rakowsky, J. Copper, R. Stockbauer, T. E. Madey, and J. L. Dehmer, Proc. of the Conference on the Applications of Accelerators in Research and Industry, IEEE Trans. on Nuclear Science NS30, 1020 (1983).

The National Bureau of Standards (NBS) Synchrotron Ultraviolet Radiation Facility (SURF-II) is used in conjunction with several high throughput monochromators to study the interaction of vacuum ultraviolet photons with solids and gases. Recent work has been concerned with the photon stimulated desorption of atomic and molecular ions from surfaces, with the effect of electric fields on molecular photoabsorption and with the study of molecular photoionization by angle-resolved photoelectron spectroscopy. These research programs yield new information about molecular bonding at surfaces, molecular dynamics near ionization thresholds, and the coupling of the electronic and nuclear motion near resonances in molecules. In addition to these programs in basic research, SURF-II is used for the calibration of transfer standard detectors over a photon energy range 20-250 eV. Calibration of monochromator systems is achieved over the photon energy range 5-250 eV by using the now calculable spectral intensity radiated by the electrons, which are confined in a nearly circular orbit.

i. "The Use of Angle Resolved Electron and Photon Stimulated Desorption for the Determination of Molecular Structure at Surfaces," T. E. Madey and R. Stockbauer, Rev. Brasil. Apl. Vac. (J. of Brazilian Vacuum Society) 3, 47 (1983).

This paper is a brief review of recent data related to the use of angle-resolved electron stimulated desorption and photon stimulated desorption in determining the structures of molecules at surfaces. Examples include a variety of structural assignments based on ESDIAD (electron stimulated desorption ion angular distributions), the observation of short-range local ordering effects induced in adsorbed molecules by surface impurities, and the application of photon stimulated desorption to both ionic and covalent adsorbate systems.

j. "Desorption of Ions from Surfaces: Mechanisms of Photon Stimulated Desorption," R. Stockbauer and T. E. Madey, Annals of the Israel Phys. Soc. 6, 483 (1983).

A review is given of the mechanisms of Photon Stimulated Desorption (PSD) from ionic, covalent and van der Waals bonded surface molecules. An interatomic Auger decay process describes desorption from ionically bonded, maximal valency compounds. The mechanism for ion desorption from covalently bonded systems is thought to involve relatively long-lived two-hole states. Ion desorption from thick molecular films presents a challenge to theory since heavy fragments (C_xH_y) desorb from some (cyclohexane) and not from others (water, methanol).

k. "Instrumentation for Photon Stimulated Desorption," R. Stockbauer, Nucl. Instr. Meth. 222, 284 (1984).

Photon stimulated desorption (PSD) refers to the ejection of ions, atoms or molecular fragments from a surface initiated by the absorption of single photons; to date, most studies have concentrated on detection of ions. The properties of PSD which make it attractive as a surface characterization tool are its extreme surface sensitivity, the ions being ejected only from the topmost layer and the rapidity with which the ions are ejected. Since the desorption is fast ($\sim 10^{-14}$ s), with respect to molecular vibrations ($\sim 10^{-12}$ s), the ion trajectory reflects the initial bonding geometry of the particle to the surface.

To study the ion desorption process, one would like to know the mass, kinetic energy distribution, angular distribution and the yield (desorption rate vs. photon energy) of the desorbing ions. Time-of-flight (TOF) analyzers are used where the time between the light pulses from the synchrotron light source is on the same order as the flight time of the ion from the surface to the detector. One can measure easily ion mass and yield but not kinetic energy or angular distributions with this class of analyzer. Electrostatic deflection analyzers are used to measure ion yields and kinetic energy distributions and, in some instruments, ion angular distributions. In general, they are useful where the time structure of the synchrotron light is too short to allow TOF analysis. Optical methods have recently been applied to the detection of excited states of neutral Li seen in PSD of LiF.

l. "Inelastic Scattering of Electrons in Solids," C. J. Powell, in Electron Beam Interactions with Solids for Microscopy, Microanalysis, and Microlithography, D. F. Kyser, H. Niedrig, D. E. Newbury and R. Shimizu, eds. (SEM Inc., Chicago), 19-31 (1984).

The principal mechanisms and available data for the inelastic scattering of electrons in solids are reviewed. The processes relevant for electron-probe microanalysis, electron energy-loss spectroscopy, Auger-electron spectroscopy, and x-ray photoelectron spectroscopy are described and examples of relevant electron energy-loss data are shown. The discussion is based on the dielectric description of inelastic scattering and treats processes important in the excitation of both core electrons and valence electrons. Information is given on the cross sections for ionization of core levels, inelastic mean free paths of Auger electrons and photoelectrons in solids, and radiation damage.

m. "Non-adiabatic Effects in Elementary Surface Reactions: State-to-State Molecular Beam Experiments as a Probe," J. W. Gadzuk, in Many-Body Phenomena at Surfaces, D. Langreth and H. Suhl, eds. (Academic Press, NY), 517 (1984).

A theory of elementary chemical reactions at solid surfaces is described in terms of surface induced diabatic transitions between "reactant" and "product" potential curves. It is then shown how the internal vibrational state distribution of a diatomic molecule scattered from a surface could provide unique dynamical information required as input to the diabatic transition theory.

n. Early Applications of Vacuum, from Aristotle to Langmuir," T. E. Madey, J. Vac. Sci. Tech. A2, 110 (1984).

Highlights of the development of vacuum science and technology from ancient times to the early twentieth century are reviewed. The view of the Greek philosophers that vacuum was an impossibility hampered understanding of the basic principles of vacuum until the mid 17th century. Verifiable vacua were first produced in Italy by Berti and Toricelli; von Guericke's dramatic experiments vividly demonstrated atmospheric pressure. Piston-like "air pumps" were widely used in England and the European continent through the 18th and early 19th centuries to produce and characterize the properties of vacuum (lack of sound transmission, inability to support life, gas discharges, etc.). The Industrial Revolution was made possible through the genius of Newcomen, who designed huge atmospheric engines (based on condensation of steam to form a vacuum beneath a piston, which was then driven by the pressure of the atmosphere). A system of "atmospheric railways" propelled by vacuum pistons was built in England in the mid 19th century. Serious scientific developments of the 19th century which necessitated vacuum included Crooke's and Faraday's gaseous discharge measurements, the first sputtering experiments by Grove, the isolation of the rare gases by Ramsey, the standards work of Miller, the discovery of the electron by Thomson and of X-rays by Rontgen. The development of the incandescent light by Edison provided a background for the remarkable achievements of Langmuir in vacuum and surface science at the dawn of the 20th century. An appendix is included which lists museums containing vacuum-related exhibits.

2. Review Articles in publication

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

a. "The Chemisorption of Carbon Monoxide by the Transition Metals," J. T. Yates, Jr., T. E. Madey, and J. C. Campuszno, The Chemical Physics of Solid Surfaces and Heterogeneous Catalysis, eds: D. A. King and D. P. Woodruff.

A comprehensive review of the adsorption of carbon monoxide by transition and noble metals is presented. The systematics of CO adsorption and dissociation are discussed, along with detailed examinations of the surface structures, electronic and vibrational spectra, and kinetic behavior of adsorbed CO.

b. "The Thermal Desorption of Adsorbed Species," J. T. Yates, Methods of Experimental Physics, ed: R. L. Park.

The experimental and theoretical basis of thermal desorption spectroscopy as a tool for surface characterization is described. Methods of analysis of thermal desorption spectra to obtain kinetic information (desorption energies, desorption order, coverages of adsorbed species) are included, together with numerous examples of desorption of small molecules from single-crystal metal surfaces.

c. "Experimental Methods in Electron and Photon Stimulated Desorption," T. E. Madey and R. Stockbauer, Methods of Experimental Physics, ed: R. L. Park.

We review experimental techniques and applications of electron stimulated desorption (ESD) and photon stimulated desorption (PSD) of atomic, molecular, and ionic species from surfaces. The physical principles of these methods, as well as details of experimental measurements and data analysis are discussed. We close with a discussion of beam damage in surface analysis.

d. "Laser Studies of Surface Chemical Reactions," R. R. Cavanagh and D. S. King, Chemistry and Physics of Solid Surfaces V, Springer-Verlag.

A review of laser studies of surface chemical dynamics with emphasis on thermal desorption processes is presented. The correlation of gas-phase and liquid-molecular dynamics with analogous surface processes is demonstrated with primary emphasis on experimental techniques for monitoring relevant quantum state populations. Recent results for the desorption of NO from Ru(001) and NO from oxidized Ru crystals are compared in terms of rotational populations, and velocity and angular flux distributions.

e. "Final-State Resolved Studies of Molecule-Surface Interactions," D. S. King and R. R. Cavanagh in New Laser and Optical Investigations of Chemistry and Structures at Interfaces, Verlag Chemie.

Quantum state-specific diagnostics as applied to surface dynamics are discussed. The NO molecule is used as an illustration of the experimental determination of gas-surface interactions. Topics reviewed included beam-surface scattering, thermal desorption, vibrational accommodation, Doppler profiles, and Fourier-transform infrared emission spectroscopy.

f. "Characterization of Surfaces Using Electron and Photon Stimulated Desorption," T. E. Madey, D. E. Ramaker, and R. Stockbauer, Ann. Rev. Phys. Chem.

We review various mechanisms of electron- and photon-stimulated desorption of ions and neutrals from surfaces. Examples include desorption from ionic surfaces, from covalent adsorbates on metal surfaces, and from layers of physically adsorbed atoms. The use of the electron stimulated desorption ion angular distribution (ESDIAD) method for determining local structures of surface molecules is described.

g. "Inelastic Mean Free Paths and Attenuation Lengths of Low-Energy Electrons in Solids," C. J. Powell, Scanning Electron Microscopy/1984.

A review is given of calculations of inelastic mean free paths and measurements of attenuation lengths of low-energy electrons in solids. The emphasis of the review is on the systematics of the dependences of these quantities on material and electron energy. Calculations of inelastic mean free paths from experimental dielectric data indicate that different dependences on electron energy occur in different materials and that deviations from simple theoretical or empirical expressions are to be expected.

h. "Innershell Ionization Cross Sections," C. J. Powell in Electron Impact Ionization, T. D. Märk and G. H. Dunn, eds., Springer-Verlag.

A review is presented of cross-sections for the ionization of inner-shell electrons by electron impact. Calculations, measurements, and empirical formulas are described and compared. Recommendations are given for the selection of cross-section data. Finally, applications of inner-shell ionization cross-section data to materials and surface analysis problems are described.

i. "Core Level Binding-Energy Shifts in Solids at Surfaces," W. F. Egelhoff, Jr., Surface Sci. Reports.

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 relative merits of the 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.

j. "Methods for Producing Clean Liquid Surfaces," J. Fine and S. Hardy, in Treatise on Clean Surface Technology, K. L. Mittal, ed.

A review of techniques which have been used to produce atomically clean surfaces on liquids is presented. Methods are discussed for the handling and pre-cleaning of liquid specimens. Ultrahigh vacuum techniques for obtaining clean liquid surfaces are divided into two types: those which do so by creating a new surface and those which act by removing impurities that are present. The techniques include a number of variations on drawing pure liquid from the interior of a reservoir, deposition of liquid films, skimming, evaporation, dissolution, chemical reactions, and sputtering by ion bombardment. A number of specific liquid systems are discussed.

3. Books
(C. J. Powell, 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 a 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 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.

Volumes 1 and 2 of the book series will describe the techniques and methods for electron spectroscopy and ion spectroscopy, respectively, which are in widespread use for surface analysis. These volumes will be concerned largely with techniques for which commercial instrumentation is available. It is hoped that writing for Volume 1 will be completed in 1984 and that for Volume 2 by early 1985.

Volume 3 will describe techniques for specimen handling and depth profiling. For specimen handling and treatment, this volume will provide a compilation of methods that have proven useful. This volume will also address the common artifacts and problems associated with the bombardment of solid surfaces by electrons and ions. Finally, a description will be given of methods for depth profiling. Authors have been selected to write chapters for this volume.

Volume 4 will bring together a description of methods for vibrational spectroscopy of molecules on surfaces. Most of the techniques are currently under active development; commercial instrumentation is available for some techniques but this situation could change in the next few years. The current state-of-the-art of each technique will be described as will the relative capabilities. An important component of the volume will be the summary of the relevant theory. Authors have been selected to write chapters for this volume.

D. Standards-Committee Activities

Three staff members of the Division hold offices on two ASTM Committees, the E-42 Committee on Surface Analysis and the D-32 Committee on Catalysts, and on the recently approved Surface Chemical Analysis Working Party established under the auspices of the Versailles Agreement on Materials and Standards. Participation in the activities of these groups provides an opportunity for leadership, for dissemination of NBS expertise, and to learn of significant measurement problems in relevant areas.

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

The ASTM Committee E-42 on Surface Analysis founded in 1976, now has some 140 members; in addition, a large 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. There is substantial activity in all of these areas.

Committee activities of the past year include approval of the following standards:

- E673-84: Standard Definitions of Terms Relating to Surface Analysis (includes additions of terms for AES, ESCA, and SIMS)
- E983-84: Standard Guide for Electron Beam Effects in Auger Electron Spectroscopy
- E984-84: Standard Guide for Identifying Chemical Effects and Matrix Effects in Auger Electron Spectroscopy
- E995-84: Standard Guide for Background Subtraction Techniques in Auger Electron Spectroscopy
- E996-84: Standard Practice for Reporting Data in Auger Electron Spectroscopy
- E1015-84: Standard Practice for Reporting Spectra in ESCA (Electron Spectroscopy for Chemical Analysis)
- E1016-84: Standard Practice for Determining and Specifying the Properties of Electrostatic Electron Spectrometers

The following proposed standards are at various stages of Committee or Subcommittee ballot:

- Additions to Standard Definitions of Terms Relating to Surface Analysis (for ESCA and Energetic Ion Analysis methods)
- Standard Guide for Specimen Handling
- Standard Practice for Reporting Depth Profile Data in Secondary Ion Mass Spectrometry

Other standards are being drafted.

The Committee sponsors two symposia each year, one at the annual Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy in the spring and the other at the National Symposium of the American Vacuum Society in the fall. Papers presented at these symposia are published. A workshop is held at each meeting to discuss particular measurement problems. At the 1983 American Vacuum Society Symposium the topic was "Case Studies in Ion Sputtering: Applications and Limitations," and the topic at the 1984 Pittsburgh Conference was "Solving Industrial Problems Using Surface Analysis."

Technical Subcommittees of the E-42 Committee have organized a number of round robins to compare the results of nominally identical measurements in different laboratories. The following round robins are currently in progress:

- Comparison at the relative intensities of Auger-electron peaks in a series of Cu-Au alloys
- Comparisons of depth distributions measured by secondary-ion mass spectroscopy (SIMS) for ^{11}B implanted in Si
- Comparisons of the relative intensities of peaks in SIMS data using metallic glasses
- Comparisons of peak intensities determined by ion-scattering spectroscopy (ISS) for Cu-Ag-Au alloys
- Comparisons of elemental sensitivity factors for ISS signals of Cu and Au
- Comparisons of core-level binding energies determined by x-ray photoelectron spectroscopy with instruments calibrated using a field-emission electron source.

The E-42 Committee created a Standard Reference Data Subcommittee during the past year. This new Subcommittee will: (i) establish needs for reference data in the area of surface analysis; (ii) develop criteria for the evaluation of data; (iii) set priorities for needed data evaluations; and (iv) identify groups and experts to perform the evaluations. It is anticipated that the Subcommittee will give advice on these matters to the Division and the NBS Office of Standard Reference Data.

Work at NBS on the production and characterization of standard reference materials for surface analysis (see Section 2.2) and on other surface-standards activities is reported to and disseminated by the E-42 Committee.

2. Surface Chemical Analysis Working Party of the Versailles Agreement on Materials and Standards

(C. J. Powell)

The "Versailles Agreement" arose from a meeting of the Heads of Government (Economic Summit) of industrialized nations at Versailles in 1982. The participants represented Canada, Federal Republic of Germany, France, Italy, Japan, United Kingdom, United States of America, and the Commission of the European Communities. A Summit Working Group on Technology, Growth, and Employment was establishing consisting of government science advisers. This group has established Working Groups in areas such as photovoltaic solar energy, food technology, advanced robotics, biotechnology, high speed trains, remote sensing from space, and advanced materials and standards. A summary of developments resulting from the Versailles Agreement was published as a News and Comment article recently in Science 224, 1317 (1984).

The Versailles Project on Advance Materials and Standards (VAMAS) has considered the establishment of Technical Working parties in specific materials areas. A proposal for a Surface Chemical Analysis Working Party was prepared by Dr. M. P. Seah of the UK National Physical Laboratory and Dr. C. J. Powell of NBS and approved by the VAMAS Steering Committee in June, 1984. The proposal described the growth and diversity of surface analysis in the development of advanced materials in modern technologies and, additionally, the use of surface analysis for improved films and coatings. The principal techniques of surface analysis in common use were identified and the technical limitations to accurate surface analyses summarized. Accurate surface analyses require: (i) knowledge of the principles of the measurement method, (ii) knowledge of the behaviour of the measuring instrument, and (iii) correct interpretation and expression of the final measured result. Standards for the measurement of surface composition with known accuracy and for the reliable determination of chemical state will thus require: (a) a base of principles, definitions of terms, and suitable equations, (b) reference procedures for the measurement of intensities and spectral features, (c) procedures and data for instrument calibrations, (d) reference data for material parameters such as elemental sensitivity factors, matrix terms, chemical state spectra, ion sputtering rates, etc., and (e) standards for specifying an analysis. Specific needs were identified for the common methods of surface analysis, Auger-electron spectroscopy, x-ray photoelectron spectroscopy, and secondary-ion mass spectrometry together with the needs for ion sputtering which is used to obtain composition versus depth information in films and coatings. Existing standards activities in the member countries were reviewed and suggestions were made for additional standards for surface chemical analysis by scientists in the member states of VAMAS.

As yet, the VAMAS Steering Committee has not developed appropriate policies concerning the mechanisms of operation of the different Working Parties. Although the precise nature of the relationship between national groups (such as the ASTM E-42 Committee) and VAMAS is not clear, it appears that VAMAS will provide the means to develop surface analysis standards on an international basis and with support from a high level in each government. There should therefore be greater participation in the development of surface analysis standards than would happen through the ASTM E-42 Committee alone. At present, technical representatives in the VAMAS nations are being contacted to identify areas for technical activities and possible experts who might contribute. Current activities of the ASTM E-42 Committee will be coordinated with corresponding VAMAS activities.

3. ASTM D-32 Committee on Catalysts
(R. D. Kelley)

The activities of the ASTM Committee D-32 on Catalysts are concerned with the physical and chemical properties of commercial catalysts and with developing suitable procedures for catalytic activity measurements. The membership of the Committee numbers approximately 120. Semi-annual meetings are attended by between 60-80 percent of the membership including West Europeans and South Americans. The Subcommittee on Chemical Analysis is chaired by R. D. Kelley.

In 1984, the committee celebrated the tenth anniversary of its founding and continues to maintain an active pace. Since its inception the Committee has focused its activities on tests which are used routinely in the buying and selling of catalysts. The types of tests which have been examined include surface area, pore-size distribution, density, crush strength, particle size, attrition and abrasion, chemical analysis, amongst others. These tests involve methods which were thought to be "well established", and thus particularly suitable for standardization. However, experience has shown that many of these tests have not yielded satisfactory results in round robin testing. Two examples of these problems can be seen in the standardization of the multipoint BET method for surface area and the chemical analysis for platinum in reforming catalysts. In both of these cases, standardization activity in progress for about six years and involving many problems in both procedures and materials has been substantially completed in 1984.

Highlights of the past year include:

- the certification of surface area standards by the NBS Office of Standard Reference Materials (to be available shortly) and the initiation of a program to certify a platinum-containing catalyst reference materials (to be completed in 1-2 years).
- completion of satisfactory round-robin testing for the chemical analysis of nickel (a wet chemical method and an atomic absorption method) and of palladium (wet chemical method) in catalysts.
- initiation of standardization of a procedure for multi-element chemical analysis of catalysts by atomic absorption, an ambitions project which will be of great value to both producers and users of catalysts.
- Twenty test methods have been submitted for Committee ballot.

3. SURFACE MEASUREMENTS PROGRAM

The Division undertakes a number of projects directed to the improved physical and chemical characterization of surfaces and surface processes. These projects meet Division objectives through the development of new measurement techniques, improvement of existing techniques, development of theories of the measurement process, applications to important scientific and national problems, development of measurement procedures, tests of the measurement system, development of new concepts, and provision of needed data.

A. Catalytic Surface Chemistry: Reaction Kinetics at High Pressures over Single Crystal Catalysts

(T. E. Madey, R. D. Kelley, T. J. Udovic, M. J. Wax)

The overall objective of this research is to provide a molecular understanding of heterogeneous catalytic chemistry. 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 molecular and electronic nature of chemisorbed species. Results of the past year are described below:

We have completed a study designed to address a controversy concerning the catalytic activity of tungsten as a methanation catalyst. We had previously found that polycrystalline W wire exhibits a high activity for CH_4 synthesis from H_2 and CO, whereas van Langeveld and Ponec have recently reported that evaporated W films are very poor methanation catalysts. In neither of these studies were surface analysis techniques used to ascertain the surface composition of the catalyst. In an attempt to resolve this controversy, a closer look was taken at the methanation activity of W(110) (the most densely-packed crystal face of W) over a range of reactant partial pressures and temperatures in conjunction with pre- and post-reaction surface analysis utilizing Auger electron spectroscopy (AES). The results of this study indicate that the W(110) surface does, indeed, have the ability to hydrogenate CO to form methane as well as higher hydrocarbons, but the appearance of this activity requires higher hydrogen partial pressures than were utilized by van Langeveld and Ponec. Figure 3(a) illustrates the methanation behavior of W(110) as compared with that of Ni(100) determined earlier in this laboratory. The plot of turnover number for methane production versus inverse temperature indicates a lower apparent activation energy for W(110) (56 kJ mol^{-1}) compared to that for Ni(100) (103 kJ mol^{-1}) as well as a higher activity for W(110) at lower temperatures. The plot of methanation turnover number versus partial pressure of hydrogen, figure 3(b), indicates the strong dependence on hydrogen partial pressure for W(110) compared to Ni(100). For low partial pressures of hydrogen (ca. 1 Torr), the regime studied by van Langeveld and Ponec, W(110) behaves like a poor methanation catalyst. For higher hydrogen partial pressures (ca. 100 Torr), the regime previously studied in this laboratory, W(110) behaves like a good methanation catalyst. These results demonstrate the importance of analyzing a wide range of reaction parameters when characterizing the catalytic activity of a surface.

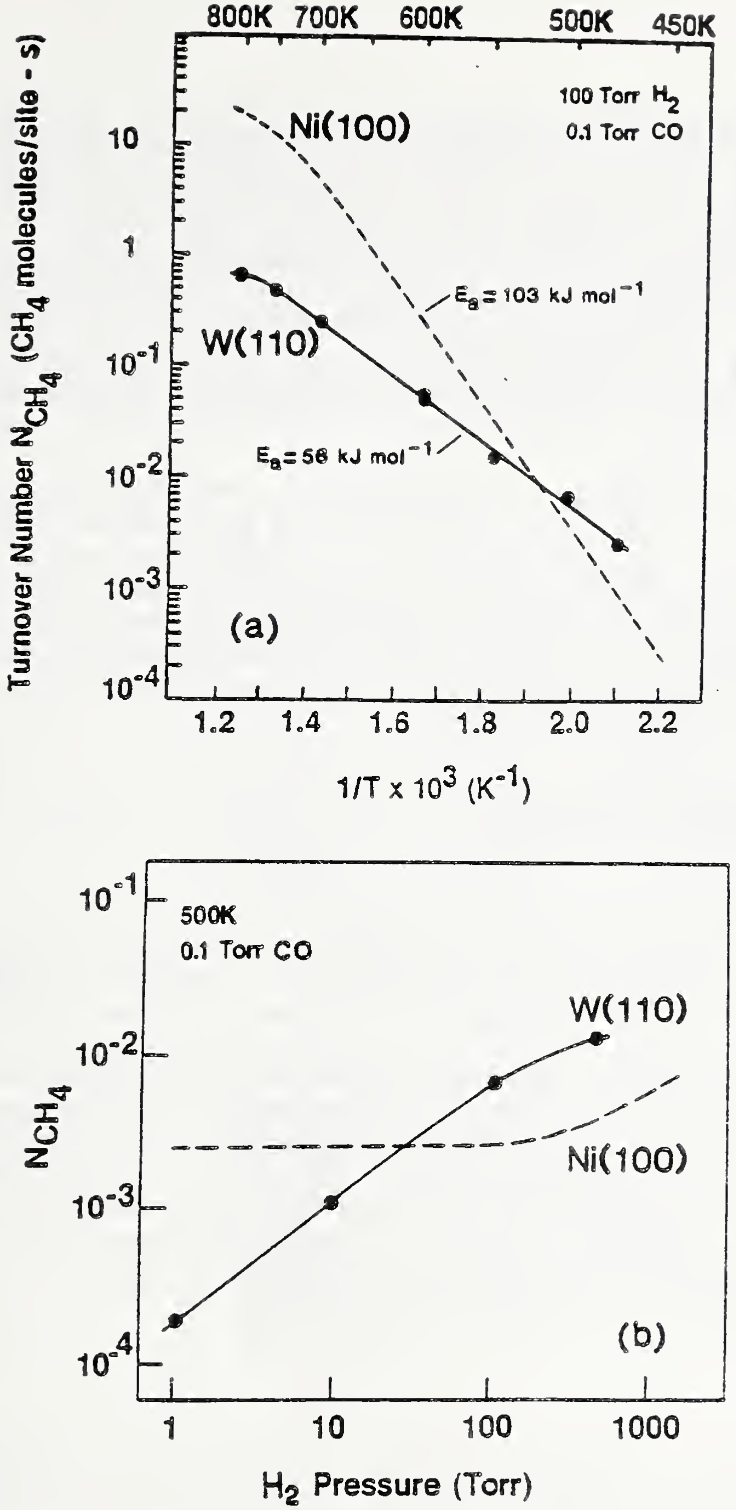

Figure 3. (a) Methanation activity as a function of temperature for W(110) and Ni(100) (partial pressure of hydrogen = 100 Torr and partial pressure of carbon monoxide = 0.1 Torr). (b) Dependence of methanation turnover number on the partial pressure of hydrogen for W(110) and Ni(100) (reaction temperature 500 K, partial pressure of carbon monoxide = 0.1 Torr).

Research has been initiated on the reactivity of model supported catalysts. Equipment has been constructed which allows controlled deposition of aluminum and platinum on tungsten single crystals. After each experiment, a clean tungsten surface may be obtained by heating above the desorption temperature of any deposited materials. Various amounts of platinum, used commercially for hydrocarbon reforming, may be evaporated directly onto tungsten, or onto thin films of alumina prepared in situ. Use of these well-defined materials will allow examination of catalytic activity as a function of support structure and of catalyst electronic structure, which, at least in the submonolayer region, varies with platinum coverage.

We plan to examine the hydrogenolysis activity of platinum deposited on tungsten and on thin layers of alumina on tungsten. We will vary the Pt particle size by appropriate heat treatment and attempt to correlate activity with particle size. We will also complete a study of the hydrogenolysis activity of two single-crystal tungsten surfaces, (110) and (100). In addition, we will study the hydrogenation of CO over refractory metal surfaces (Mo single crystals) and over alloy catalyst surfaces (e.g., Cu/Ni single crystals).

B. Electron-Stimulated Desorption: Relation to Surface Molecular Structure and Reactivity

(T. E. Madey, F. P. Netzer, K. Bange)

A continuing challenge in surface science is the determination of 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 characterize the fundamental electronic excitations resulting in the stimulated desorption of ions. ESDIAD has the advantage of being sensitive to the local bonding geometry of adsorbed molecules, even in the absence of long range order in the adsorbed layer. The present primary thrust of this project is to use ESDIAD to characterize the influence of surface additives (e.g., catalyst promoters and poisons) on the local structure of small molecules on metal surfaces. Another objective is to determine molecular structures in controversial cases.

During the last year, we found clear evidence for a local interaction between CO and Na adsorbed on Ru(001). For low coverages of Na($\theta_{Na} \leq 0.15$ ML) and saturation coverages of CO at 80 K, a fraction of the CO molecules undergo a substantial change in bonding configuration: molecular CO bound perpendicular to the Ru(001) surface changes to an "inclined" configuration in the presence of low coverages of Na. The bonding interaction which causes the tilting is believed to be primarily electrostatic in nature.

We also examined the influence of two electronegative additives, O and Br, on the structure and reactivity of H_2O adsorbed on an Ag(110) surface. The interactions of Ag + O and Ag + Br with H_2O are of interest in electrochemistry, and this study has provided a new view of the structure and kinetics.

We found that H_2O adsorbed on clean Ag(110) forms hydrogen-bonded arrays having short-range local order; H_2O desorbs in molecular form at 170 K, with no evidence for dissociation. When H_2O is coadsorbed with atomic O on Ag(110), there is evidence for new oxygen-stabilized molecular H_2O having different local structure, as well as a reaction between H_2O and O to form OH, i.e., $H_2O + O(ad) \rightarrow 2OH(ad)$. In addition, the H_2O interacts so strongly with molecular O_2(ad) that dissociation of O_2 and formation of OH appear to occur even at ~ 100 K. The OH(ad) is "tilted" on Ag(110), with the molecular axes inclined along [001] azimuths. Desorption of H_2O due to recombination of OH(ad) occurs at ~ 300 K.

In contrast, there is no hydrogen-abstraction reaction between H_2O and Br on Ag(110). The H_2O forms locally-ordered structures, and the binding energy increases, but no reaction to form OH (or HBr) occurs.

We have used ESDIAD to address a controversy concerning the structures of atomic and molecular oxygen on Ag(110). Many previous authors have suggested that both O and O_2 are adsorbed in the troughs, in high symmetry positions; O_2 was believed to be bonded with the O-O axis parallel to the surface. Our data indicate that both atomic oxygen ($T_{ads} > 300$ K) and molecular oxygen ($T_{ads} \approx 80$ K) are bonded in directions along [001] azimuths. The structures based on these measurements (e.g., molecular O_2 bonded via one O atom, and "inclined" slightly in the [001] direction) are at variance with most existing models, and provide new insights into the Ag-oxygen interaction.

There appear to be major differences in the "activity" of oxygen in promoting hydrogen abstraction on different surfaces. On Ru(001), for example, the interaction of H_2O or NH_3 with adsorbed oxygen causes an increase in molecular binding energy, but no dissociation. On Ni(110) and Ag(110), O(ad) abstracts hydrogen from H_2O to form OH(ad). During the coming year, we will examine the ability of both atomic and molecular O_2 to promote hydrogen abstraction reactions on different surfaces. Specifically, we will study NH_3 + O on Ag(110), where the oxygen is relatively weakly bound, and NH_3 + O on Fe(100), where the oxygen is more strongly bound. Other polar molecules (H_2O, CH_3OH) and other electronegative additives (Br) will also be studied.

Iron is an excellent catalyst in NH_3 synthesis, and adsorbed K is known to "promote" the reaction by increasing the rate. In an attempt to understand at the molecular level how K influences the bonding geometry of NH_3 to Fe, we will use ESDIAD to examine the structure and reactivity of NH_3 on clean Fe(100), and on K-dosed Fe(100). The influence of K on the local structure of CO will also be studied; such interactions may be relevant to Fischer-Tropsch synthesis.

Recent angle-resolved ultraviolet photoemission spectroscopy measurements have indicated that molecular O_2 is bound to a Cu(110) surface through one O atom, with the O-O axis perpendicular to the surface. These results seem to be at variance with previous measurements, in which the O_2 was presumed to be lying down. We will attempt to verify this structure using ESDIAD; we will also study the influence of additives (O, Br) on the structure and reactivity of H_2O.

We will examine the structure of H_2O on Cu(110) and the influence of additives (Na, Br, O) on the H_2O structure; these measurements will be compared with ongoing theoretical calculations of the same system by Dr. U. Landman of the Georgia Institute of Technology (and recently appointed part-time Expert to the Division staff).

C. Nucleation, Growth and Surface Atomic Structure of Ultrathin Films

(A. J. Melmed, A. Ciszewski)

There is considerable interest in the nucleation and growth of ultrathin films of metals and semiconductors. The interest is concerned with relationships between particular physical and chemical properties and the morphology and atomic structure of the film, particular for thicknesses in the monolayer range. For example, surface atoms of samarium metal have been found to be divalent, while the bulk atoms are trivalent, and this has led to the suggestion that the surface lattice parameters should be larger than the corresponding bulk values or that surface reconstruction should occur. In order to investigate the surface atomic structure of Sm, we determined the conditions for producing clean Sm surfaces by epitaxial crystal growth from the vapor. The initial work was done in a field electron microscope, and then the methods developed were transferred to a low-energy electron diffraction apparatus, where (0001) Sm crystal layers were grown on a (011) W substrate. Initial results indicate that the (0001) Sm surface is not reconstructed, but that is is expanded relative to the bulk by 4-15%, depending on layer thickness. We plan to complete the determination of surface lattice parameter for (0001) Sm during the coming year and to clarify the homogeneity of Sm coverage during the early stages of deposition on (011) W.

During the past year, methods developed earlier to prepare clean films by epitaxy from the vapor phase in the ultrahigh vacuum of a field-electron microscope were extended to relatively high-vapor-pressure materials. In collaboration with Drs. V. Maurice, O. Frank, and J. H. Block of the Fritz-Haber Institute in Berlin, the rare-earth metal europium was grown on rhenium and tungsten substrates. Growth modes, nucleation sites, and epitaxial relationships were determined. An unexpected type of film growth was observed to occur, namely the growth of fcc europium on one and only one rhenium plane [Re(203)]; this growth mode could be correlated with the surface atomic structure of Re(203).

D. Electron Spectroscopy of Surfaces

(T. J. Jach)

Preliminary experiments have been conducted in an attempt to observe the surface shifts of core-level binding energies by means of glancing-incidence x-ray photoemission. In collaboration with Drs. P. Cowan of the NBS Quantum Metrology Group and L. B. Holdeman (COMSAT), measurements have been made of photoelectron spectra of nickel and gold for x-ray angles of incidence less than and greater than the macroscopic critical angle for total external reflection in order to observe shifts in binding energies for predominantly surface or bulk atoms. Recent work has centered on the requirement to have smooth surfaces at an atomic level in order to get a significant contribution from the surface atoms. The correlation of the x-ray reflectance of the surface with other means of roughness measurement (stylus, scanning electron microscopy) may lead to a new method of measuring average surface roughness where the scale of the roughness is less than 20A.

E. Ion-Surface Collisions and Atomic Excitations

(J. Fine, R. Klein)

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 of 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 calculations to analyze these experiments, we expect that such sputtered atoms will have rather high kinetic energies - extending up to hundreds of electron volts. An experimental determination of the kinetic energy distribution and state identification of those specific atoms which have undergone Auger decay would give more information concerning the atomic excitation and collisional energy transfer mechanisms of ion collisions in solids.

In collaboration with Drs. L. J. Moore (NBS Inorganic Analytical Research Division) and T. B. Lucatorto (NBS Radiation Physics Division), a new series of experiments has been planned and designed to determine the kinetic energy distributions of specific sputtered atoms (ions) and their states of excitation. Resonance multiphoton laser-ionization schemes have been developed to detect sputtered atoms in specific excited states and time-of-flight techniques will be used to measure their kinetic energy distributions. Pulse timing and gating sequences have been designed and estimates made of signal intensity indicate that such measurements are feasible. An apparatus has been designed for the preliminary investigation of this problem. An ultrahigh vacuum chamber for ion-beam-angle dependent measurements is under construction and will be coupled to two ultraviolet pulsed laser systems. We plan to investigate atoms and ions sputtered from surfaces of Mg, Aℓ, and Si and to study the distance beneath the surface at which collisional excitation occurs.

F. Surface Theory

(J. W. Gadzuk)

The theoretical physics projects of the Division are focused on understanding both static and dynamic behavior of atoms, molecules, solids, surfaces, radiation and their mutual interactions. This understanding comes from consideration of the microscope atomic-scale properties of individual entities as well as from larger-scale statistical properties of ensembles. Based upon our studies, phenomenological model theories 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.

A large-scale theoretical effort has been underway aimed at the modeling of reaction dynamics at metallic surfaces and at interfaces of electro-chemical significance. Major focus in the past has been on the role of internal degrees of freedom (vibrational, rotational, and electronic) of molecules in determining energy flow and redistribution occuring in elementary molecular processes at surfaces. Several major advances deserve mention here.

An analytic and exact model which enables calculation of the classical trajectories for a diatomic molecular beam incident upon a surface has been constructed in collaboration with Dr. S. Holloway of the University of Liverpool, England. Account is taken of the possibility for the molecule to: i) scatter in a vibrationally excited state; ii) form an adsorbed negative-molecular-ion resonance state; iii) dissociatively adsorb; and iv) undergo electronic charge transfer than thus potential surface hopping. In the spirit of past gas-phase work of Polanyi, we have explored the ramifications of potential-energy-surface (PES) topological features in determining the outcomes of dynamic processes at surfaces. For instance, the PES shown in Fig. 4 has been useful in studying the branching ratios for competing processes:

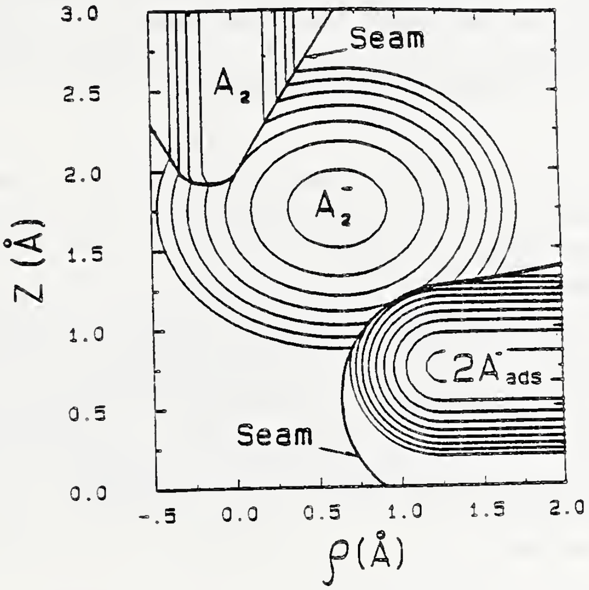

Fig. 4 Diabatic potential-energy surface for diatomic molecule A_2 approaching a solid surface with z the center-of-mass distance from the surface and ρ the intra-molecular separation relative to the neutral molecule equilibrium distance. The entrance ($z \to \infty$) and exit ($\rho \to \infty$) channels correspond to an intact molecule (A_2) and 2 adsorbed particles ($2A_{ads}$), respectively, and are separated by a negative molecular ion resonance (A_2^-). Transitions between the various states can occur along the "seam" where the potential energies of adjacent states are equal.

A_2(gas) → A_2^- (nondissoc. ads.) → A_2^*(gas),
A_2(gas) → A_2^- (nondissoc. ads.),
A_2(gas) → A_2^- (non dissoc. ads.) → 2A (dissoc. chemisorbed)

We have studied the activated dissociative chemisorption of a diatomic molecule for the case where an activation barrier exists in the exit channel along the seam (curve crossing) separating the A_2^- resonance from the dissociated state.

Due to the fact that the incident A_2 molecule first goes through the A_2^- resonance, memory of the initial partitioning of energy (normal versus parallel translational, vibrational, etc.) is erased. Consequently, activated adsorption could depend upon the total energy available, not just the normal translational component, as recently observed experimentally. This conclusion runs counter to all previous surface-science intuitive models based on one-dimensional potential-energy curves, thus demonstrating the utility of new conceptual models. We have calculated mean translational-to-vibrational energy redistributions, dissociative sticking probabilities, and have included the role of substrate viscous forces and mode mixing. We are in the process of establishing the role of chaotic versus quasi-periodic intra-molecular dynamics on surface processes.

Charge-transfer processes in molecule-surface interactions constitute a large class of events which are significant in determining chemical outcomes. From the point of view of quantum intra-molecular dynamics, charge transfer (harpooning) between a surface and an incident molecule is equivalent to potential surface hopping in which the wavepacket representing the initial state of a particular molecular degree of freedom is instantly placed at a non-equilibrium location on a new potential surface. By following the time evolution of the wavepacket, observable dynamic properties relevent both to spectroscopy and chemistry can be calculated, often in a significantly more economic way than by using traditional stationary-state techniques and almost always in a physical more transparent manner.

Adapting the wavepacket-dynamics approach developed previously by Heller to surface dynamics, we have constructed a wavepacket model for describing intra-molecular dynamics in surface scattering processes involving charge transfer. The essence of the model is shown in Fig. 5 where intra-molecular potential curves for a neutral diatomic molecule and a negative molecule ion are shown. The center-of-mass translational motion is described by some imposed surface scattering trajectory which sets the time interval τ_R. Initially the molecule A_2 is in its vibrational ground state. At time $t=0$, an electron transfers from the substrate to the molecule, the A_2^- curve is switched on, and the wavepacket propagates on the new curve until time $t=\tau_R$, when the electron returns to the solid. This event has the effect of switching back on the A_2 potential and allowing the now-moving wavepacket to propagate on the neutral curve. We have developed a quantitative theory for the vibrational excitation distribution in the scattered molecule in terms of the molecular parameters and the lifetime of the A_2^- intermediate state. A typical set of vibrational distributions is shown in Fig. 6 for bromine as a function of n, the vibrational quantum number, and with the intermediate state lifetime treated parametrically. Not only is substantial excitation experienced, which varies with τ_R, but also significant dissociation can occur due to curve hopping. The wavepacket dynamics serves as a complement to the classical studies and holds promise for being fairly easily generalized to polyatomic molecules with several degrees of freedom. Work is in progress to extend these studies to more complicated systems, and into the area of stimulated desorption.

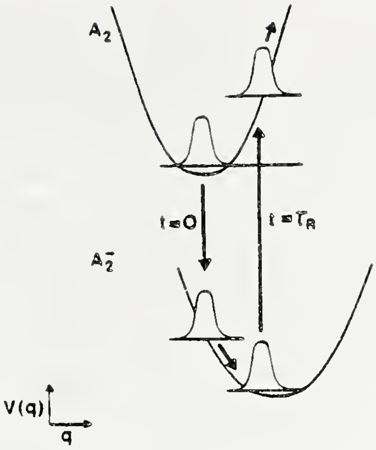

Fig. 5 Intramolecular potential energy curves illustrating the wave-packet propagation of the relative nuclear coordinates associated with the existence of a negative-molecular ion within the time interval $0<t<\tau_R$. The return of the wave packet onto the A_2 curve at $t=\tau_R$, while possessing both kinetic and potential energy, is responsible for vibrational excitation of the final state of the A_2 molecule.

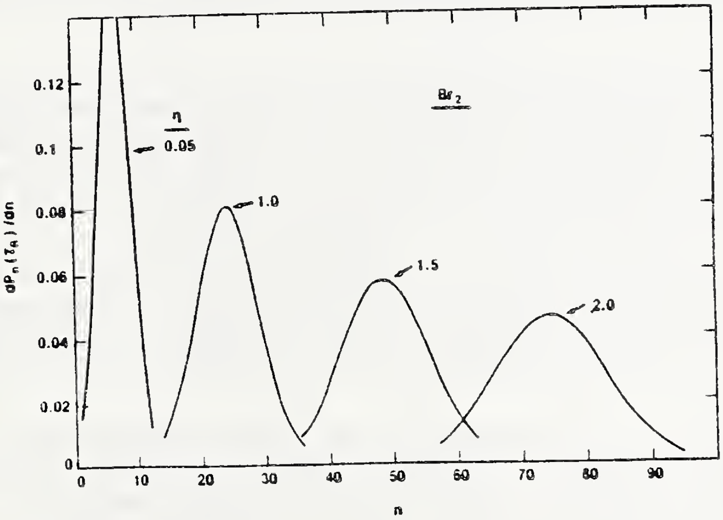

Fig. 6 Predicted vibrational excitation distributions of scattered molecules as a function of vibrational quantum number for bromine molecules which have experienced the sequence of curve hoppings shown in Fig. 5. The resonance lifetime τ_R (via $\eta = \tilde{\omega}\,\tau_R$ with $\tilde{\omega}$ the Br_2^- frequency) is treated parametrically. The curve labeled $\eta=2$ corresponds to an internal vibrational population distribution of the bromine molecule containing ~ 1eV total vibrational energy.

Vibrational spectroscopy of molecules adsorbed on solid surface is one of the dominant tools for obtaining microscopic chemical information of chemisorption systems. While the principal use has been through interpretation of the energy position of a loss feature, increasing attention has been focused on the information content of the lineshape and width. Aside from inhomogeneous broadening effects, the surface science community has, almost without exception, assumed that the linewidth is a direct measure of inelastic damping of an excited oscillator outside a surface. Many debates on the relative roles of phonon versus electron-hole pair contributions to dissipation have relied on the characteristics of the observed linewidth as the final determinant. Although elastic dephasing collisions are well known in other vibrational spectroscopies to usually be the dominant source of observed linewidths in systems involving condensed phases, their importance in surface vibrational spectroscopy has not been recognized. In collaboration with Dr. A. Luntz of the IBM Research Laboratory, San Jose, we have developed a theory based on the exchange-coupling dephasing model due to Harris, in which there is anharmonic coupling between intra-molecular ($\sim 2000 \mathrm{cm}^{-1}$) modes and large-amplitude, low-frequency modes associated with bonding to the surface. The latter modes, coupled to the stochastically fluctuating phonon both of the substrate, are responsible for dephasing collisions that can yield large (~ 10-$50 \mathrm{cm}^{-1}$) vibrational linewidths. The predicted temperature dependence of the linewidth is in accord with very recent experimentally measured values, adding strong support to our theory. From this work we conclude that the vibrational linewidths of intra-molecular adsorbates modes cannot generally be related to dissipative effects, as has been assumed previously, without independent measurements which distinguish between dissipative and dephasing broadening mechanisms.

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 under controllable dynamic and reactive conditions, and 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, neutron spectroscopy of metal hydrides, and other experimental probes of non-adiabatic effects.

G. Fabrication of Fluorescent Screens

(A. J. Melmed)

Fluorescent phosphor screens are widely used in the Surface Science Division and in other parts of NBS, and very often the phosphor screen must be custom-made. The preparation process usually requires two or more days, especially if a high-quality, uniform phosphor deposition is required.

In collaboration with Dr. O. Frank of the Fritz-Haber Institute, Berlin, a simple method was developed for preparing fluorescent screens on glass or metal substrates. Whereas the former method required a careful balance of large volumes of complex chemical solutions for maintaining proper ion and binder concentrations in the phosphor settling solution, the new process replaces the chemistry with rapid mechanical steps and smaller volumes of liquid. The entire process can be completed in about three hours.

4. SURFACE SCIENCE COMPETENCE PROGRAM

A. Introduction

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

The Surface Science Competence Program NBS Task 26103 was established with new staff 5 1/2 years ago. Initial plans envisaged new research activities in three areas: (a) chemical dynamics on surfaces, (b) ion interactions with surfaces, and (c) surface properties of novel materials; there are, however, appreciable overlaps among these areas with other Division projects. Specific projects have been selected based on a judgement of their scientific merit and on assessments of the future scientific and technical challenges requiring NBS expertise and action. Our strategy has been to involve existing Division staff in the new activities to the maximum extent possible and to implement both new experimental and new theoretical activities.

Section 4.B contains reports of the technical activities initiated as part of the Surface Science Competence Program. Section 4.C contains reports of activities by Surface Science Division staff concerned with the development of experiments at the Brookhaven National Synchroton Light Source. These experiments are being conducted as part of NBS Task 26105 which was initiated in 1980.

B. Reports of Surface Science Competence Program Activities

1. ESDIAD-EELS Studies of the Structure and Reactivity of Adsorbed Species (N. D. Shinn, T. E. Madey)

The determination of the local bonding geometry of adsorbed species on surfaces is of fundamental importance to the development of a conceptual basis of surface chemistry. Fundamental studies of adsorbate structures on single crystals are just beginning to give baseline information to technologies such as heterogeneous catalysis, corrosion prevention, electrochemistry, and semiconductor design.

We have constructed an unique apparatus combining ESDIAD (Electron Stimulated Desorption-Ion Angular Distributions) and EELS (Electron Energy-Loss Spectroscopy). These techniques in combination make a powerful facility for surface structural characterization.

This year high resolution electron energy loss spectroscopy (EELS), electron stimulated desorption ion angular distributions (ESDIAD), low energy electron diffraction (LEED) and Auger electron spectroscopy (AES) have been used to identify two distinct, sequentially populated, molecular CO binding states at 120 K on Cr(110). The first is a new molecular state

(α_1) with a substantially weakened CO bond, believed to be a precursor state to dissociation, whereas the second state (α_2) is comparable to terminally bonded CO on other transition metals. The CO stretching frequencies of the α_1 state (~ 1150-1330 cm^{-1}) are substantially shifted from the gas phase (2143 cm^{-1}), and are believed to be the lowest values ever reported for adsorbed molecular CO on any clean or promoted transition-metal surface.

Initially, CO adsorbs with a sticking probability of ~ 0.9 which decreases upon formation of a c(4x2) CO overlayer. EELS spectra reveal a weak 450 cm^{-1} loss and, surprisingly, two strong features at 1150 and 1330 cm^{-1}. All losses increase with additional CO exposure, shifting to ~ 475, 1200, and 1330 cm^{-1} at full c(4x2) CO overlayer formation. With further CO exposure, the c(4x2) LEED pattern reverts to (1x1) symmetry with high background intensity, and a new triplet of EELS loss features appears at 495, 1865, 1975 cm^{-1}. ESDIAD measurements as a function of CO exposure show atypically weak O^+ ion emission along [110], increasing in intensity only after the appearance of the latter triplet of EELS features.

These data are suggestive of α_1 CO molecules oriented nearly parallel to the Cr(110) surface, while α_2 CO molecules are oriented normal to the surface at either atop or bridge-bonded sites. Figure 7 illustrates representative EELS spectra for the sequential α_1, α_2 CO population experiment. Further investigation of the unique α_1, CO state and the decomposition of both α_1 and α_2 CO are planned.

Also this year, an EELS/ESDIAD/LEED (low-energy electron diffraction) study of O_2 adsorption on Cr(110) has found an unexpected molecular adsorption state below 200K. As seen in figure 8, the vibrational spectrum at 120 K includes losses at 615 cm^{-1} (due to atomic oxygen) and 1020 cm^{-1}, the latter being attributed to the O-O stretch of O_2(ads). At 300 K, only atomic oxygen remains with a characteristic loss at 605 cm^{-1}. Low oxygen exposures at 300 K result in the formation of a p(4x2) O overlayer and the observation of a 290 cm^{-1} loss feature, possibly due to a surface phonon of the ordered overlayer.

ESDIAD measurements of the low temperature adsorption have identified six azimuthally ordered cones of O^+ ion emission away from the surface normal. These correlate with the appearance of the O-O vibrational loss, indicating that there are six discrete tilted orientations for O_2(ads), reflecting the pseudo-hexagonal symmetry of the Cr(110) surface. In contrast, atomic oxygen results in a single [110] directed cone of O^+ emission observable at all temperatures.

In addition, an example of co-adsorbate interactions inducing a significant molecular reorientation has been found in CO/O_2 titration experiments on Cr(110). Cr(11) pre-dosed with atomic oxygen to form a p(4x2) structure completely blocks the α_1 CO adsorption state. Only the 495, 1865, and 1975 cm^{-1} CO vibrational features are seen, in addition to the Cr-O stretch at 605 cm^{-1}. A more dramatic result is found when a c(4x2) CO adlayer - i.e., the saturation coverage of the α_1 binding state - is subsequently exposed to oxygen. The stepwise increase in surface

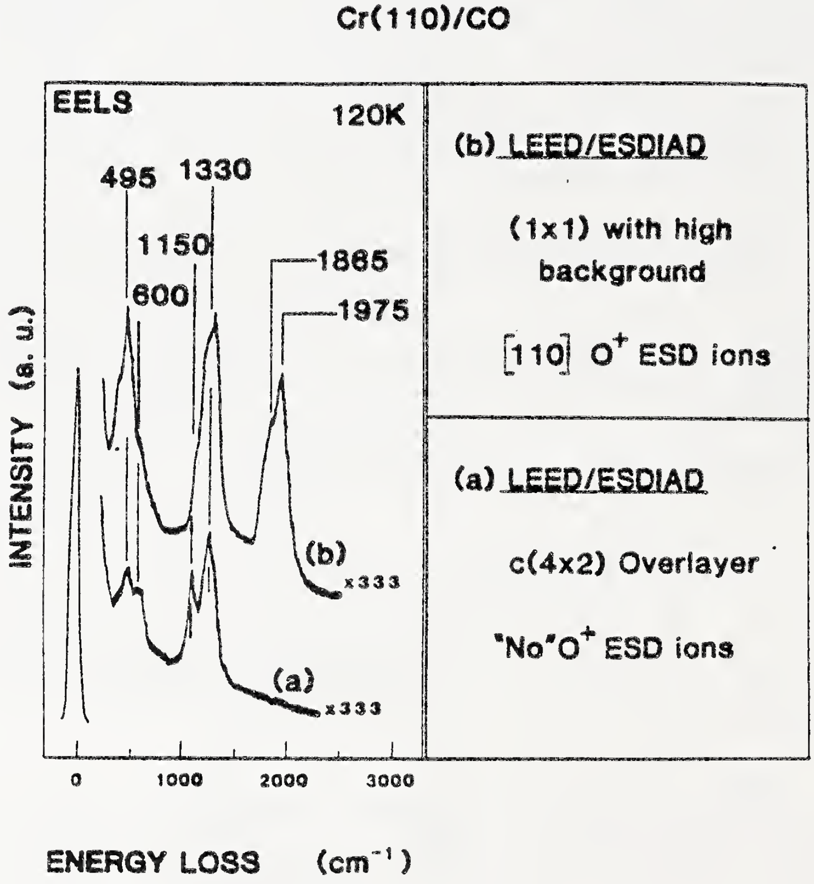

Fig. 7. Summary of EELS/ESDIAD/LEED data for CO adsorption on Cr(110) at 120 K. Panel at left shows representative spectra for two stages of chemisorption. α_1 CO is characterized by spectrum (a) with CO stretching frequencies at 1150 and 1330 cm^{-1}, as well as a Cr–CO mode at ~ 475 cm^{-1} and a residual Cr–O stretch at 600 cm^{-1}. Further CO exposure populates the α_2 CO state with corresponding, site-specific CO stretching frequencies at 1865 and 1975 cm^{-1}. The Cr–CO stretching mode is observed at 495 cm^{-1}.

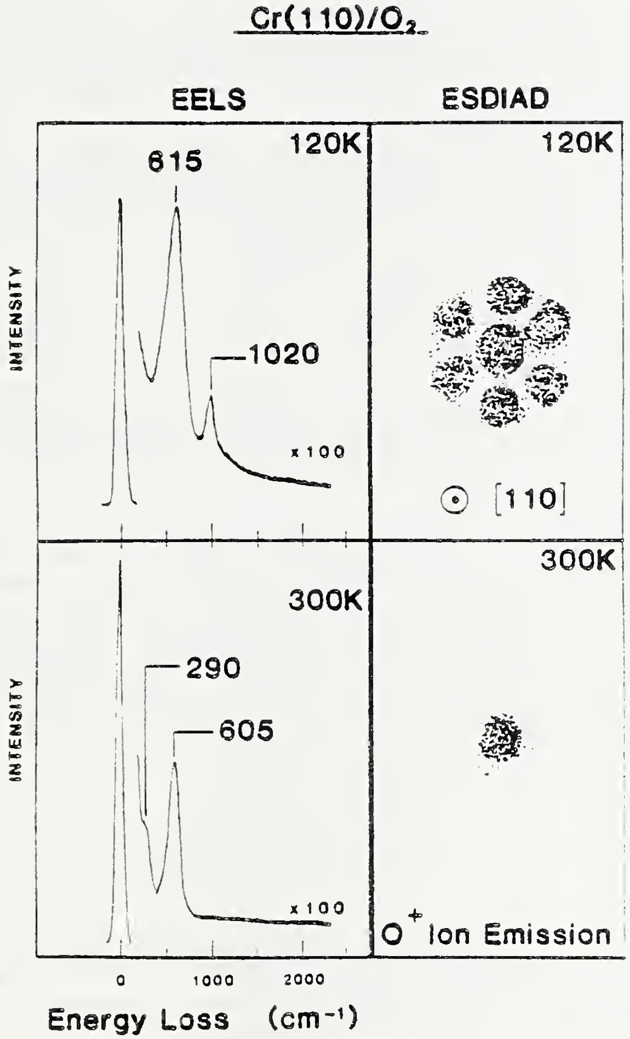

Fig. 8 Vibrational spectra for oxygen chemisorption on Cr(110) with corresponding ESDIAD patterns. At 300 K, atomic oxygen results in a single [110] directed O^+ ion beam and a Cr-O stretching frequency of 605 cm^{-1}. The 2909 cm^{-1} shoulder is observable only at low oxygen coverages. Low-temperature adsorption populates a new molecular state, with O-O stretching frequency of 1020 cm^{-1} and six new off-normal O^+ ion beams.

oxygen causes the 1200-1300 cm^{-1} CO intensity to gradually decrease while a commensurate increase is seen in loss features at ~ 470, 1865 and 1975 cm^{-1}. This oxygen-induced conversion of CO from the first binding state to the second (terminally bound) state further demonstrates the existence of two molecular CO states at 120 K. Detailed coverage-dependent studies are underway to elucidate these apparent site-blocking and site-competition effects.

We plan to continue of the Cr(110) chemisorption studies with particular attention to the effects of steps, sub-surface oxide, and contaminants. Further investigation of the complex interaction of CO and O_2 is necessary to confirm evolving models for this system. Additional experiments with N_2, CO_2, and H_2S are anticipated to assess the chemical activity of Cr(110) for dissociative adsorption and the role of common bulk impurities (N,S) in adsorbate ordering. The investigation of Cr(100) surface chemistry and adsorbate-induced surface reconstruction continues. In view of the surprising results of the Cr(110)/CO/O_2 investigation, comparable experiments are planned for the less dense Cr(100) surface in order to address the question of site-specific CO chemisorption modes on chromium. To date, the only work on molecular adsorption on single-crystal chromium surfaces is that done in this laboratory, although there is a wider interest in assessing chemisorption trends in the family of Cr, Mo, and W transition metals.

We plan to interface the high-resolution EELS spectrometer to an LSI 11 microcomputer. This will enable semi-automated data acquisition in a pulse-counting mode as well as facilitated and expanded data-manipulation capabilities. These improvements to the EELS instrument are necessary for the satisfactory performance of relevant, low-signal experiments. Initial experiments planned will probe the low coverage interactions of H_2O and O(ads) on Ag(110) and also NH_3 on oxygen pre-dosed Ni(110). In both cases, vibrational data is needed to confirm the models developed in previous ESDIAD/LEED/TDS (thermal desorption spectroscopy) studies for the respective hdyrogen abstraction reactions $H_2O + O(ads) \rightarrow 2\ OH(ads)$ (on Ag(110)) and $NH_3 + O(ads) \rightarrow NH_2\ (ads) + OH(ads)$ (on Ni(110).

We will complete the fabrication, testing, and incorporation of the "high pressure" reaction chamber and transfer mechanism to the EELS/ESDIAD system. This powerful combination of ultrahigh vacuum spectroscopic techniques and actual kinetic measurements

on the same model catalyst will allow the correlation of reaction rates to models derived from detailed chemisorption studies. Of particular interest is the hydrogenation of CO over the atomically corrugated Ni(110) and Ni(311) surfaces. Although recent studies of other structured model catalysts have revealed interesting chemisorption results, the significance of these results has not been established. Our studies will directly test the catalytic importance of an atomically rough surface as well as expand our knowledge of chemisorption on "defective" surfaces.

2. Laser Diagnostics of Surface Dynamics
(R. R. Cavanagh)

The pathways and rates of energy transfer at surfaces are not readily accessible with conventional surface-characterization techniques. A variety of laser-based techniques, however, have been applied to similar questions of molecular dynamics in both the gaseous and liquid states. In this program, the focus is on extending established laser methods and developing new laser-based techniques for addressing the issue of energy transfer at surfaces. The program includes exploitation of both the spectral and temporal resolutions available in state-of-the-art lasers.

Two types of experiments are underway in which laser diagnostics are employed to probe dynamical processes at surfaces. This work is performed in collaboration with Drs. King, Stephenson, Mantell, Heilweil, and Casassa of the NBS Molecular Spectroscopy Division.

a. Laser-Excited Fluorescence as a Probe of Surface Dynamics

Molecular desorption from surfaces is representive of chemical conversion processes which transform reactants (adsorbed molecules on surfaces) to products (gas-phase molecules and bare surfaces). In order to characterize and utilize such reaction processes, it is essential to have state-specific diagnostic probes suitable for such measurements. The focus of this work is to explore the application of laser-based probes (such as laser-excited fluorescence and multiphoton ionization) to adsorbate and desorption processes. Processes such as thermally activated desorption, chemically induced desorption, laser-induced desorption, and electron-stimulated desorption exemplify the scope of the project. This work is being performed collaboratively with Drs. King and Mantell.

A high-resolution excimer-pumped tuneable dye laser is being used to study thermal desorption in a new ultrahigh vacuum chamber. The laser operates under microprocessor control, giving single-mode tunability over 0.5 cm^{-1}, at a resolution of 0.005 cm^{-1}, or over 20 cm^{-1} at a resolution of 0.03 cm^{-1}. The output energy is typically 100 µJ at 226 nm. Combining the present tuning range of the laser (800-215 nm) with the improved surface diagnostics in the vacuum chamber, a much broader range of desorption diagnostics is possible.

Experiments to probe the spatial orientation of the NO molecular axis following thermal desorption from Ru(001) have been performed. Since inhomogeneous magnetic fields on the order of 10 mGauss are sufficient to perturb the measurements, the magnetic shielding in the new chamber was critical, as was the ability to take data only at the zero crossing of the current used to heat the Ru crystal. We have not found any preferred alignment (i.e., the molecular axis is neither predominantly perpendicular nor parallel to the crystal plane).

The influence of adsorbate-adsorbate interactions on the dynamics of thermal desorption is essentially unexplored. Our current sensitivity level of ~ 5 percent of a monolayer will permit us to examine the magnitude of such effects. In addition during the coming year thermal desorption from substrates which are inactive for NO decompostion (such as Pt(111) or Pd(111)) will be characterized. In such systems (where dissociative channels are not in competition with thermal desorption), strong polarization effects are anticipated. Laser surface heating will be explored. Heating pulses of 10 ns duration will be used to initiate molecular desorption. The resulting internal-state distribution will provide an unique characterization of the heat bath sampled during the desorption process. Also, the extension of state-specific diagnostics to molecules such as carbon monoxide or hydrogen will be initiated with the construction of the appropriate four-wave mixing facilities for working in the 150 nm wavelength region.

b. Real-Time Measurements of Energy Transfer at Surfaces

The time scale for energy transfer at surfaces remains a major uncharacterized parameter of chemistry at interfaces. The application of time-resolved laser techniques to a variety of solid surface problems holds promise for providing real-time diagnostic of relaxation mechanisms. With a variety of techniques, the surface response to laser excitation (using infrared, visible, or ultraviolet pulses) is probed in real time.

In collaboration with Drs. Stephenson, Heilweil, and Casassa, the first real-time measurements of the vibrational relaxation of a surface species have been made. The vibrational relaxation of OH (3690 cm^{-1}) groups on colloidal silica (~120Å diameter particles, 200 m^2/gm) dispersed in carbon tetrachloride has been found to be 150 ps. This relaxation time is forty times shorter than for comparable diatomic oscillators at this wavelength, yet the time is three orders of magnitude longer than that obtained from linewidth arguments. The implications of the observed lifetime will only be fully realized when a variety of systems with different chemical properties have been explored. It is already apparent, however, that in this system vibrational relaxation is slow on the time scale of rotational reorientation.

Infrared pump-probe experiments are a general method for establishing rates and mechanisms of energy transfer. Three issues will be addressed next. First, the measurement technique will be extended to pressed discs in vacuum to determine why the vibrational relaxation at the solid-liquid interface is substantially different from that at the solid-vacuum interface. Second, the relaxation rates for adsorbed OH species on other insulator surfaces such as Al_2O_3, ZnO, and zeolites will be examined to determine the correlation between vibrational relaxation and substrate. Third, two-color pump-probe techniques will be applied to establish the pathways of vibrational relaxation on surfaces.

3. Neutron Inelastic Scattering by Adsorbed Species on Surfaces (R. R. Cavanagh, R. D. Kelley, T. J. Udovic)

Neutron scattering is regarded generally as a tool of solid state physicists. Recently, however, there have been increasing neutron scattering efforts in the areas of material and chemical sciences. At NBS, the Surface Science Division has been working with the Reactor Radiation Division to apply neutron scattering to molecular processes at surfaces. Our efforts in the past year can be divided into several categories.

The Neutron Inelastic Scattering, (NIS) spectra have been measured for the first time during a steady-state catalytic chemical reaction. In this case the hydrogenation of CO to hydrocarbons. The "in situ" measurements of adsorbate vibrations have been made using a Raney nickel catalyst (a high surface area material). Reaction products were measured with gas chromatography while the vibrational spectra were being recorded. Measurements were made as a function of temperature and H_2/CO ratio. Analysis of the spectral changes which accompany changes in reaction parameters is not complete. However, it is quite clear that the introduction of CO into the hydrogen gas stream results in a substantial reduction in the concentration of atomic hydrogen on the nickel surface. Vibrational modes due to hydrocarbon species are also detected. The intensity of these modes varies in a complex way with changes in reaction conditions (partial pressure of carbon monoxide, temperature, and flow rate).

NIS from adsorbed species on platinum black is being investigated. The hydrogen spectra are being analyzed and the chemical activity of "defect" hydrogen is being probed. Present data permits the identification of H_2O formation at room temperature due to reaction of oxygen with preadsorbed hydrogen. In addition, NIS of NH_3 adsorbed on such a "defect" surface exhibits vibrational spectra in distinct contrast to that anticipated for close-packed platinum planes.

The NIS spectra of the chemisorption of C_2H_2 and C_2H_4 on Raney nickel were analyzed. Spectra were taken as a function of surface coverage, of adsorption temperature, and of subsequent heat treatment. These data indicate that at low temperatures C_2H_2 adsorbs molecularly on the nickel surface. In the case of ethylene adsorption, some bond dissociation takes place even at 120 K leading to a mixed adsorbed phase composed predominantly of a molecular C_2H_4 species. The vibrational spectra of the molecularly adsorbed species are very similar to those observed on flat Ni(111) single crystal surfaces with electron energy-loss spectroscopy. Thus, as was found on high surface area platinum in an earlier NIS study, steps and other crystal defects (which are likely to be present in a heterogeneous material like Raney nickel), have little influence on the structure of the molecularly adsorbed hdyrocarbon. However, the presence of crystal defects can account, by analogy with single-crystal work, for the low-temperature (C_2H_2, $T > 200$ K; C_2H_4, $T > 120$ K) decomposition of the molecularly adsorbed species on the Raney nickel surface.

NIS experiments have been initiated on a variety of new materials including ruthenium black and zeolite H-rho. Novel behavior of hydrogen has been observed in each case. In the zeolite, for example, a pronounced reversible conversion of bound hydrogen is apparent when the sample is heated from 275 K to 550 K. The removal of a peak at 1060 cm^{-1} is accompanied by an increase in the intensity of a peak near 200 cm^{-1}.

We plan to extend NIS adsorption studies to supported catalysts, e.g., Pt/Al_2O_3 or Pt in zeolite Y. We will examine the changes in the vibrations of chemisorbed hydrogen with particle size. The supported catalysts will be prepared and characterized in collaboration with various external laboratories. Further analysis of the material will be provided by neutron diffraction and possibly small-angle neutron scattering. We will continue the "in-situ" reaction studies of H_2/CO reactions on the nickel catalyst. Both increased and decreased reaction temperatures and increased partial pressure of CO are obvious reaction-parameter changes which could clarify the nature of the surface species which we have detected on the catalyst surface during reaction.

Next year, we will examine the adsorption of hydrogen on Pd black. Neutron scattering can distinguish between chemisorbed hydrogen and hydrogen absorbed into the bulk. We will study the vibrational spectroscopy of hydrogen on the surface and the conversion to the bulk hydride. NIS will be utilized to probe the surface chemical behavior of RuS_2, a potentially promising hydrodesulferization catalyst. The adsorptive behavior of H_2 and H_2S on both Ru black and sulfided Ru black will be further investigated. Future plans involve investigations the adsorption of thiophene on RuS_2 in an attempt to elucidate the adsorbate-surface geometry. Knowledge of the exact adsorption scheme (i.e., σ-bonded "edgewise adsorption" through the sulfur heteroatom vs. π-bonded "flatwise adsorption" through the aromatic π-cloud) provides insights concerning the type of reaction favored (i.e., hdyrogenolysis vs. hydrogenation) during hydrodesulfurization.

Further studies of adsorbate diffusion will be facilitated with the installation of a cold neutron source on the NBS reactor during the fall of 1984. Coupled with a redesigned time-of-flight spectrometer, the capability to probe a wider range of momentum transfers will be significantly enhanced. The increased beam flux, number of detector channels, and the simultaneous reduction of constraints on sample size will all increase the flexibility of the technique.

4. Photon-Stimulated Desorption and Ultraviolet Photoemission Spectroscopy Using Synchrotron Radiation

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

A major goal of this effort is to identify the electronic excitations which result in the photon-stimulated desorption (PSD) of ions from molecules adsorbed on surfaces as well as from condensed films. When possible, PSD ion yields are correlated with ultraviolet photoemission spectroscopy (UPS) of both valence states and core-electronic states of the adsorbed species. These studies provide tests of recent theoretical models of electron- and photon-stimulated desorption of ions. In addition, the synchrotron radiation techniques (PSD, UPS) are combined with other surface spectroscopies to study adsorption and reactions on solid surfaces.

Several "firsts" were achieved in FY 1984: the first studies of a single-crystal stoichiometric oxide surface (TiO_2 (110)) using synchrotron radiation, the identification of a new ion-desorption mechanism in oxidized Cr(110), and the design of a new two-dimensional display analyzer for angle-resolved PSD.

During the past year, we have used synchrotron radiation to make detailed studies of the electronic excitation spectra of the oxidized Cr(110) surface above the 3p ionization threshold ($\gtrsim$ 42 eV). We have correlated these measurements with PSD of O^+ ions, and have found a new ion-desorption mechanism: only certain core-hole states initiate ion desorption. These findings have important implications for the theory of PSD. We were the first to apply synchrotron radiation to characterize the electronic structure of a single-crystal metal oxide surface, TiO_2(110). Preliminary photoemission results have clarified the d-band contributions to the oxide valence band, and have indicated the presence of a shake-up resonance ~ 19 eV below the Fermi level. We also made the first PSD study of <u>well-characterized</u> TiO_2 single-crystal surfaces having the (110) orientation. This major test of the Knotek-Feibelman model of ion desorption reveals shortcomings in the basic theory. The studies involve "perfect" TiO_2 surfaces, and "defect" surfaces produced by Ar^+ sputtering and indicate the importance of local-site geometry in PSD and electron-stimulated desorption.

This year we installed and tested a new high-flux grazing incidence monochromator at SURF-II. The new monochromator proceeds a photon flux 20 to 50 times more intense than our present instrumentation in the photon energy range 25 to 80 eV. The range can be extended to 175 eV with a new grating. We also completed the design and initiated construction of a new display-type ion and electron energy analyzer. It is a bandpass analyzer which employs an ellipsoidal mirror; the design is based on an analyzer pioneered by Eastman. When complete, it will be the second such analyzer in operation in North America.

This coming year we plan to use variable wavelength UPS to determine, for the first time, the influence of oxide surface structure and surface defect concentration on the electronic properties of transition metal oxides. Nearly-perfect, annealed TiO_2 and Ti_2O_3 will be compared with defective, Ar^+-bombarded surfaces. Single crystals having different orientations will be studied; both thermally-stable and thermally-unstable surfaces (e.g. TiO_2 (110) and (100)) will be examined.

We will complete the construction of the new angle-resolving, display-type ion and electron energy analyzer. We will employ this special analyzer to measure the surface core-level shifts in several related series of oxidized substrates, e.g., ranging from clean Ti to oxidized Ti metal, to stoichiometric Ti_2O_3 and TiO_2. This will provide new insights into the local electronic environment of both cations and anions. We will employ the same analyzer to initiate the first angle-resolved PSD studies on both nearly-perfect and defective oxides, as well as on molecules adsorbed on these surfaces. Surface structure inferred from these studies will be correlated with other measurements.

Next year we also plan to extend extend chemisorption measurements on single-crystal oxides to the temperature range below 300 K. Surprisingly, there are virtually no chemisorption measurements reported at low temperatures. Our goal is the accurate determination of adsorption energetics and molecular structure for CO, H_2O, NH_3 on oxides.

5. Surface Chemical Physics of Single Crystals, Alloys and Ultrathin Films

(W. F. Egelhoff)

Interest in ultrathin (down to one atomic layer) metal films on the part of the surface-science community has greatly increased in the past three years as it has become clear that an understanding of such structures will contribute to solving a wide range of problems in surface science. Among these are an understanding of the differences between surface and bulk electronic structure, the changes of surface electronic structure associated with chemisorption, the basis of surface magnetism, the modification of surface-layer properties by the substrate, the relationship between electronic structure and epitaxial growth, and the surface properties of alloys. The experimental program presently underway is using an integrated approach to study single-crystal surfaces, alloys and ultrathin films to contribute to an understanding of all of the above problems.

This past year a new aspect of x-ray photoelectron spectroscopy (XPS) and Auger-electron spectroscopy (AES) of thin films was discovered that can be used to characterize the morphology of films and to provide a new approach to analyzing XPS and AES data. The phenomenon takes the form of enhanced intensities of photoelectrons or Auger electrons from an atom in the film along the internucleus axes towards neighboring atoms. This is illustrated in Fig. 9. For 2 ML of copper on Ni(100), the inner Cu layer will have its core-level peak intensities enhanced at a polar angle of 45°, as shown, due to forward scattering by the top Cu layer. Figure 10 presents experimental data of the angular distributions of the Cu $2p_{3/2}$ signal as a function of the film thickness that show a strong peak at $\theta=45°$ when the Cu film thickness exceeds 2 ML. The effect is more pronounced for electron energies greater than 500 eV; for example, in the angular profiles of the Cu AES peak several peaks are observed that can be interpreted as arising from specific layers of Cu atoms. Numerical calculations demonstrate that this type of enhancement is not due to electron channeling (the Kikuchi effect) as has been suggested previously.

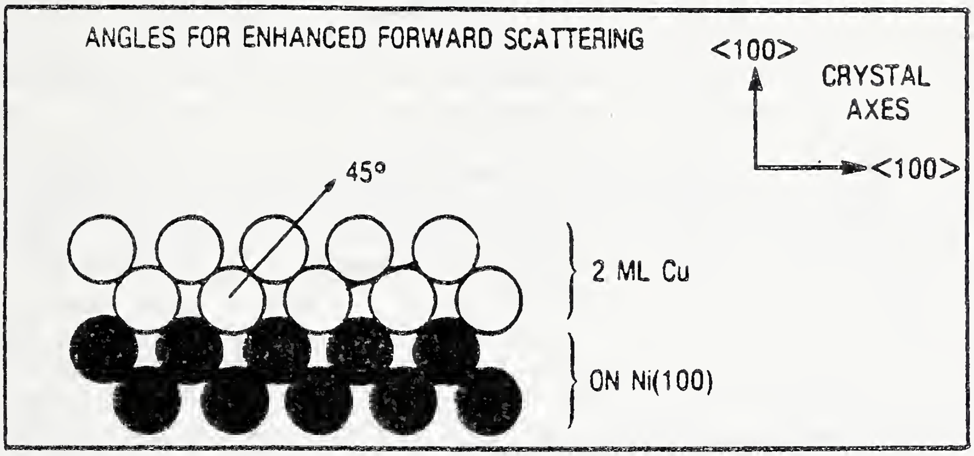

Fig. 9 Illustration of enhanced forward scattering at a polar angle of 45° from the bottom Cu layer by the top Cu layer of a 2ML copper film on a Ni(100) substrate.

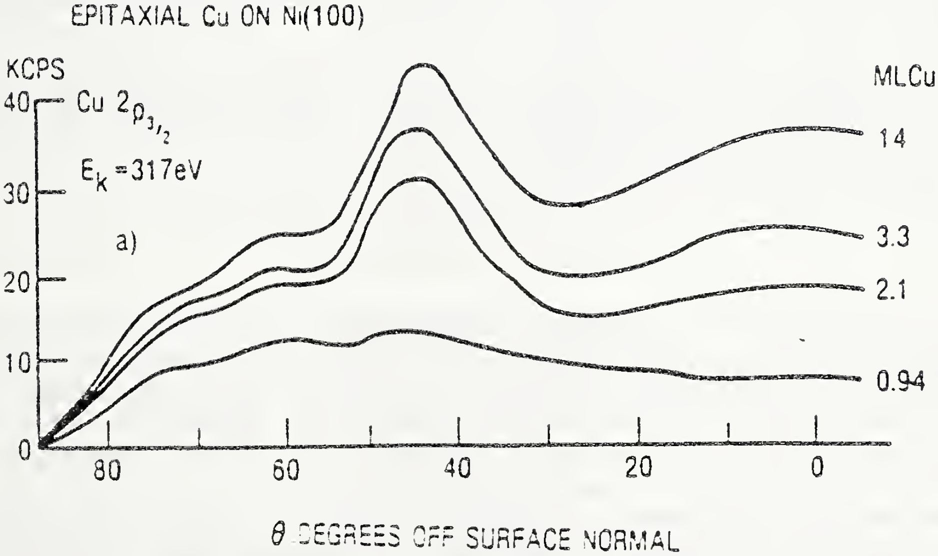

Fig. 10 Intensity of the Cu $2p_{3/2}$ XPS signal as a function of polar angle for different thicknesses of copper (in monolayers) epitaxially deposited on Ni(100).

This forward scattering phenomenon has been found to be an easily used, new approach to gaining structural information about surfaces. The enhanced intensities along internuclear axes provide a very useful diagnostic of whether epitaxy, agglomeration, surface alloying, or interdiffusion are occuring at a multicomponent surface.

The forward-scattering phenomenon can be utilized to provide additional, new data important for surface and interface science. The XPS signal originating from a particular layer can be selected by appropriate choice of angle. This provides a convenient means of measuring the core-level binding energies of surface atoms and comparing them with the binding energies of atoms in other layers and in the bulk. The phenomenon also provides a new way of determining the background in XPS and AES data; this method is described in Section 2.A.8. Finally, this work has shown that conventional methods of measuring electron attenuation lengths for quantitative surface analysis by XPS and AES can be subject to appreciable errors, as described in Section 2.A.7; the "effective" attenuation length for the analysis of thin ordered films will depend on the film morphology and crystalline perfection as well as the instrumental geometry.

A major, invited review article, "Core-Level Binding-Energy Shifts in Solids and at Surface," is currently being written for Surface Science Reports. In addition work will continue on the development of the forward-scattering effect as a tool for structural and electronic studies of surfaces and interfaces; the refinement of the use of the equivalent-core Born-Haber-cycle method for determining thermochemical quantities at surfaces and interfaces; and the initiation of a program to make nonequilibrium, exotic alloy structures such as alternating single, epitaxial atomic layers of Cu/Ni/Cu/Ni/Cu.... This plan represents an extension of the field of ordered alloy systems to a potentially unlimited number of nonequilibrium ordered systems. Novel materials such as these have not been prepared previously but are expected to have unusual physical and chemical properties.

6. Atom-Probe Field-Ion Microscopy of Materials

(A. J. Melmed, R. Klein, M. E. Twigg)

We are completing the construction of an Atom-Probe Field-Ion Microscope (APFIM) facility which will enable microscopic determinations of composition and atomic structure to be made on a wide range of materials in both the surface and the bulk regions of a sample. The atom probe facility will consist of three instruments: (1) A rapid turnover low-temperature field-ion microscope (built earlier) for initial specimen surveys and microstructure characterization; (2) A general-purpose atom probe (GPAP) for initial microcomposition surveys; and (3) A high-resolution energy-corrected atom probe (ECAP) for accurate microcompositional analyses, especially for very small (< 10 nm) precipitates, alloy phases, etc.

The general purpose atom probe (GPAP), completed last year, has been applied to the determination of the composition and the micro-structure of superalloys. With the imaging and variable-aperture capability of the

GPAP, selected ares of the alloy specimens, that is single-phase regions, have been isolated for analysis. This is important to alloy designers since the composition of microprecipitates strongly influences the properties of alloys. The GPAP is especially suited for this type of research into structures and composition for precipitates, etc. whose major dimensions are less than about 50 nm. The GPAP is thus extending our measurement capabilities to an important area of materials characterization.

An evaluation of the instrumental factors influencing the compositional analysis of alloys has been initiated and is more than half completed. This work will lead to an optimization of procedures to improve the confidence limits in determinations of composition with our GPAP.

Considerable progress has been made in the construction of the energy-corrected atom probe (ECAP). The main chamber, the straight-path detector, the energy-compensation lens, and the end-flight ion detector have been assembled. The vacuum manifold, gas-supply systems and electronic control units are being constructed.

During the past year, a nickel-base superalloy, RSR 143 (Ni,Al,Mo,Ta), has been analzyed with the GPAP and an analytical transmission electron microscope (TEM). The compositions of the three phases of this alloy, namely the γ matrix, the γ' cuboids and the DO_{22} platelets were determined, and it was found that the platelets (fine-scale precipitates) were rich in aluminum and tantalum. The conclusion is that both elements provide for the stabilization of the precipitates in this alloy.

The alloy RSR 224A (Ni,Al,Mo,W) has been studied in cooperation with the Pratt and Whitney Company. It was found that W is present in excess in the small precipitates and indeed is absent from the surrounding matrix. The inference is that further addition of W should provide additional precipitate growth, so that particular mechanical properties may be enhanced.

In conjunction with the comparisons of analyses made using the GPAP and TEM, calculations have been made of the effect of bremsstrahlung-induced fluorescence on x-ray micro-analysis in the TEM. This fluorescence should not be overlooked in the analysis of thin-foil specimens composed primarily of heavy elements.

Measurements have been made on Ni_3Al to assess factors influencing the analysis of composition with the GPAP. As found by others, increasing the ratio of pulse voltage to dc bias voltage (from 10 percent to 40 percent) results in increases of the measured Ni/Al ratio towards the nominal value. Further analysis of these experiments is in progress.

During the next year we will initiate micro-diffusion measurements for metal/metal and metal/semiconductor systems. We plan the completion of construction and testing of the ECAP and its application to grainboundary segregation studies in nickel-base superalloys and to interdiffusion measurements of metal layers on semiconductors. We will also continue studies establishing and extending the confidence limits of atom-probe analysis of complex systems.

7. Surface Theory

(S. M. Girvin, P. K. Lam, T. J. Jach, D. E. Ramaker)

Theoretical research is conducted in areas judged useful for the experimental program and to develop a conceptual base for surface and interface properties, processes, interactions, and measurements.

A principal area of investigation has been the quantum Hall effect. This phenomenon occurs in a two-dimensional electron gas (inversion layer) found at an atomically smooth interface between two semiconducting materials. At very high magnetic fields (10T) and low temperatures (1K), the Hall resistance of such devices is found to take on universal quantized values h/e^2i where h is Planck's constant and e is the elementary charge. The quantum number i can be an integer or a simple rational fraction.

The main problem of current interest is to develop an understanding of the origin of the fractional quantum numbers. These are believed to arise from a collective many-body ground state due to Coulomb interactions. A new formalism has been developed for doing quantum mechanics in high magnetic fields in two dimensions. The work centers on the use of coherent states which allow formulation by semi-classical wave packet dynamics. This method reduces the complexity of computer calculations which so far have limited the number of interacting particles for which the Schroedinger equation can be solved. We are presently in the process of applying this formalism to the fractional quantum number problem using both analytical and numerical Monte Carlo methods.

This year we have predicted the critical value of magnetic field for the liquid-solid transition (Wigner crystallization) of the inversion layer. For this work, a new variational wave function was developed to describe the solid phase. This wave function includes correlations and is thus an improvement over previous Hartree-Fock results. Numerical evaluation of the ground state energy shows that above a critical magnetic field corresponding to 6.5 flux quanta per electron, the inversion layer solidifies (see Figure 11) and the fractional quantum Hall effect will no longer be observed. This prediction is in good agreement with the limited experimental data presently available and has stimulated considerable new interest in attempts to directly observe Wigner crystallization in inversion layers.

Work also continued on the elucidation of the mechanisms that can give rise to electron- and photon-stimulated desorption of ions from adsorbates on surfaces as well as from single crystals. Particular attention was given to the competitive core-hole decay processes (i.e. resonant photoemission and Auger decay) either before or after escape of the excited electron. The adsorption systems studied included OH and H_2O

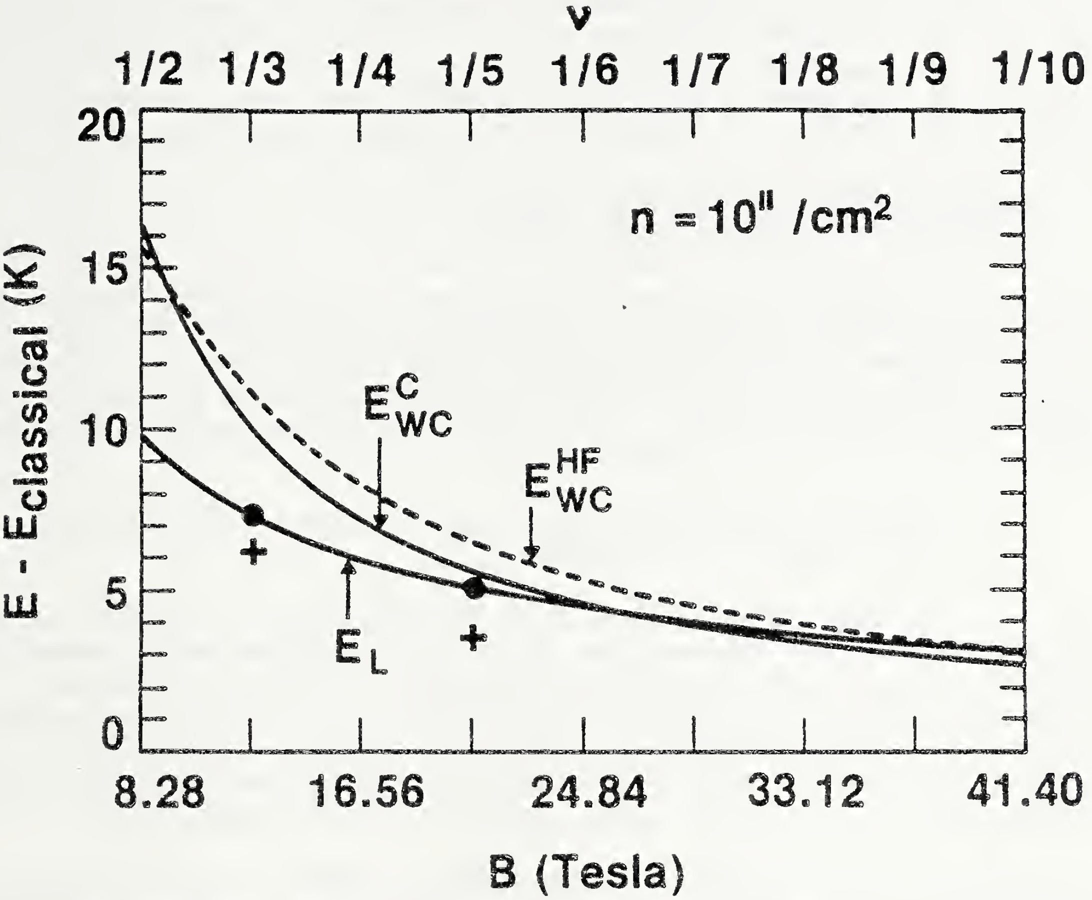

Fig. 11 Ground state energy vs. magnetic field B at an electron density of $10^{11}/cm^2$. The corresponding Landau level filling factor ν is shown on the upper horizontal axis. The dashed line is the Hartree-Fock energy for the solid. The solid line labelled E_{WC}^{C} is the improved solid energy incorporating correlations. E_L is the liquid state energy. Note that for $\nu^{-1} > 6.5$, the solid is more stable than the liquid.

on Ti(001), Cr(110), and Cu(100) and O on Cr(110). A study has also begun to explain the relative O^+ desorption yields from single-crystal and ion-sputtered TiO_2 surfaces. All of these systems have been studied experimentally at NBS (Section 4.B.4). The role of excitonic or defect-like states in the localization of either the initial excited electrons or the two final-state holes, and hence in the desorption process, will be further studied.

Next year we plan to complete the analytic and numerical Monte Carlo descriptions of the fractional quantum number ground state and see the application to inversion layer systems of the semi-classical wave-packet techniques pioneered by Keller for chemical physics problems. Work will continue (in collaboration with Prof. M. W. Cole of the Pennsylvania State University) to develop a scattering theory formalism to describe the repulsive part of the rare-gas metal-substrate interaction.

C. Surface Science Experiments at the Brookhaven National Synchrotron Light Source

A major undertaking since FY 1981 has been the initiation of an NBS-Naval Research Laboratory collaboration to establish four beam lines at the Brookhaven National Synchrotron Light Source (NSLS). The Surface Science Division is directly involved in experiments on two of the four beam lines on the x-ray ring. These experiments have been delayed due to machine difficulties at Brookhaven.

1. Photon-Stimulated Desorption and Photoemission Spectroscopy
(T. E. Madey, R. Stockbauer)

This work is an extension of the experiments performed at the NBS SURF-II facility (see section 4.B.4) to the higher photon energies and more intense light available at the NSLS. Light from a unique, extended-range monochromator (5-5000 eV) will be used to study surface structure and surface bonding of adsorbed molecules. Experimental probes will include photoemission spectroscopy, surface extended x-ray absorption fine structure, and, particularly, photon-stimulated desorption.

The main experimental ultrahigh vacuum chamber has been designed and constructed, and the sample preparation chamber has been designed and acquired. Ancillary electronics and uhv apparatus (manipulator, LEED/ESDIAD optics, argon ion gun, etc.) have been purchased. The first efforts will be to characterize the roles of both core-level and valence excitations in the photon-stimulated desorption (PSD) of ions from covalently-bonded surface molecules.

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

The NBS Quantum Metrology Group under the direction of Dr. R. D. Deslattes is developing an experiment to study electronic effects associated with core-level ionization in atoms, molecules, and simple solids. Specific effects to be studied include dynamical effects in inner-shell vacancy production, relaxation of the extra-atomic environment, and production of multiple vacancies with or without ionization. One member of the Surface Science Division staff has been assigned to work half-time on this project.

The experiment will consist of a high-resolution crystal monochromator designed to operate between 0.8 and 5 eV in an ultrahigh vacuum. It is planned to study photoemission, Auger-electron emission, and x-ray fluorescence from gas and solid targets, particularly in the vicinity of thresholds for core-level ionization. The facility will also be used for extended x-ray absorption fine structure and x-ray standing-wave studies of clean surfaces and interfaces.

We have become the first user group to obtain radiation from a port on the NSLS x-ray ring. Present work involves the extensive modification and positioning of our beam output facilities in collaboration with machine physicists at NSLS. We have developed a new generation of photodiodes particularly designed for x-ray synchrotron experiments. These diodes are compatible with ultrahigh vacuum (UHV) systems and are bakeable. We are designing the second-generation UHV experimental chamber for surface-sensitive x-ray experiments. This chamber will be particularly suited for x-ray standing wave, surface diffraction, and reflectance studies. It will include a manipulator capable of being set to very small angles with high accuracy.

5. PUBLICATIONS

(a) Publications of Past Year

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6. TALKS

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Fine, J., "Standard Reference Materials for Sputter Depth Profile Analysis," NBS Research Advisory Committee Symposium on Surface Science, National Bureau of Standards, Gaithersburg, MD, September 13, 1984.

Gadzuk, J. W., "Sixty Years of Surface Physics," Institut fur Festkorperforschung, KFA, Jülich, W. Germany, September 15, 1984.

Gadzuk, J. W., "Non-Adiabatic Effects in Elementary Surface Reactions: State-to-State Molecular Beam Experiments as a Probe," Chemical Physics Seminar, California Institute of Technology, Pasadena, CA, November 1, 1984.

Gadzuk, J. W., "Non-Adiabatic Effects in Elementary Surface Reactions: State-to-State Molecular Beam Experiments as a Probe," Surface Science Colloquium, Univ. of California, Berkeley, CA, November 3, 1983.

Gadzuk, J. W., "Textbook Time-Dependent Quantum Mechanics not Taught in Textbooks: Some Applications in Surface Physics," Howard University, Washington, D.C., November 16, 1983.

Gadzuk, J. W., "Non-Adiabatic Effects in Elementary Surface Reactions," Physics Department Colloquium, Pennsylvania State University, University Park, PA, November 21, 1983.

Gadzuk, J. W., "Dephasing, Pairs, and Phonons or Why my Lineshapes are so Broad," Institute of Theoretical Physics, Chalmers University of Technology, Göteborg, Sweden, January 17, 1984.

Gadzuk, J. W., "Energy Redistribution in Molecule-Surface Collisions Involving Charge Transfer/Surface Hopping," American Physical Society Meeting, Detroit, MI, March 26, 1984.

Gadzuk, J. W., "Energy Redistribution and Dissociative Adsorption on Molecule-Surface Collisions," Greater Washington Surface Science Seminar, National Bureau of Standards, Gaithersburg, MD, April 30, 1984.

Gadzuk, J. W., "Russian Reflections," Sandy Springs Friends School, Olney, MD, May 9, 1984.

Gadzuk, J. W., "The Vibrational Lineshape of CO Chemisorbed on Ni(111): Dephasing in Action," Physical Electronics Conference, Princeton University, Princeton, NJ, June 20, 1984.

Gadzuk, J. W., "Dynamic Effects in Electronic Excitation and Molecular Scattering," International Centre for Theoretical Physics, Trieste, Italy, June 28, 1984.

Gadzuk, J. W., "On Vibrational Lineshapes of Adsorbed Molecules," Consiglio Nazionale della Ricerche, Rome, Italy, July 2, 1984.

Gadzuk, J. W., "Dynamics of Molecular Processes at Surfaces: I. Charge Transfer and Internal Excitation, II. Energy Redistribution and Dissociative Adsorption," Consiglio Nazionale della Ricerche, Rome, Italy, July 3, 1984.

Gadzuk, J. W., "Communicating Scientific Concepts," Third Electrochemical Study Group, Fritz-Haber Institute, Berlin, W. Germany, July 16, 1984.

Gadzuk, J. W., "Surface Science Concepts of Charge Transfer Reactions," Third Electrochemical Study Group, Fritz-Haber Institute, Berlin, W. Germany, July 18, 1984.

Gadzuk, J. W., "Dynamic Effects in Electronic Excitation and Molecular Scattering at Surfaces," Solid State Physics Group, Cornell University, Ithaca, NY, August 6, 1984.

Gadzuk, J. W., "Dynamic Effects in Electronic Excitation and Molecular Scattering at Surfaces," NBS Research Advisory Committee Symposium on Surface Science, National Bureau of Standards, Gaithersburg, MD, September 13, 1984.

Gadzuk, J. W., "Molecular Scattering, Energy Redistribution and Dissociative Adsorption," Workshop on Interactions of Molecular Beams with Solid Surfaces, Cambridge, England, September 27, 1984.

Girvin, S. M., "Rough Surfaces and Random Interfaces: Scattering of Light and Electrons," Statistical Engineering Division Seminar, National Bureau of Standards, Gaithersburg, MD, October 11, 1983.

Girvin, S. M., "The Quantum Hall Effect," Chalmers University, Gothenburg, Sweden, November 17, 1983.

Girvin, S. M., "The Quantum Hall Effect," Physics Department Colloquium, Purdue University, W. Lafayette, IN, February 2, 1984.

Girvin, S. M., "The Quantum Hall Effect," Physics Department, Brown University, Providence, RI, March 8, 1984.

Girvin, S. M., "The Quantum Hall Effect," Physics Division, National Research Council of Canada, Ottawa, Canada, May 18, 1984.

Girvin, S. M., "Review of the Present Status of the Quantum Hall Effect," Aspen Center for Physics Workshop, Aspen, CO, July 3, 1984.

Kelley, R. D. (coauthors: R. R. Cavanagh, J. J. Rush, and T. E. Madey), "Neutron Spectroscopic Studies of the Adsorption and Decomposition of C_2H_2 and C_2H_4 on Raney Ni," Physical Electronics Conference, Princeton University, Princeton, NJ, June 19, 1984.

Kurtz, R. L., "The Influence of O_2 and H_2O on the Surface Electronic Structure of Corundum Transition-Metal Oxides," American Vacuum Society 30th Annual Symposium, Boston, MA, November 1, 1983.

Kurtz, R. L., "Electron Mean-Free Path Measurements in Condensed Molecular Layers," American Physical Society Meeting, Detroit, MI, March 26, 1984.

Kurtz, R. L., "Use of Synchrotron Radiation to Determine Electron Mean-Free Paths in Condensed Molecular Solids," Greater Washington Surface Science Seminar, National Bureau of Standards, Gaithersburg, MD, April 30, 1984.

Kurtz, R. L., "Photon-Stimulated Desorption of O^+ from TiO_2: Evidence for New Mechanisms," Physical Electronics Conference, Princeton University, Princeton, NJ, June 18, 1984.

Kurtz, R. L., "Surface Studies of the Oxides of Titanium: Electronic Structure, Chemisorption, and Desorption from Ti_2O_3 and TiO_2," Naval Research Laboratory, Washington, D.C., September 19, 1984.

Lam, P. K., "Correlation Energy of a Two-Dimensional Wigner Crystal in a Quantizing Magnetic Field," American Physical Society, Detroit, MI, March 28, 1984.

Madey, T. E. (coauthor: C. Benndorf), "The Dynamics of Electron and Photon Stimulated Desorption Processes," International Conference on Solid Surfaces, Madrid, Spain, September 26, 1983.

Madey, T. E., "Early Applications of Vacuum, From Aristotle to Langmuir," American Vacuum Society 30th Annual Symposium, Boston, MA, November 1, 1983.

Madey, T. E. (coauthors: D. L. Doering and S. Semancik), "Coadsorption of Water and Sodium on the Ru(001) Surface," Materials Research Society 1983 Annual Meeting, Boston, MA, November 15, 1983.

Madey, T. E., "Early Applications of Vacuum, From Aristotle to Langmuir," University of Maryland, College Park, MD, November 29, 1983.

Madey, T. E., "Structure of Surface Molecules using Electron Stimulated Desorption," Pennsylvania State University, University Park, PA, January 19, 1984.

Madey, T. E., "History of Vacuum, From Aristotle to Langmuir," American Vacuum Society Chapter, Houston, TX, January 31, 1984.

Madey, T. E., "History of Vacuum Technology," American Vacuum Society Florida Chapter, Clearwater, FL, February 6, 1984.

Madey, T. E., "History of Vacuum Technology," Case Western Reserve University, Cleveland, OH, February 23, 1984.

Madey, T. E., "Electron and Photon Stimulated Desorption," Case Western Reserve University, Cleveland, OH, February 23, 1984.

Madey, T. E. (coauthor: C. Benndorf), "Influence of Oxygen and Sodium on the Structure of NH_3 on Ni(110)," Sixth European Conference on Surface Science, York, England, April 2, 1984.

Madey, T. E., "Electron and Photon Stimulated Desorption," American Physical Society Meeting, Storrs, CT, May 30, 1984.

Madey, T. E., "Mechanisms and Applications of Electron Stimulated Desorption," Surface Canada 1984, Montreal, Canada, June 1, 1984.

Madey, T. E. (coauthors: C. Benndorf, D. L. Doering, and S. Semancik) "Influence of Surface Additives, Sodium and Oxygen on the Structure and Bonding of H_2O to Metal Surfaces," Third Electrochemical Study Group, Berlin, W. Germany, July 16, 1984.

Madey, T. E., "The Uses and Limitations of ESDIAD for Determining the Structure of Surface Molecules," First International Conference on the Structure of Surfaces, Berkeley, CA, August 14, 1984.

Madey, T. E., "The Structure and Kinetics of Water Adsorbed on Clean and Impurity-Dosed Metal Surfaces," American Chemical Society, Philadelphia, PA, August 27, 1984.

Melmed, A. J. "The Complimentary Use of APFIM and TEM in Materials Research," Fritz-Haber Institute, W. Berlin, Germany, January 23, 1984.

Melmed, A. J., "Field Ion Mass Spectroscopy at the Atomic Level," University of Bonn, Bonn, W. Germany, April 6, 1984.

Melmed, A. J., "Investigation of Ni-based Superalloy Compostructure by TEM and APFIM," Chalmers University of Technology, Goteborg, Sweden, May 24, 1984.

Melmed, A. J., "Scanning Tunneling Microscopy: Some Reviewer's Comments," Fritz Haber Institute, Berlin, Germany, June 4, 1984.

Melmed, A. J., "The Complementary Use of TEM and APFIM in Materials Research, Technical University, Münich, W. Germany, June 15, 1984.

Melmed, A. J., "Rare-Earth Crystal Growth From the Vapor: Eu/Re and Eu/W," 31st Field International Field Emission Symposium, Paris, France, July 15, 1984.

Melmed, A. J., "The Complementary Use of APFIM an Analytical TEM for Studying Ni-Base Superalloys," 31st International Field Emission Symposium, Paris, France, July 16, 1984.

Melmed, A. J., "Epitaxial Growth and Some Properties of Samarium Crystals on Tungsten," 31st Field International Field Emission Symposium, Paris, France, July 16, 1984.

Powell, C. J. (coauthor: N. E. Erickson), "Comparison of L_3-Shell Excitation Energies of 3d Transition Metals Obtained by XPS, AEAPS, and EELS," American Vacuum Society 30th Annual Symposium, Boston, MA, November 1, 1983.

Powell, C. J., "Inelastic Mean Free Paths of Low-Energy Electrons in Solids," American Physical Society Meeting, Detroit, MI, March 26, 1984.

Powell, C. J., "Inelastic Mean Free Paths and Attenuation Lengths of Low-Energy Electrons in Solids," Symposium on Microprobe Surface Analytical Techniques, Scanning Electron Microscopy/1984, Philadelphia, PA, April 16, 1984.

Powell, C. J., "Quantitative Surface Spectroscopy," Symposium of the Ohio Chapter of the American Vacuum Society, Case Western Reserve University, Cleveland, OH, May 16, 1984.

Powell, C. J., "Lectures on Surface Analysis," Shanghai Institute of Testing Technology, Shanghai, China, May 24-June 5, 1984.

Powell, C. J. (coauthor: N. E. Erickson), "Electron Spectroscopy of Core Levels," Department of Physics, Waseda University, Tokyo, Japan, May 21, 1984.

Powell, C. J. (coauthor: N. E. Erickson) "Quantitative Auger-Electron Spectroscopy and Development and Applications of Appearance-Potential Spectroscopy," Shanghai Branch of Chinese Vacuum Society, Shanghai Science Hall, Shanghai, China, May 29, 1984.

Powell, C. J., "Emerging Methods of Surface Characterization," Shanghai Metrological Society, Shanghai Institute of Testing Technology, Shanghai, China, June 4, 1984.

Powell, C. J., "Quantitative Surface Characterization by Auger-Electron Spectroscopy and X-ray Photoelectron Spectroscopy," Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China, June 12, 1984.

Powell, C. J. (coauthor: N. E. Erickson), "Electron Spectroscopy of Core Levels," Applied Physics Department, Osaka University, Osaka, Japan, June 14, 1984.

Powell, C. J., "Energy Dependence of Inelastic Mean Free Paths of Low Energy Electrons in Solids," Gordon Research Conference on Electron Spectroscopy, Wolfeboro, NH, July 18, 1984.

Powell, C. J. (coauthor: N. E. Erickson), "Comparisons of L_3-Shell Binding Energies of Ti-Ni as Measured by XPS, EELS and APS," Gordon Research Conference on Electron Spectroscopy, Wolfeboro, NH, July 18, 1984.

Shinn, N. D. (coauthors: J. F. Morar and F. R. McFeely), "Spectroscopic Characterization of Fluorinated Silicon Surfaces," American Vacuum Society 30th Annual Symposium, Boston, MA, November 2, 1983.

Shinn, N. D., "Oxygen Induced CO Reorientation on Cr(110)," Surface Science Group, Massachusetts Institute of Technology, Cambridge, MA, June 1, 1984.

Shinn, N. D. (coauthor: T. E. Madey), "Observation of a New Molecular CO Binding State on Cr(110)," Physical Electronics Conference, Princeton University, Princeton, NJ, June 18, 1984.

Shinn, N. D., "Chemisorption on Cr(110); Uncommon Results for O_2 and CO," IBM T.J. Watson Research Center, Yorktown Heights, NY, June 25, 1984.

Shinn, N. D. (coauthor: T. E. Madey), "From Molecular Chemisorption to Initial Surface Oxidation; an EELS Study of Cr(110)," American Chemical Society Meeting, Philadelphia, PA, August 27, 1984.

Shinn, N. D., "Vibrations of Adsorbed Molecules Probed by Electron Energy Loss Spectroscopy," NBS Research Advisory Committee Symposium on Surface Science, National Bureau of Standards, Gaithersburg, MD, September 13, 1984.

Stockbauer, R., "Photon Stimulated Desorption of Ions from Surfaces: Mechanisms and Applications," Solid State Physics Seminar, University of Maryland, College Park, October 24, 1983.

Stockbauer, R., "Surface Science at SURF," NBS Research Advisory Committee Symposium on Synchrotron Radiation, National Bureau of Standards, Washington, D.C., October 20, 1983.

Stockbauer, R., "Photon and Electron Stimulated Desorption of Ions from Surfaces: Mechanisms and Applications," Physical Chemistry Seminar, University of North Carolina, Chapel Hill, NC, November 14, 1983.

Stockbauer, R., "Photon and Electron Stimulated Desorption of Ions from Surfaces: Mechanisms and Applications," Department of Chemistry Seminar, Boston University, Boston, MA, April 23, 1984.

Twigg, M. E., "A Microanalytical Study of Secondary Precipitation in Ni-Base Superalloys," Bell Laboratories, Murray Hill, NJ, November 17, 1983.

Twigg, M. E., "A Microanalytical Study of Ni-base Superalloys," Case Western Reserve University, Cleveland, OH, November 21, 1983.

Twigg, M. E., "An Analytical Study of Ni-base Superalloys," Michigan Technological University, Houghton, MI, January 12, 1984.

Twigg, M. E., "An Analytical Study of Ni-base Superalloys," University of Utah, Salt Lake City, UT, January 23, 1984.

Twigg, M. E., "An Analytical Study of Ni-base Superalloys," Rensselaer Polytechnic Institute, Troy, NY, January 26, 1984.

Twigg, M. E., "A Microanalytical Study of Nickel-base Superalloys," Auburn University, Auburn, AL, February 2, 1984.

Twigg, M. E., "A Microanalytical Study of Nickel-base Superalloys," The Metals Society-American Institute of Metallurgical Engineering Meeting, Los Angeles, CA, February 27, 1984.

Twigg, M. E., "A Microanalytical Study of Nickel-base Superalloys," Department of Metallurgy, Lehigh University, Bethlehem, PA, March 5, 1984.

Twigg, M. E. (coauthors: A. J. Melmed and R. Klein), "Atom-Probe Field Ion Microscopy and Analytical Transmission Electron Microscopy of Nickel-Based Super Alloys," Greater Washington Surface Science Seminar, National Bureau of Standards, Gaithersburg, MD, April 30, 1984.

Twigg, M. E., "Microanalytical Study of Superalloys," 1984 Meeting of Microbeam Analysis Society, Lehigh University, Bethlehem, PA, July 16, 1984.

Twigg, M. E., "Electron Trajectories in Monte Carlo Calculations," 1984 Meeting of Microbeam Analysis Society, Lehigh University, Bethlehem, PA, July 17, 1984.

Twigg, M. E., "Bremsstrahlung Fluorescence in AEM," 1984 Meeting of Microbeam Analysis Society, Lehigh University, Bethlehem, PA, July 20, 1984.

Udovic, T. J., "The Catalytic Activity of Clean and Modified W(110)," American Chemical Society, St. Louis, MO, April 11, 1984.

Udovic, T. J., "Catalysis by a Single-Crystal Surface: Hydrogenation Reactions over W(110)," Greater Washington Surface Science Seminar, National Bureau of Standards, Gaithersburg, MD, April 30, 1984.

Wax, M. J. (coauthor: R. G. Bergman), "Mechanism of a Molybdenum Hydride/Molybdenum Alkyl Dinuclear Reductive Elimination," American Chemical Society, St. Louis, MO, April 9, 1984.

7. SURFACE SCIENCE DIVISION SEMINARS

Avery, N., University of Melbourne, Parville, Australia, "EELS Study of the Bonding and Reactivity of Molecules on Metal Surfaces," October 7, 1983.

Bange, K., Fritz Haber Institute, Berlin, W. Germany, "Electrochemistry and UHV Systems: Coadsorption of Water with Positive and Negative Ions on Metal Surfaces," January 5, 1983.

Binnig, G., IBM Zurich Research Laboratory, Ruschlikon, Switzerland, "Scanning Tunneling Microscopy of Surfaces," October 31, 1983.

Burgess, D., Northwestern University, Evanston, IL, "Laser Induced Thermal Desorption as a Probe of Surface Processes," March 20, 1984.

Caflisch, R., Massachusetts Institute of Technology, Cambridge, MA, "Renormalization Group Studies of Adsorption, Fluid Mixtures and Liquid Crystals," February 21, 1984.

Castleman, A. W., Pennsylvania State University, University Park, PA, "Aggregated State of Matter: From Nucleation to Photoionization," October 11, 1983.

Cavanagh, R. R., National Bureau of Standards, Gaithersburg, MD, "Chemical Dynamics at Surfaces: Cold Rotations and Hot Vibrations," September 12, 1984.

Cohen, P. I., University of Minnesota, Minneapolis, MN, "RHEED Studies of Morphology of GaAs Surfaces Prepared by Molecular Beam Epitaxy," December 9, 1983.

Cole, M., Pennsylvania State University, University Park, PA, University Park, PA, "Physical Adsorption: Theory and Reality," May 15, 1984.

Comsa, G., Institut fur Grenzflachenforschung und Vakuumphysik, Jülich, W. Germany, "Island Formation and 2-D Phase Transitions Studied by Thermal He Scattering," June 8, 1984.

DePristo, A., Iowa State Univeristy, Ames, IA, "Energy Transfer in Diatomic and Triatomic Scattering from Smooth and Structured Non-Rigid Surfaces," June 21, 1984.

Dhere, N., Institute of Military Engineering, Rio de Janeiro, Brazil, "Thin Film Solar Cells," June 27, 1984.

Doering, D., University of Florida, Gainesville, FL, "Rotational Epitaxy and Periodic Lattice Structures," June 13, 1984.

Dose, V., Universität Würzburg, Würzburg, W. Germany, "Inverse Photoemission," April 13, 1984.

Forstman, F., Institute of Theoretical Physics, Free Univrsity, Berlin, W. Germany, "Plasma Waves in Electro-Reflectance: An Optical Measurement of the Bulk Plasmon Dispersion," June 12, 1984.

Friend, C., Harvard University, Cambridge, MA, "Surface Chemsitry of Modified W(110)," August 17, 1984.

Hamers, R. J., Cornell University, Ithaca, NY, "Multiphoton Ionization Studies of Inelastic Molecular Scattering at Surfaces," March 21, 1984.

Hofmann, S., Max Planck Institut fur Metallforschung, Stuttgart, W. Germany, "Prefrential Sputtering in Oxides," April 9, 1984.

Huse, D., Bell Laboratories, Murray Hill, NJ, "Melting Transition of Krypton on Graphite," September 21, 1983.

Kleinman, L., University of Texas, Austin, TX, "Initial Stages of the Oxidation of Aluminum," May 18, 1984.

Landman, U., Georgia Institute of Technology, Atlanta, GA, "Molecular Dynamics Study of Surface Diffusion," October 13, 1983.

Lam, P. K., National Bureau of Standards, Gaithersburg, MD, "Nature of Metallic Binding," February 15, 1984.

Marcus, P., Ecole Nationale Superieure de Chimie de Paris, Paris, France, "Chemisorption of Sulphur on Metal and Alloy Surfaces," October 13, 1983.

Muller, J., Institut fur Festkorperforschung, Jülich, W. Germany, "Cluster Study of the Interaction of an H_2O Molecule with Al Surfaces," October 14, 1983.

Myers, L. L., Air Force Office of Scientific Research, Bolling Air Force Base, D.C., "Air Force Basic Research in Chemistry and Surface Science," May 3, 1984.

Netzer, F., University of Innsbruck, Innsbruck, Austria, "Electronic Structure of Rare Earth Metal Surfaces by Electron Energy Loss Spectroscopy," October 27, 1983.

Netzer, F., University of Innsbruck, Innsbruck, Austria, "Electron Energy Loss Spectroscopy of Rare Earths," July 11, 1984.

Nowotny, J., Polish Academy of Sciences, Karakow, Poland, "Surface Properties of Metal Oxides at Elevated Temperatures," May 24, 1984.

Pfnuer, H. E., IBM Research Laboratory, San Jose, CA, "Activated Adsorption of CH_4 and N_2 on W(110): The Effects of Kinetic Energy, Angle of Incidence and Surface Temperature on the Dissociative Adsorptive Probability," November 23, 1983.

Powell, C. J., "Status of Quantitative Surface Analysis by Auger-Electron Spectroscopy and X-Ray Photoelectron Spectroscopy," September 5, 1984.

Preston, R., Chemical Process Metrology Division, National Bureau of Standards, Gaithersburg, MD, "Decomposition Reactions on Chemically-Modified Tungsten Single-Crystal Surfaces," March 22, 1984.

Tully, J., Bell Telelphone Laboratories, Murray Hill, NJ, "Dynamics of Vibrational Energy Flow at Surfaces," May 25, 1984.

Umbach, E., Technical University of Munich, Munich, W. Germany, "Recent Developments of High Resolution Auger Spectroscopy from Adsorbates," July 26, 1984.

Wax, M., National Bureau of Standards, Gaithersburg, MD, "Metal Hydride Induced Migratory Insertion in Molybdenum Carbonyl Alkyls," November 17, 1983.

Zhang, C.-S., University of California, Berkeley, CA, "The Interaction of Oxygen with the Mo(100) and Mo(111) Single Crystal Surfaces: Chemisorption and Oxidation at High Temperature," September 10, 1984.

8. TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Cavanagh, R. R.
Surface Science Division Safety Officer
Molecular Spectroscopy Division Seminar Chairman

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.
Treasurer, General Committee of the Physical Electronics Conference
Member, Editorial Advisory Board, "Progress in Surface Science"

Girvin, S. M.
Election Teller, American Physical Society Division of Condensed Matter Physics, December, 1983

Kelley, R. D.
Chairman, Subcommittee D-32.03 on Chemical Analysis of ASTM Committee D-32 on Catalysts

Madey, T. E.
Member, Executive Committee of the Governing Board of the American Institute of Physics, member of AIP Committee on Corporate Associates, and member of committee on AIP-Society relations

U.S. Representative to Surface Science Division of the International Union of Vacuum Science, Techniques and Applications (IUVSTA) and Secretary of Committee

Program Chairman, International Vacuum Congress and International Conference on Solid Surfaces, Baltimore, MD, October, 1986

Member, Organizing Committee, 11th Conference on Atomic Collisions in Solids, Washington, D.C., August, 1985

Member, International Advisory Committee, First International Conference on the Structure of Surfaces, Berkeley, CA, August, 1984.

Member, International Advisory Committee, Sixth European Conference on Surface Science, York (United Kingdom), April, 1984

Member, International Advisory Committee, Second Workshop on Desorption Induced by Electronic Transitions, Garmisch, W. Germany, October, 1984

Chairman, "History of Vacuum" Exhibit Committee, American Vacuum Society National Symposium, November, 1983

Co-Editor, "History of Vacuum Science and Technology", a monograph to commemorate the 30th Anniversary of the American Vacuum Society

Member, ASTM Committee E-42 on Surface Analysis

Member, Editorial Board, "Methods of Surface Characterization"

Member, Editorial Board, Journal of Vacuum Science and Technology

Melmed, A. J.

Secretary, Steering Committee, International Field Emission Symposium

Powell, C. J.

General-Chairman, Physical Electronics Conference

Chairman, ASTM Committee E-42 on Surface Analysis

Cochairman, Surface Chemical Analysis Working Party, Versailles Agreement on Materials and Standards

Member, Board of Trustees, Gordon Research Conferences; Vicechairman of Board

Chairman, American Vacuum Society Surface Science Division

Trustee, American Vacuum Society Scholarships and Awards Committee

Instructor, American Vacuum Society Short Course: "Surface Analysis: Electron and other Emerging Spectroscopies"

Chairman, Local Committee, Meeting of American Physical Society, Baltimore, MD, March, 1985

Member, Editorial Board, "Applications of Surface Science"

Member, Editorial Board, "Surface and Interface Analysis"

Member, Editorial Board, "Methods of Surface Characterization"

Stockbauer, R.

Assistant Program Chairman, International Vacuum Congress and International Conference on Solid Surface, Baltimore, MD, October, 1986.

9. PROFESSIONAL INTERACTIONS, CONSULTING AND ADVISORY SERVICES

Cavanagh, R. R.

Collaborating with Dr. D. S. King of the NBS Molecular Spectroscopy Division on state-specific diagnostics of molecular desorption processes

Collaborating with Dr. J. C. Stephenson of the NBS Molecular Spectroscopy Division on real time measurements of vibrational relaxation processes at surfaces

Collaborating (with R. D. Kelley and T. J. Udovic) with Dr. J. J. Rush of the NBS Reactor Radiation Division on neutron inelastic scattering studies of adsorbates on high surface area materials

Collaborating with Dr. J. J. Rush of the NBS Reactor Radiation Division and Dr. G. D. Stucky of E. I du Pont de Nemours on vibration and diffusion properties of hydrogen in zeolite H-rho.

Collaborating (with T. J. Udovic) with Dr. J. J. Rush of the NBS Reactor Radiation Division and Dr. B. J. Tatarchuk of Auburn University on neutron inelastic scattering measurements from adsorbates on dispersed ruthenium catalysts

Egelhoff, W. F.

Collaborating with Dr. R. A. Armstrong of the National Research Council, Ottawa, Canada on a theoretical analysis of the role of electron forward scattering in the angular intensity distributions of Auger-electron spectra and x-ray photoelectron spectra

Erickson, N. E.

Worked on assignment as a Program Manager with the Air Force Office of Scientific Research, October 1983 to February 1984, on three programs: optical thinfilm preparation and characterization, optical signal processing materials preparation, and spacecraft survivability

Fine, J.

Collaborating with Profs. M. L. Roush and T. D. Andreadis of the University of Maryland on computer simulations of ion bombardment and sputtering phenomena in order to obtain angular distributions of ejected atoms

Collaborating with Prof. B. Navinsek of the J. Stefan Institute, Ljubljana, Yugoslavia on the effect of surface topography on measurements of sputtering yields, on depth resolution at interfaces, and on the fabrication and characterization of standard reference materials for surface analysis. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.

Collaborating with Drs. D. G. Simons and M. D. Brown of the Naval Surface Weapons Center, White Oak, MD, on the use of Rutherford backscattering spectroscopy to characterize thin film standard reference materials for surface analysis.

Collaborating with Dr. L. J. Moore of the NBS Inorganic Analytical Research Division and Dr. T. Lucatorto of the NBS Radiation Physics DIvision on the use of laser multiphoton ionization techniques to identify sputtered atoms and to determine their kinetic energies.

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. S. C. Hardy of the NBS Metallurgy Division on the evaluation of methods for producing atomically clean surfaces on liquids.

Collaborating with Dr. P. A. Lindfors of the Physical Electronics Division of Perkin-Elmer Corp. on the interface depth resolution of sputter-profiled Ni/Cr interfaces.

Collaborating with Dr. R. F. Fleming of the NBS Inorganic Analytical Research Division on thin-film thickness measurements of standard reference materials for surface analysis.

Gadzuk, J. W.

Collaborating with Prof. M. Sunjic of the Rudor 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 theoretical and experimental physicists (Drs. S. Andersson, B. Kasemo, B. Lundqvist) at Chalmers University of Technology, Gothenburg, Sweden and with J. Norskov at NORDITA (Nordic Institute of Theoretical Atomic Physics), Copenhagen, Denmark, on theories of dynamical processes near free and electrochemical surfaces.

Collaborating with Prof. U. Landman of the Georgia Institute of Technology on theoretical modeling of rotational excitation in molecular processes a surfaces, electron- and photon-stimulated desorption, and on stochastic processes related to surface diffusion.

Collaborating with Dr. L. J. Moore of the NBS Inorganic Analytical Research Division and Dr. T. B. Lucatorto of the NBS Radiation Physics Division on laser detection and analysis of thermally desorbed atoms from surfaces.

Collaborating with Dr. S. Holloway, University of Liverpool, England on classical trajectory theories of molecular processes at surfaces.

Collaborating with Dr. E. Hood, California Institute of Technology, on a theory of polarized metastable helium de-excitation spectroscopy at surfaces of magnetic materials.

Collaborated with Dr. A. Luntz, IBM Research Laboratory, San Jose, CA, on a study of vibrational lineshapes of adsorbed molecules.

Invited lecturer and participant at the Third Electrochemistry Study Group, Fritz-Haber Institute, Berlin, July 9-20, 1984.

Girvin, S. M.

Collaborating with Drs. M. E. Cage, R. F. Dziuba and B. F. Field of the NBS Electricity Division on aspects of the quantum Hall effect.

Collaborating with Dr. M. Jonson of Chalmers University of Technology, Gothenburg, Sweden on the theory of transport in inversion layers.

Collaborating with Dr. G. B. Arnold of the University of Notre Dame on studies of scattering of electrons and photons at disordered interfaces.

Collaborating with Dr. D. R. Penn of the NBS Radiation Physics Division on studies of spin-polarized secondary-electron cascades in ferromagnets.

Collaborating with Dr. J. MacFadden of the NBS Mathematical Analysis Division and Prof. P. J. Stiles of Brown University on the modeling of inversion-layer capacitance experiments.

Collaborating with Prof. M. W. Cole of the Pennsylvania State University on studies of atom-metal surface interactions.

Invited participant, Workshop on the Quantum Hall Effect, Aspen Institute of Physics, July 2-15, 1984.

Jach, T. J.

Collaborating with Dr. P. Cowan of the NBS Quantum Metrology Group and with Dr. L. B. Holdeman of COMSAT on glancing incidence x-ray excitation of surface atoms to measure surface core-level binding-energy shifts.

Collaborating with Drs. P. Cowan and S. Brennan of the NBS Quantum Metrology Group on the development of a beamline at the National Synchrotron Light Source, Brookhaven and on experiments to study electronic effects associated with core-level ionization in atoms, molecules, and solids. This effort also includes collaboration with Drs. R. Williams and J. Rife of the Naval Research Laboratory on methods to extract focussed soft x-rays from the synchrotron light source.

Collaborating with Drs. P. Cowan and S. Brennan of the NBS Quantum Metrology Group and with Drs. G. Materlik and M. Bedzik of the German Electron Synchrotron Laboratory DESY, Hamburg on surface and interface x-ray diffraction experiments at DESY using glancing incidence.

Consulting with Dr. L. B. Holdeman of COMSAT on efforts to determine sources of contamination on clean and photoresist-covered silicon surfaces for semiconductor process lines.

Collaborating with Drs. G. Hembree and T. Vorburger of the NBS Mechanical Production Metrology Division on determinations of the relationships between surface roughness measured by stylus and reflected light techniques, scanning electron microscope observations, and x-ray reflectance measurements.

Collaborating with Dr. J. Pena of the Center for Research and Advanced Studies, National Polytechnic Institute of Mexico to study the surface constituents of gallium arsenide thin films produced as amorphous photovoltaic devices.

Kelley, R. D.

Collaborating (with R. R. Cavanagh and T. J. Udovic) with Dr. J. J. Rush of the NBS Reactor Radiation Division on neutron inelastic scattering measurements of adsorbates on optically opaque high-surface-area metal and metal-oxide catalysts.

Kurtz, R. L.

Collaborated (with T. E. Madey and R. Stockbauer) with Mr. N. Usuki of Sumitomo Metals, Amagasaki, Japan on measurements of electron attenuation lengths in condensed molecular layers using synchrotron radiation.

Collaborating with Prof. V. E. Henrich of Yale University on studies of the chemisorption of molecules of catalytic interest on $Fe_2O_3(001)$.

Collaborating (with T. E. Madey, D. E. Ramaker, and R. Stockbauer) with Dr. E. Bertel of the University of Innsbruck, Austria on studies of the mechanisms involved in the production and desorption of ions from solid surfaces.

Madey, T. E.

Collaborating with Drs. I. Terzic, J. Vukanic and Z. Miskovic of the Boris Kidric 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.

Collaborating (with R. Stockbauer) with Drs. R. Williams, J. Rife, and W. R. Hunter of the Naval Research Laboratory on the design and instrumentation for an ultrahigh vacuum beamline at the Brookhaven National Synchrotron Light Source, to study chemisorbed molecules on clean metal surfaces with photoemission spectroscopy and photon-stimulated desorption.

Collaborated (with R. L. Kurtz and R. Stockbauer) with Mr. N. Usuki of Sumitomo Metals, Amagasaki, Japan on measurements of electron attenuation lengths in condensed molecular solids.

Collaborating with Dr. J. L. de Segovia, Institute for Materials Research of the National Research Council of Spain, Madrid, under the auspices of the joint U.S.-Spanish Cooperative Program. The joint effort is in the area of adsorption and electron-stimulated desorption of small molecules on surfaces.

Invited lecturer and participant at the Third Electrochemistry Study Group, Fritz-Haber Institute, Berlin, July 9-20, 1984.

Collaborating with Drs. J. Sass and K. Bange of the Fritz-Haber Institute, Berlin, on fundamental studies of electrochemical phenomena with emphasis on the interaction between water and surfaces.

Collaborating with Dr. N. Tolk of Bell Communications Research on studies of electron stimulated desorption of excited alkali neutral atoms from surfaces.

Collaborating 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.

Collaborating (with R. Kurtz, D. E. Ramaker, and R. Stockbauer) with Dr. E. Bertel of the University of Innsbruck, Austria on studies of the mechanisms for the stimulated desorption of ions from surfaces.

Melmed, A. J.

Collaborating as a co-principal investigator with Prof. W. R. Graham of the University of Pennsylvania on studies of atomic reconstruction of metal and semiconductor surfaces.

Collaborating with Dr. C. Hayek of the University of Innsbruck, Austria on a morphological characterization of catalytically active platinum particles on silicon substrates.

Worked at the Fritz-Haber Institute, Berlin in the laboratories of Prof. J. H. Block from November, 1983 to August 1984. During this assignment, several collaborations were initiated: with Dr. W. Drachsel on studies with synchrotron radiation of photo-field ionization of gases; with Dr. Drachsel on a comparative study of photo-illumination and onset potential in field ionization from silicon with and without metallic overlayers; with Drs. M. Grunze and G. Strasser on measurements of weakly bound adsorption states of nitrogen on (111) iron using low-energy electron diffraction, Auger-electron spectroscopy, and thrmal desorption spectroscopy; and with Drs. W. A. Schmidt, O. Frank, and J. H. Block on sudies with field-ion mass spectrosocpy of silicon, gold, and sulfur adsorption on silver.

Powell, C. J.

Invited lecturer and consultant at the Shanghai Institute of Testing Technology, Shanghai, May 22-June 8, 1984, under the sponsorship of the United Nations Industrial Development Organization.

Member of Solid State Physics Review Panel for Office of Naval Research

Shinn, N. D.

Collaborating with Drs. B. Roop, S. Joyce and J. I. Steinfeld of the Massachusetts Institute of Technology on the temperature-programmed desorption of fluorosilyl species from fluorinated silicon surfaces.

Stockbauer, R.

Collaborating with Dr. A. Flodström of Lund University, Dr. R. Nyholm of the University of Uppsala, and Drs. J. Schmidt-May, C. Kunz and F. Senf of the University of Hamburg on resonant photoemission and photon stimulated ion desorption from metal oxides using synchrotron radiation from the DESY storage ring in Hamburg, W. Germany.

Collaborating with Drs. A. C. Parr, D. L. Ederer and S. Southworth of the NBS Radiation Physics Division, Dr. J. L. Dehmer of the Argonne National Laboratory, Dr. K. Codling of Reading University, U.K., and Drs. J. B. West and D. Holland of the Daresbury Synchrotron Radiation Laboratory, U.K. on studies of gas-phase molecules using triply differential photo-electron spectroscopy with synchrotron radiation from the NBS SURF-II facility.

Collaborating with Drs. A. C. Parr and J. Butler of the NBS Radiation Physics Division and Dr. S. Lias of the NBS Chemical Kinetics Division on measurements of the fragmentation of molecules using photoelectron-photoion coincidence techniques.

Collaborating (with T. E. Madey) with Drs. R. Williams, J. Rife and W. R. Hunter of the Naval Research Laboratory on the design and instrumentation of an ultrahigh vacuum beamline at the Brookhaven National Synchrotron Light Source, and on the study chemisorbed molecules on clean metal surfaces with photoemission spectroscopy and photon stimulated desorption.

Collaborating (with R. Kurtz, T. E. Madey, and D. E. Ramaker) with Dr. E. Bertel of the University of Innsbruck, Austria on studies of the mechanisms for the stimulated desorption of ions from surfaces.

Collaborating (with J. Barth) with Dr. D. Ederer of the NBS Radiation Physics Division on the characterization of a new high-flux toroidal grating monochromator recently installed on the NBS SURF synchrotron light source.

Collaborating (with R. L. Kurtz and T. E. Madey) with Mr. N. Usuki of Sumitomo Metals, Amagasaki, Japan on measurements of electron attenuation lengths in condensed molecular solids.

Twigg, M. E.

Collaborating with Dr. E. Aigeltinger of Pratt and Whitney on measurements of the microcomposition of nickel-based superalloys

Udovic, T. J.

Collaborating (with R. R. Cavanagh and R. D. Kelley) with Dr. J. J. Rush of the NBS Reactor Radiation Division on neutron inelastic scattering studies of adsorbed molecules on catalyst materials.

Collaborating (with R. R. Cavanagh) with Dr. J. J. Rush of the NBS Reactor Radiation Division and with Dr. B. J. Tatarchuk of Auburn University on neutron inelastic scattering measurements of the adsorptive behavior of hydrodesulferization catalysts.

10. VISITING SCIENTISTS

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

Bange, K., of the Fritz-Haber Institute, Berlin, W. Germany worked at NBS for three months in the winter of 1984. He and and Dr. Sass from the same institute studied the structure and bonding of water to an Ag(110) surface and the influence of additives (O, Br) on the structure and chemistry of the adsorbed water.

Barth, J., of the University of Hamburg, W. Germany worked at NBS for ten weeks in early 1984 on the installation and testing of a new high-flux toroidal-grating monochromator at the NBS SURF synchrotron radiation facility.

Benndorf, C., of the University of Hamburg, W. Germany, spent two months at NBS in late summer 1984 initiating studies of the structure and chemistry of ammonia on an alkali-promoted Fe(110) surface.

Chambers, G. P., a graduate student at the University of Maryland, has worked at NBS since January 1983 under a cooperative agreement. He has been involved in computer software development for quantitative surface analysis by Auger-electron spectroscopy and in sputter-depth-profile measurements of thin-film standard reference materials using this technique.

Ciszewski, A., of the Institute for Experimental Physics, University of Wroclaw, Wroclaw, Poland was awarded the 1982-83 Welch Foundation Scholarship to work at NBS for one year beginning November, 1982. He investigated the nucleation and growth of several rare-earth metals on tungsten surfaces.

Doering, D., of the University of Florida spent part of June 1984 studying rotational ordering in overlayers of lithium on a Ru(001) surface.

Heise, W., a graduate student at Auburn University, worked at NBS from April 1984 to May 1984 under a cooperative agreement. He participated in neutron inelastic scattering experiments involving the adsorption of hydrogen on ruthenium black.

Holloway, S., of the University of Liverpool, United Kingdom, was a visiting scientist for 6 weeks during the summer of 1984. He worked on theoretical modeling of reactive molecular processes at solid surfaces via detailed trajectory studies that include the role of electronic transitions and non-linear chaotic intra-molecular motion.

Netzer, F. P., of the University of Innsbruck, Austria worked at NBS for two months in the autumn of 1983. He studied the influence of sodium on the local structure of CO on Ru(001) and found evidence that CO "inclines" in the presence of Na.

Sass, J., of the Fritz-Haber Institute, Berlin, W. Germany worked at NBS for one month in the winter of 1984. He and Dr. Bange of the same institute studied the structure and bonding of water on an Ag(110) surfaces and the influence of additives (O, Br) on the structure and chemistry of the adsorbed water.

Usuki, N., of the Sumitomo Metals Company, Japan worked at NBS from October, 1983 to March, 1984 on measurements of electron attenuation lengths in condensed molecular films using synchrotron radiation from the NBS SURF facility.

11. Surface Science Division Staff

As of June 30, 1984 the Surface Science Division was staffed as follows:

C. J. Powell, Chief
S. K. Brereton,° Secretary
M. L. Burns+
R. R. Cavanagh
W. F. Egelhoff, Jr.
N. E. Erickson
J. Fine
J. W. Gadzuk
S. M. Girvin
T. J. Jach**
R. Klein
P. K. Lam*
A. J. Melmed
M. E. Twigg*

Surface Structure and Kinetics Group

T. E. Madey, Group Leader
L. M. Johnson, Secretary
P. M. Connelly#
R. D. Kelley
R. L. Kurtz*
E. O. Neitzel#
A. Pararas++
D. E. Ramaker@
N. D. Shinn*
R. L. Stockbauer
M. J. Wax*

° On detail to Office of Science and Technology Policy
* NBS-NRC Postdoctoral Research Associate
@ Expert, Part-Time
\# Engineering Technician
\+ Student Appointment
++ Contractor
** Half time with Quantum Metrology Group

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C.J. Powell

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10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)*

This report summarizes technical activities of the NBS Surface Science Division during Fiscal Year 1984. 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)*

Surface chemistry; surface physics; surface science; surface standards

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