

NBSIR 80-2166

Technical Activities 1980
Surface Science Division
Reprinted from NBSIR 80-2132

C. J. Powell, Chief

Surface Science Division
Center for Thermodynamics and Molecular Science
National Measurement Laboratory
National Bureau of Standards
U.S. Department of Commerce
Washington, DC 20234

October 1980

Prepared for:
National Bureau of Standards
Department of Commerce
Washington, DC 20234

NBSIR 80-2166

**TECHNICAL ACTIVITIES 1980
SURFACE SCIENCE DIVISION
REPRINTED FROM NBSIR 80-2132**

C. J. Powell, Chief

Surface Science Division
Center for Thermodynamics and Molecular Science
National Measurement Laboratory
National Bureau of Standards
U.S. Department of Commerce
Washington, DC 20234

October 1980

Prepared for:
National Bureau of Standards
Department of Commerce
Washington, DC 20234



U.S. DEPARTMENT OF COMMERCE, Philip M. Klutznick, *Secretary*

Luther H. Hodges, Jr., *Deputy Secretary*

Jordan J. Baruch, *Assistant Secretary for Productivity, Technology, and Innovation*

NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

ABSTRACT

This report summarizes technical activities of the NBS Surface Science Division during Fiscal Year 1980. These activities include experimental and theoretical research in surface science, the development of improved measurement methods, the provision of needed data, the development of reference materials, applications to important scientific and national problems, and surface-standards work. 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, 1979 to September 30, 1980. The report was prepared as part of the Annual Report of the Center for Thermodynamics and Molecular Science within the National Measurement Laboratory of NBS. Much of the writing was done in June and July of 1980 so not all of the actual accomplishments for the year have been included.

The technical work of the Division is separated formally into a "Surface Measurements Program" and a "Surface Science Competence Program." The basis for this separation is described briefly in the Introduction (Section 1) and in the reports for these two programs (Sections 2 and 3). Within each program are a number of technical projects. Information is given on project objectives, results obtained during the past year, and the nature of planned activities.

Sections 4 and 5 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 6. The involvement of Division staff on professional committees is shown in Section 7 while internal and external scientific collaborations are described in Section 8. Visiting scientists who have worked in the Division during the year are identified in Section 9 and the Division staff is listed in Section 10.

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, Washington, D.C. 20234.

TABLE OF CONTENTS

ABSTRACT	i
FOREWORD	ii
1. Introduction	1
2. Surface Measurements Program	5
2.1 Introduction	5
2.2 Characterization of Surface Reactions and Processes	5
2.2a Catalytic Chemistry for Synthetic Fuels	5
2.2b Infrared Studies of Chemisorbed Species	6
2.2c Field-ion Microscopy Studies of Stress-Corrosion Cracking	7
2.3 Physical Characterization of Surfaces	9
2.3a Electron-Stimulated Desorption	9
2.3b Electron Spectroscopy of Surfaces	9
2.3c Ion-Induced Electron Spectroscopy of Surfaces	11
2.3d Liquid-Metal Surfaces	11
2.3e Microcompositional Analysis of Semiconductor Surfaces	12
2.3f Investigation of Surface Atomic Structure	12
2.4 Theoretical Descriptions of Surface Processes	13
2.4a Surface Theory	13
2.5 Surface Standards	14
2.5a Measurement of Absolute Ion Sputtering Yields	15
2.5b Development of Prototype Standard Reference Materials	15
2.5c Standards Committee Activities	16
2.5d Review Articles and Books	18

3.	Surface Science Competence Program	19
3.1	Introduction	19
3.2	Report of Technical Activities	20
3.2a	ESDIAD-EELS Studies of the Molecular Structure of Adsorbed Species	20
3.2b	Laser Fluorescence as a Probe of Surface Dynamics . .	21
3.2c	Neutron Inelastic Scattering from Adsorbed Species on Surfaces	22
3.2d	Angle-Resolved Photon-Stimulated Desorption - A New Tool for Surface Characterization	22
3.2e	Photoemission Studies of Materials	23
3.2f	Atom-Probe Field-Ion Microscopy of Materials	25
3.2g	Surface Theory	26
4.	Publications	28
5.	Talks	35
6.	Seminars	45
7.	Technical and Professional Committee Participation and Leadership	49
8.	Professional Interactions, Consulting and Advisory Services	51
9.	Visiting Scientists	55
10.	Surface Science Division Staff	57

SURFACE SCIENCE DIVISION

C.J. Powell, Chief

SUMMARY OF ACTIVITIES

Fiscal Year 1980

1. INTRODUCTION

(a) Background

Surface science is a rapidly growing, exciting field offering many scientific and technological challenges. The growth is evident in the large number of national and local meetings of major professional societies (e.g., American Physical Society, American Chemical Society, American Vacuum Society), of many other groups (e.g., Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Conference on Metallurgical Coatings, Materials Research Society, Applied Surface Analysis Symposium, Physical Electronics Conference, Conference on Plasma-Surface Interactions), of over a dozen Gordon Research Conferences in 1980 concerned with surface phenomena, and in both journal and book publications. The excitement in the field is evident from the enthusiasm of the practitioners, the numerous articles reporting new phenomena in many different journals (particularly, for example, in Physical Review Letters, Chemical Physics Letters), and in the widespread realization that the availability of new experimental and theoretical tools offers opportunities to probe, at a fundamental atomic and molecular level, the physics and chemistry of complex surface processes. It is also clear that surface characterization is now an integral part of many technologies and industries (e.g., catalysis, coatings, corrosion, semiconductors, semiconductor devices, computer, automobile, communications) for many different applications (e.g., failure analysis, quality control, process and device development). Characterization of surface properties and processes is similarly important in many areas of national concern (e.g., defense, energy, environment, space).

The nature of the required surface characterization in the above areas varies tremendously. For the more fundamental investigations, it is often necessary to determine the surface composition, surface atomic structure, and the surface electronic structure of carefully prepared surfaces (e.g., single-crystal samples, single-crystal samples with steps, small clusters or particles, surfaces with various amounts of adsorbed gases or deposited atoms or molecules) and to evaluate the physical and chemical properties in terms of current theories and other knowledge. For the more applied investigations, it is often necessary to determine the surface composition and surface morphology of an extremely wide range of samples (e.g., catalysts, polymers, semiconductor devices, metals, alloys, compounds, coatings, thin-

film devices, laser windows, display devices, solar devices, memory devices, contacts, biomaterials, adhesives, seals, wear surfaces, composites, energy-storage devices, Tokamak-wall parts, building materials, flyash, automobile parts) and to relate the measured surface properties to other characteristics of the sample. In many instances, other surface properties need to be measured for both fundamental and applied work (e.g., roughness, surface defects, and the mechanisms and kinetics for morphological and chemical transitions).

Although there have been many successes in surface science and surface technology, many measurement-related problems and limitations remain. Among these problems and limitations are: many of the widely used instruments for the measurement of surface composition are not sufficiently accurate; most analyses of surfaces are qualitative, not quantitative; there are virtually no standard procedures, reference data, or reference materials to ensure reliable surface measurements by the commonly used techniques; there is inadequate knowledge of the "measurement process" for many methods of surface characterization; the rates of irreversible damage to a surface during surface characterization are not well established; structural information can be obtained with some difficulty for ordered surfaces but methods to obtain short-range atomic structures are not established; little kinetic data exists for important surface processes under well-controlled conditions; and most surface-characterization measurements have to be performed in a low-pressure (usually ultrahigh-vacuum) environment rather than in situ.

(b) Goal and Objectives

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 a task titled "Develop Measurement Methods for Surface Properties." Work performed during the year for this task is reported in Section 2. Objective (4) is being met as a result of the recently established NBS Competence Program through a task titled "Surface Science." A separate report on these activities is given in Section 3.

(c) Technical Output and Professional Interactions

Sections 4 and 5 of this report contain listings of the publications and talks, respectively, for the past year by Surface Science Division staff. Although these listings were prepared before the end of the fiscal year, the quantity of the technical output is high both in absolute terms and in comparison with the previous year.

An innovation this year has been the establishment of a joint mailing list by the Surface Science Division and the NBS Electron Physics Group. In both December 1979 and June 1980, a listing of recent publications and of publications in progress was sent to over 800 individuals whose names and addresses were compiled in an ad hoc way largely from attendance lists at recent meetings. The response has been extremely gratifying. Over 50% of those receiving the mailing sent back a postcard requesting copies of designated publications; other scientists have asked for their names to be placed on our mailing list while others have indicated that they appreciate receiving listings of the recent work (and make use of the information in their own libraries). Some 400 responses were received to the first mailing; there were 100 to 150 requests for copies of each of six review articles while there were typically 30 to 70 requests for each of most of the remaining publications. The mailing list has proven to be an effective means of disseminating the recently published work of the Division to those who can use it and also provide a means of documenting the fact that a substantial "clientele" exists for the services now being provided by the Division. The mailing list is also an effective means of publicizing NBS work in surface science. It is planned to continue these mailings at a frequency of approximately two per year.

Many members of the Division staff hold leadership positions in professional societies and groups, as listed in Section 7. 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.

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 8. 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 nine visiting scientists work at NBS for varying periods during the past year, as indicated in Section 9. 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. In the annual competition for 1980, the Surface Science Division received 11 applications for Postdoctoral awards out of about 75 for the entire NBS; two awards to this Division were made.

Interest in surface science and surface characterization at NBS continues to grow. The Division has had an active Seminar program, as indicated in Section 6, and these seminars have been attended by other NBS staff. A third one-day course on surface analysis was presented at NBS in February 1980; this course was attended by 36 scientists from 16 different NBS organizational units. Since this course was first offered in 1978, over 100 NBS scientists have taken the course or expressed interest in it. Members of the Division staff are consulted on a wide range of NBS problems such as: fracture mechanisms and crack growth in materials; leaching of toxic elements from flyash; material transport at the interfaces of electrical contacts; artifacts in eddy-current standards for non-destructive evaluation of materials; and surface effects on proposed secondary mass standards.

(d) Laboratory Automation

During the past year, a number of the experimental projects in the Division have been interfaced to microcomputer systems and other projects are being similarly automated. It is believed that these changes will lead to more efficient operations, more accurate and reliable experimental data, and to new types of experiments being undertaken that would previously not have been feasible.

2. SURFACE MEASUREMENTS PROGRAM (13 staff years)

2.1 Introduction

The Division's work for the task titled "Development of Measurement Methods for Surface Properties" is divided into a number of individual projects. 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, the development of new concepts, the provision of needed data, and the development of reference materials. The reports of the technical projects have been divided into four groups to provide a clear relationship to different surface-measurement problem areas and to the Division objectives. It should be recognized, however, that many of the projects have outputs extending beyond the particular category in which they have been placed.

2.2 Characterization of Surface Reactions and Processes

(a) Catalytic Chemistry for Synthetic Fuels - The Hydrogenation of CO (Yates, Madey, Kelley, Goodman, Kiskinova)

The overall objective of this research is to provide a molecular understanding of heterogeneous catalytic chemistry in areas of importance to energy-related technologies, particularly the generation of synthetic fuels. Among these areas are the catalytic synthesis of hydrocarbons from carbon oxides and hydrogen on metal surfaces, the mechanism of catalytic poisoning, and the molecular and electronic nature of chemisorbed species.

Results of past year include:

- (1) A comparison of the absolute reaction rate of CH_4 synthesis on Ni(100) and Ni(111) has been completed. Within experimental error, both the rate and activation energy are identical on the two crystal surfaces. Similar conclusions have also been reached in comparison of two Ru crystal surfaces for this reaction. This work suggests that structure factors are unimportant and that for this reaction it is likely that electronic factors within the catalytic substrate govern the kinetic behavior.
- (2) Quantitative studies of S poisoning and alkali metal promotion have been carried out. In both cases it appears that electronic effects govern the behavior of the doped surface, and that major rate changes may be induced in this manner.
- (3) A new method for studying interactional effects on surface binding of CO to Ni(100) has been devised. Desorption of one isotopic species

of CO into a high flux beam of a second isotope of CO has been directly employed to observe the effect of elevated CO coverage on the desorption process.

- (4) A second high pressure chamber, complete with an Auger spectroscopy facility for surface analysis, has been completed.

Future plans include the following:

- (i) Search for catalytic methanation activity among elements outside of group VIII. Among the candidates are: W, Mo, and Sm.
- (ii) Exploratory studies of classes of catalytic poisons and their relative influence on the rate of synthesis of CH₄. Examples are S, N and P.
- (iii) Study of the decomposition of organic molecules by surfaces using isotopic labeling methods, (alcohols, aldehydes), in order to produce a systematic picture of organic functional group stabilities on surfaces.

(b) Infrared Studies of Chemisorbed Species (Yates, Cavanagh, Griffin)

Infrared spectroscopy provides a means for gaining structural information about chemisorbed species. It is important in studies of technical surfaces of catalytic importance and is an important component of an NBS effort to make comparative studies of chemisorption processes and surface reactions on three types of substrates: (i) highly dispersed atoms on a support (by IR spectroscopy); (ii) macroscopic single-crystals (by high-resolution electron energy-loss spectroscopy; and (iii) high-area practical catalyst materials (by neutron inelastic-scattering spectroscopy).

Accomplishments of the past year include:

- (1) Identification of atomically dispersed Rh sites on an Al₂O₃ support. These sites exhibit different chemisorptive properties from Rh sites present in crystalline Rh.
- (2) Development and use of methods for controlling the distribution of the two classes of Rh sites.
- (3) Discovery of an infrared spectroscopic method for observing the electrostatic interaction of a surface dipolar oscillator with its image in the underlying substrate.
- (4) Extension of infrared spectroscopy to the investigation of electronic analogs to CO and establishment of a firm linkage between transition metal chemisorption and organometallic chemistry (isocyanide chemisorption)

- (5) Demonstration of the concept that anchor ligands may be used to orient functional groups to surfaces in a controlled manner.
- (6) Study of through-metal electronic interactions between adsorbed species.
- (7) Direct spectroscopic observation of ligand-induced displacement effects between coadsorbed species.
- (8) Study of the spillover of chemisorbed hydrogen atoms produced on metal sites to the oxide support.
- (9) Correlation of IR and thermal desorption techniques for hydrogen chemisorption on a ZnO surface.

It is planned to continue IR work in the following areas:

- (i) Study of phenylisocyanide chemisorption with the objective of anchoring an ultraviolet-absorbing chromophore for possible use in surface photolytic studies.
- (ii) Exploratory studies of the effect of solvents on the infrared behavior of adsorbed molecules as they are covered. This could lead the way to IR studies of electrode surfaces exposed to the electrolyte.
- (iii) Search for a transient intermediate in the desorption of CO from a Rh surface, i.e., $\text{Rh}(\text{CO})_2 \xrightarrow{-\text{CO}(\text{g})} [\text{Rh}(\text{CO})] \xrightarrow{-\text{CO}(\text{g})} \text{Rh}$.
- (c) Field-Ion Microscopy Studies of Stress-Corrosion Cracking (Melmed, Carroll)

The objective of these studies is to examine on an atomic scale the early stages of stress-corrosion cracking, a phenomenon leading to premature failure of metals under apparently innocuous conditions. Surface chemistry as well as defect properties are important factors to be understood in the interplay between stress-assisted cracking and crack promoting agents, such as hydrogen.

The work carried out in the past year sought to extend the application of field ion microscopy (FIM) to new alloy systems and pure metals with the aim of examining the occurrence of hydrogen/stress-induced metal defects.

Results of the past year include:

- (1) Work with three titanium-palladium alloys resulted in an evaluation of their susceptibility to stress-corrosion cracking. The FIM results indicated that the susceptibility to stress-corrosion cracking in titanium was not reduced by the addition of palladium.

- (2) Work with vanadium resulted in the observation of an unexpected effect due to the interaction with hydrogen under stress. Field ion micrographs indicate that the material's normally-imaged impurities were removed in the top-most 10-15 layers by exposing specimens to hydrogen imaging conditions at temperatures less than 30 K. The technique may be adaptable to larger, single crystal vanadium samples where the attainment of clean vanadium surfaces in the past proved to be a formidable achievement.
- (3) Work was started with a high purity aluminum-5.5% zinc-2.5% magnesium alloy to study the initial stages of its hydrogen embrittlement behavior. Previous SEM studies have shown that the aluminum matrix contains aggregated constituent phases with a wide distribution of sizes. Field ion micrographs indicate that this distribution contains clusters as small as a few atoms. In addition, and perhaps more importantly, micrographs indicate that the aluminum matrix has a high distribution of a defect structure (tentatively identified as partial dislocation pairs) that sometimes are as little as five layers deep.
- (4) The first clear field ion micrographs of alpha-uranium were obtained that show atomic details of many orthorhombic crystal planes. Micrographs indicate that a surface hydride phase is formed readily under hydrogen imaging conditions; some micrographs indicate possible hydride particle precipitation at a major crystal defect boundary. No evidence was found, however, of hydrogen/stress-induced surface cracks.

Future studies will be directed toward obtaining FIM characterizations of:

- (i) the Al-Zn-Mg alloy charged with hydrogen sufficient to promote hydrogen embrittlement to determine whether there is a positive or negative correlation between the observed dislocation pairs and the initial stages of crack formation.
- (ii) a wide range of electroless nickel-phosphorous alloys and their interaction with hydrogen and stress.

Future atom-probe FIM investigation should provide chemical identification of corrosion products at surface crack sites in zirconium and titanium, and in Ti-Pd and Al-Zn-Mg alloys.

2.3 Physical Characterization of Surfaces

(a) Electron-Stimulated Desorption (Madey, Houston)

A key problem 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.

During the last year, progress has been made in the following areas:

- (1) We have completed a detailed study of the influence of surface structure on molecular bonding geometry, by examining the adsorption of CO on both planar surfaces and on surfaces containing monatomic steps. The data demonstrate that there are profound differences in molecular bonding at step sites compared to adsorption on flat surfaces.
- (2) We have probed the mechanisms of electron-stimulated desorption (ESD) by studying the enhancement of ion desorption yields at energies above deep-core excitation thresholds in surface molecules.
- (3) We have initiated a study of NH₃ adsorption on Ni(111) to compare ESDIAD-determined structures with the structure determined using angle-resolved ultraviolet photoemission spectroscopy. The results indicate that there are differences in the methods which require detailed investigation.

Future plans include:

- (i) Study orientational order-disorder processes.
- (ii) Probe the mechanism of ESD by assessing the effect of deep core ionization on ion desorption from adsorbed molecules.
- (iii) Measure yields and angular distributions of negative ions.
- (iv) Examine the relationship between surface bond angle and ion desorption angle with adsorbed molecules of "known" structure.

(b) Electron Spectroscopy of Surfaces (Powell, Jach)

The objective of this project is to apply and extend techniques of electron spectroscopy for the determination of surface composition, other surface properties, and the dynamics of electron-surface interactions.

Activities of the past year include:

- (1) The L_3VV Auger-electron spectra of Ni and Cu have been measured as a function of incident-electron energy near the threshold for ionization of electrons in the L_2 -subshell. At the lower incident energies, the observed spectra are shown to be substantially free of perturbing satellites. The L_3VV spectrum of Ni consists of two features, one due to atomic final states and the other due to band effects. Shifts in the position of the L_3VV Auger features as a function of incident energy imply a systematic difference in core-electron binding energies measured under adiabatic and sudden conditions. One cannot therefore directly use "absolute" binding energies determined by appearance-potential spectroscopy for calibration of x-ray photoelectron spectroscopy instruments.
- (2) Measurements have been made of the electron energy-loss spectra associated with excitation of the 2p and 3p core levels of Ni and Cu. Although Ni and Cu have very different band structures, the Ni and Cu 3p loss spectra are very similar in shape, the Ni and Cu 2p loss spectra show similarities near the threshold for excitation, while there is a considerable difference in the 3p and 2p loss spectra for each metal. In addition, weak features in the 3p loss spectra of Ni and Cu change as a function of incident electron energy in the range 150 to 1000 eV.
- (3) Thirteen types of intraocular lenses manufactured for human implantation were examined by x-ray photoelectron spectroscopy (XPS) in a search for possible surface contaminants that could be harmful. Apart from signals due to carbon and oxygen, the only other elements detected were chlorine on one sample and nitrogen on another.
- (4) Extensive XPS measurements have been made of a series of pollutant particles both after insertion into the instrument and after varying periods of ion bombardment to remove layers of sample material. Many elements have been detected and it has been found that the relative concentrations of most elements vary as a function of depth from the original surface. Comparisons of XPS data with average bulk compositions show that some elements (e.g., Sb, As, V, P, and Cl) can be located close to the virgin surface.
- (5) In collaboration with scientists in the NBS Polymer Science and Standards Division, Auger-electron spectroscopy studies have been made of dental alloys to understand wear mechanisms and of polymer films to optimize procedures for uniform film deposition and to develop protective polymer coatings.

Future work includes:

- (i) Further studies of core-level electron energy-loss spectra (e.g., Co, Zn, Ag, Au) to identify excitation mechanisms.
 - (ii) Studies of surface phase changes on stepped crystals of magnetic materials near the Curie temperature.
 - (iii) Use of secondary-ion mass spectroscopy to identify trace elements in pollutant particles and to detect ionic fragments from different individual particles excited by an incident electron beam.
- (c) Ion-induced Electron Spectroscopy of Surfaces (Fine, Andreadis)

The collision of energetic ions (1 keV) with solid surfaces gives rise to a number of interactions within the solid which result in the ejection of atoms, ions, photons, and electrons. Ejected atoms and ions have been used extensively to monitor sputtering and secondary-ion emission processes but there has been very little work to correlate the ejected electrons with these collision processes. Although the kinetic ejection of electrons by ions and the ejection of Auger electrons are recognized effects, little is known about the interactions which generate them.

Measurements have been recently made of the total secondary-electron yield and the secondary-electron energy distribution in the 0-200 eV range for Ga, Ge, In, and Sn samples bombarded by 0.5-5 keV argon ions. These energy distributions show the onset of a collisional process which is capable of producing secondary electrons of rather high energy (greater than 100 eV); these electrons are not Auger electrons. It seems likely that these electrons are the result of an ion (atom)-atom collision in the target rather than one between an ion (atom) and the target conduction atoms.

Future work will include:

- (i) Secondary-electron energy-distribution measurements of additional elements excited by different ions to identify various atomic excitation mechanisms.
 - (ii) Similar measurements with higher ion energies (up to 20 keV) and with ions of metallic elements.
- (d) Liquid-Metal Surfaces (Fine, Andreadis)

A collaborative project is underway with the NBS Metallurgy Division to examine surface properties of liquid metals and, in particular, to correlate measurements of surface tension with amounts of surface impurities.

A new way has been found in initial test measurements to generate a clean liquid gallium surface. It has been found that a small-diameter (1 mm) argon-ion beam can effectively remove impurity precipitates from a large surface area (about 50 mm²). Impurity particles can be seen to flow into the ion-impact region from distances of many millimeters. This cleaning method may be a useful means for cleaning other liquid surfaces.

An uhv instrument dedicated to surface-tension measurements and with the capability for Auger-electron spectroscopy is being assembled. Surface-tension measurements of elemental liquid metals and of liquid-metal alloys will be correlated with processes such as surface segregation and the growth of solid oxide overlayers.

(e) Microcompositional Analysis of Semiconductor Surfaces (Melmed)

An outstanding problem in semiconductor characterization is the measurement of impurity concentrations at low levels (e.g., 1 ppm of carbon). It is believed that the time-of-flight atom-probe field ion microscope (APFIM) could be utilized to determine impurity or dopant concentrations at these low levels.

In a collaboration with scientists at the Pennsylvania State University, the practical upper limit of resistivity for semiconductor analysis has been extended from about 10 ohm cm with commonly used APFIM instruments to about 2×10^4 ohm cm. This development allows the full analytical capability of the APFIM to be applied to a wide range of semiconductor materials.

(f) Investigations of Surface Atomic Structure (Melmed)

The atomic structure of a surface is an important parameter for understanding surface properties. For many materials, the surface atomic structures have been shown not to be simple continuations of the bulk atomic structure; in such cases, the surface is said to be reconstructed.

In collaboration with scientists at the University of Pennsylvania, it has been found:

- (1) Similar to previous work on the W[001] surface, it has been found with field-ion microscopy (FIM) that the Mo [001] surface is reconstructed over a wide temperature range (15-500 K). This result is consistent with recent low-energy electron diffraction (LEED) measurements except that no evidence has been found for a structural phase transition in this temperature range.
- (2) In contrast to the results for W and Mo, FIM observations of a Nb [001] surface show no evidence of reconstruction (again over a wide temperature range). LEED measurements with a Nb[001] sample are in progress for comparison with the FIM results.

It is planned to examine other metals and semiconductors and other crystal planes to determine the systematics of reconstruction phenomena.

2.4 Theoretical Descriptions of Surface Processes

(a) Surface Theory (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 microscopic atomic-scale properties of individual entities as well as from larger-scale statistical properties of ensembles. Based upon our studies, phenomenological or 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 lineshapes, satellite structures, etc. provide additional information on system dynamics are of considerable interest.

Recent accomplishments include:

- (1) A significant goal of surface science is to provide insights needed to control reaction rates in a desired way. We have initiated a large scale theoretical study into the modelling of reaction dynamics at metallic surfaces which include, in a very fundamental and necessary way, intrinsic non-adiabatic effects due to the electronic excitations of the substrate. Model studies in which analogies are drawn with deep level spectroscopies of solids have demonstrated the important role of substrate-excited states in determining reaction rates. In addition to model studies, a formal reaction theory has been constructed from which well-defined specific simplifications can be made.
- (2) Semi-classical scattering theory, based upon some trajectory approximations has been an extremely useful tool for describing gas-phase molecular-collision events involving non-adiabatic electronic behavior. We have developed theoretical techniques for applying such theory to problems associated with the coupled electron-nuclear motion behavior of atomic or molecular scattering from surfaces. We have constructed a trajectory-like theory for such encounters in which the quantized nature of the "classical trajectory" can be treated within a "Franck-Condon-like" picture. Applications of this theory to the problem of atom sticking to surfaces has been carried out. Ways in which state-of-the-art infrared and electron energy-loss vibrational spectroscopy can provide necessary input into such a description of surface collisions has been detailed.

- (3) An extremely transparent theory for a generic class of time-dependent quantum-mechanical problems has been developed which should enable experimentalists to do certain theoretical analyses without theorists. The class of problems involves an initial excitation and the subsequent decay of a portion of a quantum system. While in the excited state, the coupling of the subsystem to the remainder of the system is altered and, depending upon the excitation lifetime of the intermediate state, this altered coupling can significantly affect experimental observables. The single theory has been applied to gas-phase resonance Raman spectroscopy, shape resonances in molecular photoionization, XPS-Auger coincidence electron energy distributions, resonance photoionization lineshapes, stimulated desorption, and atom sticking probabilities. By drawing attention to the common link in this diverse collection of physical phenomena, workers in one field should be better able to avail themselves of relevant information provided by research output in the other fields.

Work planned for the future includes:

- (i) Continuation of work in the significant new area of reaction dynamics with near term emphasis on the interrelationship between substrate electronic excitations and surface vibrational structure. Incorporation of vibrational data into trajectory-based semi-classical scattering theory and path-integral formulations of surface-rate processes is anticipated.
- (ii) Model field theories with prescribed dynamical coupling constants will be explored. Work in progress includes a theory for substrate electron-hole pair renormalization of adsorbed intra-molecular vibrationally excited states in which level shifts and widths will be deduced and models capable of treating stimulated desorption over the entire dynamic range, adiabatic to sudden, in the excitation process will be developed.
- (iii) Analysis will be made, whenever possible, of novel experimental results. Current work includes a study of the vibrational structure and lineshape in photoionization spectra of shape resonances in diatomic molecules.

2.5 Surface Standards

The term "surface standards" is intended to cover a broad range of activities that are directed to improving the quality of surface-characterization measurements.

(a) Measurement of Absolute Ion Sputtering Yields (Fine, Andreadis)

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-analysis 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.

A dynamic method of making sputtering-yield measurements has been developed that will allow in situ measurements of sputtering yield as a function of ion dose. As a result of some difficulties encountered with previous quartz-oscillator microbalance measurements of sputter yields, new oscillator design parameters have been chosen to assume greater stability and a new set of quartz crystals has been fabricated. These crystals were specially polished to produce the ultrasmooth surfaces (with an rms surface roughness 1 nm) needed to eliminate initial surface-topography effects on the yield. It is planned to calibrate the crystals by means of neutron activation analysis. With the particular quartz-crystal oscillator head that has been designed, it is possible to monitor concurrently mass change as well as total ion dose. Both of these measurements are made with frequency counters which have recently been interfaced to a small computer that has been programmed to output yield and total-dose data continuously. This data will be correlated with Auger-electron spectra and x-ray yield data as thin-film samples are sputtered.

It is planned to measure absolute sputter yields of gold, silver, nickel, and chromium bombarded by 0.5-5 keV argon ions in the near future.

(b) Development of Prototype Standard Reference Materials (Fine, Andreadis)

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

We are presently preparing two prototype sets of reference materials. One of these reference materials will be a thin film (~ 70 nm) Ta_2O_5 sputter deposited onto a polished silicon crystal; the outer surface will be protected by a very thin layer (~ 10 nm) of sputter deposited amorphous silicon. The other reference material will be a multi-layered metal thin film structure (A B A B ... sandwich) also to be sputter deposited onto a silicon substrate. The metals selected, Ni and Cr, have reported sputtering yields which are very similar and thus there should be minimal effects of preferential sputtering. The choice of these reference materials

was decided upon as a result of inputs from ASTM Committee E-42 on Surface Analysis and the Surface Analysis Reference Committee in Europe (SARCE).

The fabrication of these specimens will be a part of a new collaborative research project under a new joint U.S./Yugoslavia program between J. Fine at NBS and B. Navinsek at the J. Stefan Institute in Ljubljana. The laboratory in Yugoslavia has a sputter-deposition apparatus capable of producing very uniform thin films under good vacuum conditions and we plan to fabricate our reference materials in this apparatus. The materials will be characterized and calibrated at NBS by means of Auger depth-profile analysis, the quartz oscillator weight-loss method, and x-ray fluorescence. Other groups may participate in the calibrations.

We expect that in the development of such Standard Reference Materials that the measured depth profiles should correlate with the "true" layer structures. However, the effect of ion bombardment on the depth resolution at interfaces is not now completely understood. One approach to learning more about this depth resolution effect is through computer modelling of the sputtering process. As part of a Cooperative Program with the University of Maryland, the sputtering of multiple layered materials is being modelled using a Monte-Carlo code. These results should allow a more complete analysis to be made of our depth profile measurements.

(c) Standards-Committee Activities (Powell, Fine, Kelley)

Three staff members hold offices on ASTM Committees E-42 on Surface Analysis and D-32 on Catalysts. Participation in the activities of these committees not only provides an efficient means to disseminate our expertise to those who need it and to exert a leadership role in important areas but provides us with current information on significant measurement problems facing those who are using surface-analysis equipment (E-42) or who are characterizing catalyst properties (D-32).

Recent activities have included:

- (1) The development of Standard Practices. Draft documents concerning Auger terminology, specimen handling, qualitative elemental identification in Auger-electron spectroscopy, energy calibration in x-ray photoelectron spectrometers, and specifying the performance of electrostatic electron spectrometers will be balloted in August, 1980. Other documents concerning electron-beam damage effects, identification of chemical states by Auger-electron spectroscopy, measurement of performance of electron spectrometers, ESCA terminology and quantification in Auger spectroscopy and ESCA are being discussed.
- (2) Surveys to determine desirable characteristics of prototype standard reference materials. Information has been collected recently concerning reference materials for the calibration of depth scales in depth-

profile measurements with surface-analysis instrumentation. One class of useful reference materials has been identified: electrochemically analyzed oxides on metals. These oxides have the virtue of being easily fabricated but there is not now available a set of procedures for preparing high-purity metal oxides. Work has started on assembling and evaluating a set of procedures in order to prepare a document on recommended thin-film anodization methods.

- (3) Contacts have been made with a small group of European scientists who have formed a Surface Analysis Reference Committee in Europe (SARCE) that is loosely associated with the Bureau Committee de Reference, an official part of the European Economic Community. Efforts will be made to coordinate the activities of the ASTM E-42 Committee on Surface Analysis with the SARCE group to increase the effectiveness of both groups and to minimize possible duplications of effort. The SARCE group was formally established at a Symposium on Quantitative Surface Analysis in London in October, 1979; at this meeting a survey of the attendees showed a strong desire for the development of a broad range of surface standards (e.g., calibration and operating procedures, reference materials, reference data, recommended procedures for data analysis, methods for quantification).
- (4) Organization of an Evening Workshop on Quantitative Surface Analysis at the 1980 Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy. This workshop involved discussion between a panel of invited speakers who gave presentations to an earlier formed Symposium and the audience on key questions which affect the accuracy of practical surface analyses (e.g., specific practical problems with particular analysis techniques, problems with the associated methodology, needs for additional reference data and materials, extent of sample damage during analysis, and sources of errors and mistakes). The workshop was judged successful by many of the attendees and a similar format and program are planned for forthcoming Pittsburgh Conferences.
- (5) Recommended methods have been developed for the analysis of base-metal and precious-metal catalysts and for the determination of catalyst-surface areas. An NBS-analyzed Co-Mo catalyst have been employed as a standard for calibration of analytical procedures.

Similar activities will continue in the coming year.

- (i) One planned activity is a test of the transmission properties of a limited number of x-ray photoelectron spectrometers of the same type. As a followup to the recently conducted ESCA roundrobin, tests will be made to determine the extent of differences in analyzer transmission properties for instruments that have been as carefully checked, aligned, and operated as possible. Such measurements will provide a baseline for comparisons with other instruments of the same type and from the other manufacturers.

(ii) Another planned activity is the sputter depth profile characterization of a multi-layered thin film (sandwich-type) structure in order to establish a method for calibrating sputtering rates for depth profile analysis. The use of such a layered structure should enable the user to eliminate the uncertainty of initial surface contaminants on the ion-erosion rate and should therefore provide a practical means for converting absolute sputtering yield data into a sputter depth measurement.

(d) Review Articles and Books

Review articles are an excellent means of disseminating information on measurement methods and reference data in selected areas. Although the preparation of a good review article is time-consuming, it is clear from the response to the division's mailing list (Section 1) that such articles are considered valuable.

A good example of the utility of review articles is the recent selection of a 1971 review article by T. E. Madey and J. T. Yates as a "citation classic" by the publisher of the Science Citation Index. This article, "Electron-Stimulated Desorption as a Tool for Studies of Chemisorption: A Review," was prepared at a time when electron-stimulated desorption (ESD) was of scientific interest for characterizing the nature of adsorbed species on surfaces and was of practical importance in affecting the accuracy of pressure measurements in the ultrahigh vacuum regime. Since then, electron-beam methods such as low-energy electron diffraction and Auger-electron spectroscopy have grown appreciably in use as surface-characterization techniques and ESD and related electron-damage effects have been recognized as a factor limiting the accuracy of measurement for many types of samples.

Review articles by Division staff that have been published since 1979 include:

- (1) "Electron Spectroscopy and Chemical Bonding," T. N. Rhodin and J. W. Gadzuk, in The Nature of the Surface Chemical Bond, ed. by G. Ertl and T. N. Rhodin (North-Holland, 1979).
- (2) "Chemical Information in Auger Spectroscopy," R. R. Rye, J. E. Houston, D. R. Jennison, T. E. Madey, and P. H. Holloway, *Ind. Eng. Chem. Prod. Res. Dev.*, 18, 2 (1979).
- (3) "Recent Progress in the Quantification of Surface Analysis Techniques," C. J. Powell, *Appl. Surface Sci.*, 4, 492 (1980).
- (4) "Prospectives for Surface Chemistry," J. T. Yates, and T. E. Madey, *Proc. of Fourth Symposium on Fluid/Solid Interactions* (Naval Research Laboratory, 1980).

Review articles in the course of publication include:

- (5) "Nitric Oxide Reduction," W. F. Egelhoff, in The Chemical Physics of Solid Surfaces and Heterogeneous Catalysis, ed. by D. A. King and D. P. Woodruff.
- (6) "The Methanation Reaction," R. D. Kelley and D. W. Goodman, in The Chemical Physics of Solid Surfaces and Heterogeneous Catalysis, ed. by D. A. King and D. P. Woodruff.
- (7) "The Thermal Desorption of Adsorbed Species," J. T. Yates, in Methods of Experimental Physics, ed. by R. L. Park.
- (8) "Experimental Methods in Electron and Photon Stimulated Desorption," T. E. Madey in Methods of Experimental Physics, ed. by R. L. Park.
- (9) "Electron Beam Damage in Auger Electron Spectroscopy," C. G. Pantano and T. E. Madey, to be published in Applications of Surface Science.

While there are many books and review articles on different aspects of surface science and its applications, there is a dearth of information on how to make reliable surface-characterization measurements. There is, in essence, a large information gap between review articles in which the latest scientific advances are discussed and manufacturers handbooks in which the operation of commonly used surface-characterization equipment is described. Negotiations are currently underway with a commercial publisher to produce a series of books which will address this need. Three NBS staff members (Powell, Madey, Yates) and two other scientists will constitute an editorial board that will oversee the production. Current plans call for several books that will include extensive descriptions of the commonly used methods of surface analysis, the practice of ion sputtering to obtain depth-profile information, specimen preparation, and vibrational-spectroscopy methods of characterizing surface molecules.

3. SURFACE SCIENCE COMPETENCE PROGRAM (9 staff years)

3.1 Introduction

The Surface Science Competence Program is a part of the recently established 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 initial plans for the Surface Science Competence Program 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 will, however, be appreciable overlaps among these areas and with other Division projects. Specific projects have

been selected based on a judgement of their scientific merit and on assessments of impacts with other NBS Divisions and of the future scientific and technical challenges requiring NBS expertise and action. Our strategy has been to involve the existing Division staff in the new activities to the maximum extent possible, to attract additional high-quality staff to NBS, to seek staff at both junior and senior levels, to implement both new experimental and new theoretical activities, and to retain flexibility to meet future needs by filling some positions on a non-permanent basis.

3.2 Reports of Technical Activities

Details are given here of projects which have been initiated. Other projects are currently being developed.

(a) ESDIAD-EELS Studies of the Molecular Structure of Adsorbed Species (Yates, Madey, Ceyer)

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 of importance to technologies such as heterogeneous catalysis, corrosion prevention, electrochemistry, and semiconductor design.

We are constructing an instrument to combine two powerful techniques for studying adsorbate structures - ESDIAD (Electron Stimulated Desorption Ion Angular Distribution) and EELS (Electron Energy Loss Spectroscopy). The two-level apparatus, magnetically shielded, is almost completed. The EEL-spectrometer is operating at optimal resolution and beam current and has been tested at resolutions as low as 4.5 meV (36 cm^{-1}) in the direct beam. When finished the apparatus will have provision for molecular beam dosing of the crystal with adsorbates (to maintain high purity), Auger spectroscopy, thermal desorption spectroscopy, angular dependent EELS, and ESDIAD, including mass spectrometric detection of the ionic fragments. It will be a unique experimental facility for structural studies on surfaces. The areas of planned research include:

- (i) Study of C_2H_4 and O_2 chemisorption and interaction on Ag surfaces
- (ii) Study of the catalytic reduction of chemisorbed oxygen by hydrogen on Rh surfaces searching for adsorbed OH intermediates
- (iii) The influence of substrate crystallography on the bonding of CO to transition metals
- (iv) Exploratory studies of laser-induced dissociation of chemisorbed molecules

- (v) Study of the orientation and vibrational spectrum of the CH_3NC molecule on Rh surfaces. Preliminary IR studies on dispersed Rh indicate the molecule chemisorbs via the NC group (as expected) and this mode of bonding provides an anchor for CH_3 groups. It is planned to study the CH_3 orientation and its freedom to rotate about the C_3V axis.
 - (vi) Study of CO bonding at ZnO single crystal surfaces, to correlate with recent photoemission studies, as well as recent IR studies at NBS.
- (b) Laser Fluorescence as a Probe of Surface Dynamics (Yates, Cavanagh)

Surface science has long been concerned with understanding the kinetics of thermal desorption. To date, no complete studies of the distribution of internal energy (vibration, rotation) in desorbing molecules have been done. Such information is of importance in modeling desorption at the quantum mechanical level, and will be important to the understanding of a crucial step in catalysis (desorption of the product molecule).

Laser fluorescence techniques are well known to be useful for studies of the internal energy distribution of free molecules. In collaboration with Drs. J. Stephenson and D. King of the NBS Molecular Spectroscopy Division, we have designed an experiment for determining the internal energy distribution of molecules desorbed thermally from surfaces. Particular care has been taken to ensure that the laser excites molecules desorbing from the sample rather than returning from the apparatus walls.

The ultrahigh vacuum optical cell has been built and tested. It has been shown that a single desorption state of NO from Ru(001) occurs at 480 K in agreement with earlier thermal desorption studies elsewhere. The optical portion of the experiment is currently under test.

We plan initially to study the thermal desorption of NO from Ru(001). The activation energy for desorption is about 10000 cm^{-1} while the vibrational frequency of the free molecule is about 1900 cm^{-1} , and we will determine whether the desorbing molecule is vibrationally or rotationally hot. Since the initial state of the chemisorbed NO is known (site location, vibrational dynamics), the determination of the internal energy distribution of the desorbing molecule in its "final state" should permit a detailed theoretical description of the dynamics of the desorption process to be constructed. NO desorbing from a molecular NO state on Ru(001) will be compared with NO desorbing from recombination of N(ads) and O(ads) on Ir(100). In addition, transient species in catalytic reactions on surfaces may possibly be detected by laser fluorescence studies in the gas phase (i.e., OH(g) from H(ads) + O(ads) on the surface), and exploratory studies in this direction are planned.

(c) Neutron Inelastic Scattering from Adsorbed Species on Surfaces
(Madey, Kelley, Cavanagh)

An important challenge to surface science is the characterization of surfaces in their working environments, e.g., high temperature and high pressure. To this end we are developing neutron inelastic scattering (NIS) at the NBS 10 MW Reactor as a tool for determining the vibrational spectra of hydrogen-containing molecules on the surfaces of high-area transition-metal catalysts. Neutron scattering is particularly sensitive to hydrogen vibrations, is ideally suited for optically opaque samples, and is useful under high pressure conditions as an in situ surface characterization tool.

Dr. J. J. Rush and his colleagues in the NBS Reactor Radiation Division have constructed a new neutron analyzer/detector system to provide a factor of 6 increase in signal-to-background over our initial measurements. A new cryostat and portable uhv system permit adsorption studies to be carried out over a wide temperature range. Using these facilities, we have studied the adsorption and decomposition of C_2H_4 over Raney Ni in the range 77-300 K; this is the first reported use of NIS for studying hydrocarbon chemisorption by a metal surface.

Future plans include:

- (i) Study of the adsorption and decomposition of small hydrocarbon molecules on Raney Ni catalysts; use these data to help identify intermediates in CO hydrogenation reactions.
- (ii) Examine low-frequency torsional modes of $-CH_3$ and $-CH_2$ ligands. These non-optically active modes cannot be easily detected using other methods and their presence or absence is essential to structural assignments of molecular fragments on surfaces.
- (d) Angle-Resolved Photon-Stimulated Desorption - A New Tool for Surface Characterization (Madey, Stockbauer)

NBS surface scientists have collaborated in a crucial and successful test of a recent theory by Knotek and Feibelman in which ion desorption from surfaces was postulated to be initiated by core-hole ionization of surface atoms. The first measurements of angular anisotropy in the photon-stimulated desorption (PSD) of positive ions from adsorbed layers on a metal surface have been made in a joint effort between the NBS group and scientists from IBM and Yorktown Heights. These experiments were conducted with soft x-rays from the University of Wisconsin Synchrotron Radiation Facility in Stoughton, Wisconsin and with a unique display-type energy analyzer designed by Dr. D. E. Eastman of IBM. In the collaborative experiments, the NBS/IBM group extended the range of the analyzer (originally designed for angular resolved photoelectron emission) to detect the PSD of O^+ ions from an adsorbed oxygen monolayer

on a tungsten (111) oriented single crystal surface. PSD ion angular distributions, energy distributions, and photon excitation spectra for O^+ desorption from W(111) have been measured for oxygen coverages ranging from a fractional monolayer to a multilayer oxide, and for photon energies in the range 8 to 120 eV. A direct comparison of PSD with ESD revealed identical angular distributions indicating that the excitation mechanisms are the same in each case. This work confirms the Knotek-Feibelman theory, which postulates that ion desorption is initiated by core-hole ionization of surface atoms, whether ionization is produced by electron or photon bombardment.

The use of photon excitation rather than electron excitation for the desorption of ions has the advantage that the ion signal can be identified with a particular bond. By tuning the photon energy, it is possible to correlate a photon-energy threshold for the emergence of a particular ion signal with a specific bond (e.g., for ions emerging from a composite surface). In the recent experiments, the angular distribution of O^+ ions and the ion yields as a function of photon energy provided detailed information about the directions of surface bonds and the site from which desorbing ions originated. Angle-resolved PSD thus offers an exciting new means of characterizing the electronic and geometric properties of specific surface bonds. Similar experiments are being initiated at the NBS SURF II facility in collaboration with Dr. R. P. Madden and his colleagues of the NBS Radiation Physics Division. The collaboration with the IBM scientists is continuing. Planning has also been initiated for related work at the Brookhaven National Synchrotron Light Source.

Plans for the next year include:

- (i) PSD of covalently bonded surface species to assess the role of valence-type excitations in ion desorption (CO, hydrocarbons adsorbed on transition-metal surfaces)
- (ii) Application of PSD to oxygen adsorption and oxide formation on metals known to be catalytically active; characterization of the structure and bonding of OH groups on oxides using angle-resolved PSD
- (e) Photoemission Studies of Materials (Egelhoff)

A series of photoemission experiments is in progress with basically two different goals. One goal is to gain a deeper understanding of the physical phenomena that govern the characteristics of the photoemission process itself. This work has yielded a better understanding of electronic processes and electron dynamics in the rare-earth elements from analysis of photoemission resonances. The other goal is to use photoemission as a tool to study novel surface properties of materials. Among the properties under consideration are the electronic and geometric structure

of monolayer and submonolayer metal overlayers on metal substrates, changes in the electronic structure for surface atoms, and information on the electronic structure of small metallic particles ranging in size from single atoms to several hundred atoms.

The following experiments are in progress:

- (1) The study of materials by photoemission using synchrotron radiation is at present a rapidly growing field. One phenomena of particular interest recently has been photoemission resonances. These resonances can be used, for example, to establish differences in valence between surface and bulk rare-earth atoms. Our aim has been to gain a deeper understanding of the general principles governing these resonances. Prior to our work it was not understood why the intensity profile of the photoemission resonances in the lanthanide-series rare-earth elements was directly proportional to the photon absorption coefficient.

Experiments have been conducted at the Stanford Synchrotron Radiation Laboratory in collaboration with Dr. G. G. Tibbets of the General Motors Research Laboratories and Mr. M. H. Hecht and Prof. I. Lindau of Stanford University. Measurements have been made of photoemission spectra of thulium in the 150 to 250 eV photon-energy range. The results indicate the $4d \rightarrow 4f$ absorption cross section is directly proportional to the strength of an autoionization resonance which is thus believed to be the predominant decay channel associated with excitation from the 4d shell. Decay by the alternative channel of escape of an excited electron does not occur readily because of a significant angular-momentum barrier constraining the 4f electrons to the atom core.

It is believed that similar behavior will be observed in other rare-earth elements and compounds. Further experiments are planned at Stanford and at the new Brookhaven National Synchrotron Light Source to examine the dynamics of electron excitation.

- (2) Recent breakthroughs in the use of binary alloys as industrial catalysts demonstrate the need for an improved understanding of the chemical physics of adatoms on one metal on a substrate of another metal. It is planned to make careful studies of the properties of Ni, Co, Fe, Cu, Pt, and Pd evaporated onto single-crystal surfaces of Fe, Ni, Al, and Cu. The surface geometry will be studied by low-energy electron diffraction with an emphasis on surface-phase transitions, ordered overlayers, and diffusion into the bulk. The electronic structure will be studied by x-ray photoemission with an emphasis on gaining an understanding of effects produced by changes in the geometric structure. The effects of gases such as CO, NO, and hydrocarbons adsorbed on binary alloy surfaces will also be studied. By investigating such systems under carefully controlled conditions, we anticipate the development of a set of

general principles for the electronic and geometric structures binary-alloy catalyst surfaces. It is noteworthy in this context that no one to date has applied photoemission to study an ordered overlayer of one metal on a single-crystal surface of another metal.

- (3) The subject of ultrasmall metallic particles is currently receiving considerable attention due to established and anticipated novel surface properties. We plan to use photoelectron spectroscopy to investigate changes in the valence-electronic structure for metallic particles as a function of particle size. Metallic particles, particularly rare-earth elements such as Eu, Sm, and Yb, will be produced by evaporation onto an amorphous carbon substrate with the average size being controlled by the substrate temperature and subsequent annealing. Particular attention will be paid to possible changes in 4f-shell occupancy as a function of size. Further studies will be made of changes in electronic structure as the particles are exposed to different gases. Such experiments should be very illuminating as the surface atoms of the particle can be an appreciable fraction of the total and as structural changes could be visible through changes in molecular-bonding configurations.

Extensive modifications and additions have been made to an existing x-ray photoelectron spectrometer for experiments in the second and third categories above. A sample-preparation chamber has been designed in which a range of samples can be prepared by vacuum evaporation and characterized by low-energy electron diffraction. The samples can then be transferred to the spectrometer.

(f) Atom-Probe Field-Ion Microscopy of Materials (Melmed, Martinka)

We are constructing 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 surface and bulk regions of the sample. There are three types of atom-probe instruments, namely time-of-flight (ToF), imaging, and magnetic sector, which each have specific advantages and limitations. The magnetic-sector type appears to have few applications in the microanalysis of solid materials so it has been decided to build a facility of ToF and imaging atom-probe instruments.

The ToF APFIM is designed with an energy-compensation stage to have a mass resolution $\Delta M/M = 1/2000$ in the mass range of most metallic elements. The main application of this instrument will be the surface analysis and depth-profile analysis of small areas and volumes, respectively, of solid materials. The spatial resolution in surface analysis will be variable from 15 nm to an atomic spacing while a depth resolution of one atomic layer over a depth range of $1\mu\text{m}$ will be attainable.

The imaging APFIM produces displays of the spatial distribution of selected elements on a sample surface. The mass resolution of the instrument is about 1/50 and the lateral resolution is about 0.3 nm. It is also possible to use the imaging instrument in the ToF mode with a mass resolution of about 1/150.

The ToF and imaging APFIM instruments are currently under construction. Both instruments incorporate a number of novel features. The instruments will be fully computerized to enable rapid data acquisition and real-time data analysis.

We plan to use the APFIM instruments for a wide range of surface and bulk materials problems:

- (i) Composition and structure: microanalysis of new materials, platings, metallic glasses, alloys, etc.
- (ii) Segregation: alloy constituents, gas, grain-boundary diffusion.
- (iii) Radiation Implantation: surface damage, dopant penetration.
- (iv) Corrosion: hydrogen interactions, aqueous media damage.
- (v) Gaseous adsorption: site-specific adsorption, reaction-product identification.
- (g) Surface Theory (Gadzuk, Girvin, Matthew, Metiu)

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

The Division has been fortunate to have as visiting scientists during the 1980 summer Prof. J.A.D. Matthew from the Physics Department, University of York, England and Prof. H. I. Metiu from the Chemistry Department, University of California at Santa Barbara. Each visitor gave three tutorial lectures which were appreciated by large audiences. While at NBS, Prof. Matthew worked on a comparative study of Auger-electron spectra excited by ions, electrons, and photons. Prof. Metiu has investigated mechanisms of electron-stimulated desorption of adsorbates from surfaces and the role of roughness in surface spectroscopies.

Other accomplishments include:

- (1) A theory for molecular reaction-rate processes at surfaces has been developed. A paper presenting the formal theory of surface rate processes together with model examples has been completed. Another paper emphasizing the role that vibrational spectroscopy can play in the reaction-rate theory has also been written.

- (2) The photoemission and Auger spectra of a material is often directly interpretable in terms of a one-body density of states. In some instances, however, one must consider the many-body dynamics of the measurement process in detail. Striking examples of the latter are the resonant satellites in several d-band materials which have been observed in photoemission near the photon-energy threshold for core-hole production. Near threshold, the Auger decay spectrum of the core-hole may be significantly modified by the presence of the spectator electron which is a by product of the creation of the core hole. A clarification of the physics of this phenomenon and its possible relationship to observed photoemission satellites has been made and an approximate analytic solution for a model describing the dynamics of the process has been obtained.

A general program of study of the statistical mechanics of adsorbed layers is underway. The capability to determine orientation of molecules by ESDIAD (Electron-Stimulated Desorption of Ion-Angular Distribution) has prompted a study of orientational ordering in adlayers on substrates of various symmetries. Another area of investigation is the analytic study and numerical Monte-Carlo simulation of interaction effects in the thermal desorption spectroscopy of adlayers. A general investigation of equilibrium phase transitions in two dimensions is planned.

4. PUBLICATIONS

(a) Publications of Past Year

- Carroll, J. J., Melmed, A. J., and Kruger, J., Technical Report to ONR, "Hydrogen Interactions with Stressed Titanium-Palladium Alloys and Stressed Vanadium Explored with Field Ion Microscopy."
- Carroll, J. J., Klein, R., and Melmed, A. J., "Thorium Field-ion Microscopy," Surface Science, 93, L93-L97 (1980).
- Duncan, T. M., Yates, J. T., Jr., and Vaughan, P. W., " ^{13}C - NMR Studies of CO Chemisorbed on Rh dispersed on Al_2O_3 ," J. Chem. Phys., 71, 3129 (1979).
- Dunlap, B. I. and J. W. Gadzuk, "Surface Plasmon Relaxation Energies for CO Adsorbed on Jellium," Surf. Sci., 94, 89 (1980).
- Gadzuk, J. W., "Hole Recoil, Vibrational Shake-up, and Photoelectron Lineshapes," Phys. Scripta, 21, 570 (1980).
- Goodman, D. W., Kelley, R. D., Madey, T. E., and Yates, J. T., Jr., "Kinetics of the Hydrogenation of CO over a Single Crystal Nickel Catalyst," J. Catal., 63, 226 (1980).
- Goodman, D. W., Madey, T. E., and Yates, J. T., Jr., "Interaction of Hydrogen Carbon Monoxide, and Methanol with Ni(100)," Surface Science, 93, L135 (1980).
- Goodman, D. W., Kelley, R. D., and Madey, T. E., "Kinetics of Carbon Deposition from CO on Ru(110) and Ni(100)," J. Vac. Sci. Tech., 17, 143 (1980).
- Goodman, D. W., and White, J. W., "Measurement of Active Carbon on Ru(110): Relevance to Catalytic Methanation," Surface Science, 90, 201 (1979).
- Holloway, P. H., Madey, T. E., Campbell, C. T., Rye, R. R., and Houston, J. E., "Electron Spectroscopy of Condensed Multilayers: Line Shape Changes due to Beam Damage and Excitation Mode," Surface Science, 88, 121 (1979).
- Kelley, R. D., and Goodman, D. W., "Catalytic Methanation over Single Crystal Nickel and Ruthenium: Reaction Kinetics on Different Crystal Planes," Division of Fuel Chemistry, ACS, Vol. 25, #2, March, 1980.
- Madey, T. E., Yates, J. T., Jr., Bradshaw, A. M., and Hoffman, F. M., "Evidence for "Inclined" CO on Pd(210)," Surface Science, 89, 370 (1979).

- Madey, T. E., "The Role of Steps and Defects in Electron Stimulated-Desorption: Oxygen on Stepped W(110) Surfaces," *Surface Science*, 94, 483 (1980).
- Melmed, A. J., Tung, R. T., Graham, W. R., and Smith, G.D.W., "Evidence for Reconstructed [001] Tungsten Obtained by Field-Ion Microscopy," *Phys. Rev. Letters*, 43, 1521 (1979).
- Melmed, A. J., and Carroll, J. J., "Ellipsometry Data Analysis Aided by Derivative Plots in N,K-Space," *Applied Optics*, 19 (1980) 1735-1736.
- Powell, C. J., Recent Progress in Quantification of Surface Analysis Techniques, *Appl. of Surf. Science*, 4, 492 (1980).
- Powell, C. J., "Application of Auger-Electron Spectroscopy and X-ray Photoelectron Spectroscopy to the Characterization of Pollutant Particles," *Characterization of Particles*, edited by K.F.J. Heinrich, NBS Special Technical Publication 533, p. 131, (1980).
- Powell, C. J., Erickson, N. E., and Madey, T. E., "Results of a Joint Auger/ESCA Round Robin Sponsored by ASTM Committee E-42 on Surface Analysis, Part I." *ESCA Results J. Elect. Spect.*, 17, 361 (1979).
- Thiel, P. A., Yates, J. T., Jr., and Weinberg, W. H., "The Interaction of Oxygen with the Rh(111) Surface," *Surface Science*, 82, 22 (1979).
- Thiel, P. A., Yates, J. T., Jr., and Weinberg, W. H., "The Co-Adsorption of Oxygen and Hydrogen on Rh(111)," *Surface Science*, 90, 121 (1979).
- Thiel, P. A., Williams, E. D., Yates, J. T., Jr., and Weinberg, W. H., "The Chemisorption of CO on Rh(111)," *Surface Science*, 84, 199 (1979).
- Thiel, P. A., Weinberg, W. H., and Yates, J. T., Jr., "A Determination of Adsorption Site Symmetry on Surfaces via Electron Energy Loss Spectroscopy: Co-Adsorption of CO and NO on Ru(001)," *J. Chem. Phys.*, 71, 1643 (1979).
- Thiel, P. A., Weinberg, W. H., and Yates, J. T., Jr., "The Adsorption of Nitric Oxide on Ru(001)," *Chem. Phys. Letters*, 67, 403 (1979).
- West, J. B., Parr, A. C., Cole, B. F., Ederer, D. L., Stockbauer, R., and Dehmer, J. L., "Shape-Resonance-Induced Non-Franck-Condon Vibrational Intensities in 3 Photoionization of N₂," *Journal of Physics B Letters; Atom. Molec. Phys.*, 13, L105 (1980).
- Williams, E. D., Thiel, P. A., Weinberg, W. H., and Yates, J. T., Jr., "Segregation of Co-Adsorbed Species - Hydrogen and Carbon Monoxide on the (111) Surface of Rh," *J. Chem. Phys.*, 72, (1980) 3496-3505.

- Yates, J. T., Jr., Thiel, P. A., and Weinberg, W. H., "The Catalytic Reaction between Adsorbed Oxygen and Hydrogen on Rh(111)," Surface Science, 82, 45 (1979).
- Yates, J. T., Jr., Duncan, T. M., Worley, S. D., and Vaughan, R. W., "Infrared Spectra of Chemisorbed CO on Rh," J. Chem. Phys., 70, 1219 (1979).
- Yates, J. T., Jr., Worley, S. D., Duncan, T. M., and Vaughan, R. W., "Catalytic Decomposition of Formaldehyde on Single Rhodium Atoms," J. Chem. Phys., 70 1225 (1979).
- Yates, J. T., Jr., Zinck, J. J., and Weinberg, W. H., "Preparation and Purity Measurement of Extremely Pure Helium Gas," Review of Scientific Instruments, 50, 132 (1979).
- Yates, J. T., Jr., Zinck, J. J., Sheard, S., and Weinberg, W. H., "Search for Vibrational Activation in the Chemisorption of CH₄," J. Chem. Phys., 70, 2266 (1979).
- Yates, J. T., Jr., Williams, E. D., Weinberg, W. H., "Does Chemisorbed Carbon Monoxide Dissociate on Rhodium?", Surface Science, 91 (1980) 562-570.
- Yates, J. T., Jr., Duncan, T. M., and Vaughan R. W., "Infrared Spectroscopic Study of Activated Surface Processes: CO Chemisorption on Supported Rh," J. Chem. Phys., 71, 3908 (1979).
- Yates, J. T., Jr., Thiel, P. A., and Weinberg, W. H., "The Chemisorption of Hydrogen on Rh(111)," Surface Science, 84, 427 (1979).

(b) Publications in Progress

- Antoniewicz, P. R., Cavanagh, R. R., and Yates, J. T., Jr., "Temperature Effects on the Infrared Spectrum of Chemisorbed CO," J. Chem. Phys., accepted.
- Carroll, J. J., Madey, T. E., Melmed, A. J., and Sandstrom, D. R., "The Room Temperature Adsorption of Oxygen, Hydrogen and Carbon Monoxide on (1120) Ruthenium: An Ellipsometry-LEED Characterization," To be published in Surface Science 96 August 1980.
- Cavanagh, R. R., and Yates, J. T., Jr., "Hydrogen Spill-over on Alumina - A Study by Infrared Spectroscopy, J. of Catalysis, accepted.
- Cavanagh, R. R., and Yates, J. T., Jr., "Site Distribution Studies of Ph supported on Al₂O₃ - An Infrared Study of Chemisorbed CO," J. Chem. Phys., in press.
- Cavanagh, R. R., and Yates, J. T., Jr., "Infrared Spectra of Methyl Isocyanide Chemisorbed on Rhodium," Surface Science, accepted.

- Cole, B. E., Ederer, D. L., Stockbauer, R., Codling, K., Parr, A. C., West, J. B., Poliakoff, E. D., and Dehmer, J. L., "Wavelength and Vibrational-State Dependence of Photoelectron Angular Distributions. Resonance Effects in 5 Photoionization of CO," J. Chem. Physics, to be published.
- Egelhoff, W. F., "Nitric Oxide Reduction," in The Chemical Physics of Solid Surfaces and Heterogeneous Catalysis, King, D. A., and Woodruff, D. P., editors, Elsevier, London, in press.
- Fine, J., "Absolute Sputtering Yield Measurement Methods - A Review," Proceedings of the Tenth Symposium on the Physics of Ionized Gases, Dubrovnik, Yugoslavia (1980).
- Fine, J., Hardy, S. C., and Andreadis, T. D., "The Generation of Clean Liquid Gallium Surfaces by Ion Bombardment," Contributed Papers of the Tenth Symposium on the Physics of Ionized Gases, Dubrovnik, Yugoslavia (1980).
- Gadzuk, J. W., and Metiu, H., "Theory of Electron-Hole Pair Excitations in Unimolecular Processes at Metal Surfaces. I. X-ray Edge Effects," Phys. Rev. B, in press.
- Gadzuk, J. W., and Metiu, H., "Aspects of Reaction Dynamics at Metal Surfaces," Proc. of IVth Int. Conf. on Solid Surfaces, Cannes, France, September, 1980.
- Girvin, S. M., and Jonson, M., "Dynamical Electron-Phonon Interaction and Conductivity in Random Metal Alloys," Phys. accepted.
- Girvin, S. M., and Penn, D. R., "Theory of Coherence Effects in Photo-induced Auger Events: Resonant Satellites in Metals with Filled d-Bands," to be published in Phys. Rev. B.
- Goodman, D. W., Kelley, R. D., Madey, T. M., and White, J. M., "Measurement of Carbide Buildup and Removal Kinetics on Ni(100)," J. Catal., accepted.
- Jach, T. J., and Powell, C. J., " $L_{2,3}VV$ Auger-Electron Lineshapes and Peak Positions for Near-Threshold Electron Excitation in Nickel and Copper," submitted for publication, Phys. Rev. Letters.
- Jach, T. J., and Powell, C. J., "Application of X-ray Photoelectron Spectroscopy and Auger-Electron Spectroscopy for the Surface Characterization of Pollutant Particles," to be published in the Summary Report of the DOE Program Review on Physics and Chemistry of Atmospheric Pollution, Harpers Ferry, W. Va., May 28-30, 1980.
- Kelley, R. D., Cavanagh, R. R., Rush, J. J., and Madey, T. E., "Neutron Inelastic Scattering Study of C_2H_4 Adsorbed on Raney Nickel," Surface Science, accepted.

- Kelley, R. D., and Goodman, D. W., "Catalytic Methanation over Single Crystal Nickel and Ruthenium: Reaction Kinetics on Different Crystal Planes," Division of Fuel Chemistry, ACS, Vol. 25, #2, March, 1980.
- Klein, R., and Fine, J., "Desorption of Cesium from Molybdenum (111); Positive Ion Thermal Desorption Spectroscopy and Neutral Lifetime Measurements," Proceedings of the Eighth International Vacuum Congress and Fourth Intl. Conference on Solid Surfaces, Cannes, France (1980).
- Lehwald, S., Yates, J. T., Jr., and Ibach, H., "Adsorption and Dissociation of NO on Ni(111)," Proceedings of Fourth International Conference on Solid Surfaces, to be published in Le Vide.
- Madey, T. E., Goodman, D. W., Fisher, G. B., and Yates, J. T., Jr., "Structure and Kinetics of Surface Species," Proceedings Fourth Symposium on Fluid-Solid Surface Interactions, in press.
- Madey, T. E., "Determination of the Structures of Surface Molecules Using ESDIAD (Electron Stimulated Desorption Ion Angular Distribution)," to be translated into German and published in "Nova Acta Leopoldina."
- Madey, T. E., Stockbauer, R., van der Veen, J. F., and Eastman, D. W., "Angle Resolved Photon Stimulated Desorption of Oxygen Ions from a W(111) Surface," Physical Review Letters, accepted.
- Madey, T. E., Houston, J. E., and Dahlberg, S. C., "Bonding Geometry of CO on Planar and Stepped Single Crystal Surfaces," Le Vide, (Proceedings of 4th International Conference on Solid Surfaces, Cannes, France, September 1980).
- Melmed, A. J., Sakurai, T., Kuk, Y., and Givargizov, E. I., "Feasibility of ToF Atom-Probe Analysis of Silicon," submitted for publication, Surface Science.
- Metiu, H., and Gadzuk, J. W., "Theory of Rate Processes at Metal Surfaces. II. The Role of Substrate Electronic Excitations," J. Chem. Phys., to be published.
- Parr, A. C., Stockbauer, R., Cole, B. E., Ederer, D. L., Dehmer, J. L., and West, J. B., "An Angle Resolved Photoelectron Spectrometer for Atoms and Molecules," Nucl. Instrum. Methods, to be published.
- Williams, E. D., Thiel, P. A., Weinberg, W. H., and Yates, J. T., Jr., "Two Dimensional Phase Separation - Coadsorption of Hydrogen and Carbon Monoxide on Rh(111)," Conference on Surface Dynamics, La Jolla (1979), accepted.
- Yates, J. T., Jr., and Cavanagh, R. R., "Vibrational Spectroscopic Studies of Chemisorbed Species on Metals," Proceedings of Fourth International Conference on Solid Surfaces, to be published in Le Vide.

Yates, J. T., Jr., and Madey, T. E., "Prospectives for Surface Chemistry," in Proceedings of Fourth Symposium on Fluid-Solid Surface Interactions, (1978).

(c) Recent Publications of New Staff Members (Cavanagh, Egelhoff, Girvin, Griffin, and Stockbauer) describing Work in Previous Positions

Cavanagh, R. R., Altman, R. S., Herschbach, D. R., and Klemperer, W., "Molecular Beam Electric Deflection Analysis of $(\text{SN})_x$ Vapor. Evidence for a Nonpolar Tetramer," J. Am. Chem. Soc., 101 4734 (1979).

Egelhoff, W. F., Jr., and Tibbetts, G. G., "Valence Changes in a Ytterbium-Aluminum Alloy During Autoionization and Auger Electron Emission," Phys. Rev. Lett. 44, 482 (1980).

Girvin, S. M., and Mahan, G. D., "Thermoelectric Power in Half-filled Bands," Phys. Rev. B 19, 1302 (1979).

Girvin, S. M. and Mahan, G. D., "Exact Results for the Quantum Diffusion of Many Particles in a Stochastic Medium," Phys. Rev. B 20, 4896 (1979).

Griffin, G., and Andres, R. P., "Microscopic Capillarity Approximation: Free Energies of Small Clusters," J. Chem. Phys. 71, 2522 (1979).

Griffin, G., and Andres, R. P., "Microscopic Capillarity Approximation: Application to Homogeneous Nucleation Theory," J. Coll. and Interface Science, accepted.

Inghram, M. G., Hanson, G. R., and Stockbauer, R., "The Fragmentation of C_2F_6^+ ," Int'l J. Mass Spectrom. Ion Phys. 33, 253 (1980).

Jonson, M., and Girvin, S. M., "Electron-Phonon Dynamics and Transport in Random Metal Alloys," Phys. Rev. Lett. 43, 1447 (1979).

Parr, A. C., Jason, A. J., and Stockbauer, R., "Photoionization and Threshold Photoelectron - Photoion Coincidence Study of Cyclopropene from Onset to 20 eV," Int'l J. Mass Spectrom. Ion Phys. 33, 243 (1980).

Parr, A. C., Jason, A. J., Stockbauer, R., and McCulloh, K. E., "Photoionization and Fragmentation Study of Cyclopropene," Advances in Mass Spectrometry Vol. 8, Proceedings of 8th International Mass Spectrometry Conference, 12-18 August 1979, Oslo, Norway, to be published.

Rosenstock, H. M., Stockbauer, R., and Parr, A. C., "Kinetic Shift in Chlorobenzene Ion Fragmentation and the Heat of Formation of the Phenyl Ion," J. Chem. Phys. 71, 3708 (1979).

- Rosenstock, H. M., Stockbauer, R., and Parr, A. C., "Photoelectron-Photoion Coincidence Study of Benzonitrile," Journal de Chimie Physique, to be published.
- Rosenstock H. M., Stockbauer, R., and Parr, A. C., "Photoelectron-Photoion Coincidence Study of The Bromobenzene Ion," J. Chem. Phys., to be published.
- Stockbauer, R., "The Formation of High Vibrational States of Ions by Photoionization," Advances in Mass Spectrometry Vol. 8, Proceedings of 8th International Mass Spectrometry Conference, 12-18 August 1979, Oslo, Norway, to be published.
- Stockbauer, R., "Observation of the OH^+ Fragment Threshold in the Threshold Photoelectron Spectra of Water," Journal Chemical Physics, to be published.
- Tibbetts, G. G., and Egelhoff, W. F., Jr., "Mixed Valent Ytterbium - Aluminum Films," J. Vac. Sci. Technol., 17, 458 (1980).
- Zhdan, P. A., Schepelin, A. P., Boronin, A. I., Borekov, G. K., Weinberg, W. H., and Egelhoff, W. F., Jr., "Photoelectron Spectroscopic Evidence for the Oxidation of Ir(111)," J. Catal. 62 180 (1980).
- Zhdan, P. A., Borekov, G. K., Boronin, A. I., Schepelin, A. P., Egelhoff, W. F., Jr., and Weinberg, W. H., "Nitric Oxide Adsorption and Decomposition on the (111) and (110) Surfaces of Iridium," J. Catal. 60, 93 (1979).

5. TALKS

- Cavanagh, R. R., "Infrared Spectra of Chemisorbed Isocyanide Species on Rhodium," Staff of the Office of Naval Research and Contractors, Case Western Reserve University, Cleveland, Ohio, May, 1980.
- Cavanagh, R. R., "Spectroscopic Comparison of CO and Isocyanide Chemisorption on Supported Metal Catalysts," ACS Meeting, Houston, TX, March, 1980; Phillips Petroleum, Bartlesville, OK, May, 1980; ONR, Cleveland, Ohio, May, 1980; General Motors, Warren, Michigan, May, 1980; Bell Labs, Murray Hill, New Jersey, June, 1980.
- Ceyer, S., "Dynamics of Gas-Surface Scattering," IBM Research Labs, San Jose, CA, Feb., 1980; Dept. of Chemistry, Harvard University, Cambridge, MA, March, 1980; Dept. of Chemistry, M.I.T., Cambridge, MA, June, 1980.
- Egelhoff, W. F., Jr., "Electronic Effects in Nitric Oxide Adsorption on Tin Oxide," Northeast ESCA Users Group Meeting, Brookhaven, NY, November, 1979.
- Egelhoff, W. F., Jr., "Photoelectron Spectroscopies Studies Using Resonance Lamp and Synchrotron Radiation of Thulium, Ytterbium, and an Aluminum Ytterbium Alloy," Physics Dept., College of William and Mary, Williamsburg, VA, April, 1980.
- Egelhoff, W. F., Jr., "Photoemission Studies on a Yb-Al Alloy," Sixth International Vacuum Ultraviolet Radiation Physics Conference, Charlottesville, VA, June, 1980.
- Fine, J., "Measurement Methods and Calibration Techniques for Making Absolute Sputtering Yield Measurements at NBS," Boris Kidric Institute, Belgrade, Yugoslavia, October, 1979.
- Fine, J., "Absolute Sputtering Yields for Depth Profile Analysis," and "Visual Ion Beam Images Produced by Electron and Ion Beam Interaction on Surfaces," J. Stefan Institute, Ljubljana, Yugoslavia, October, 1979.
- Fine, J., "Sputtering and Surface Analysis," Short Course in Surface Analysis organized by C. J. Powell, given at NBS, February, 1980.
- Fine, J., "Absolute Sputtering Yield Measurement Methods - A Review," Tenth Symposium on the Physics of Ionized Gases, Dubrovnik, Yugoslavia, August, 1980.
- Fine, J., "The Generation of Clean Liquid Gallium Surfaces by Ion Bombardment," Tenth Symposium on the Physics of Ionized Gases," Dubrovnik, Yugoslavia, August, 1980.

- Fine, J., "Desorption of Cesium from Molybdenum (111); Positive Ion Thermal Desorption Spectroscopy and Neutral Lifetime Measurements," Eighth International Vacuum Congress and Fourth International Conference on Solid Surfaces, Cannes, France, September, 1980.
- Gadzuk, J. W., "An Introduction to the Theory of Atomic and Molecular Sticking at Metal Surfaces," Conference on "The Chemisorption Bond: Electronic Structure and Formation Mechanisms," Aspenasgarden, Sweden, October, 1979.
- Gadzuk, J. W., "Relaxation Effects in Electron Spectroscopies of Molecules, Solids, and Surfaces," Physics Colloquium, Rice University, Houston, TX, November, 1979.
- Gadzuk, J. W., "Theory of Electron-hole Pair Excitations in Unimolecular Processes at Metal Surfaces," Institute für Theoretical Physics of University of Hamburg, Hamburg, W. Germany, January, 1980; Rudor Boskovic Institute, Zagreb, Yugoslavia, January, 1980.
- Gadzuk, J. W., "Surface Science as Practiced at NBS," P. N. Lebedev Physics Institute, Moscow, USSR, January, 1980.
- Gadzuk, J. W., "Basic Principles for Phenomenological Modeling of Dynamical Processes in Molecules, Solids and Surfaces; Dynamical Relaxation Effects in Photoelectron Spectroscopy of Molecules, Surfaces and Adsorbates; Dynamics of Irreversible Unimolecular Processes at Metallic Surfaces," Institute for Catalysis, Novosibirsk, USSR, January, 1980.
- Gadzuk, J. W., (co-author H. Metiu) "Theory of Electron-Hole Pair Excitations in Unimolecular Processes at Metal Surfaces," American Physical Society Meeting, New York, NY, March, 1980.
- Gadzuk, J. W., "Dynamical Processes at Solid Surfaces," M.I.T., Cambridge, Mass., April, 1980.
- Gadzuk, J. W., "Role of Electron-Hole Pair Excitations in Unimolecular Processes at Metal Surfaces," Cornell University, Ithaca, NY, May, 1980.
- Gadzuk, J. W., "Why do Atoms Stick to Surfaces?" Interdepartmental Catalysis Colloquium, Argonne National Laboratory, Argonne, IL, June, 1980.
- Gadzuk, J. W., "Time Dependent Quantum Mechanics Made Simple," and "Theory of Reaction Rates at Metallic Surfaces," Institute of Theoretical Physics, Chalmers University of Technology, Goteborg, Sweden, September, 1980.

- Gadzuk, J. W., "The Role of Molecular Vibrations and Franck-Condon Factors in Surface Reaction Dynamics," International Conference on Vibrations at Surfaces, Namur, Belgium, September, 1980.
- Gadzuk, J. W., "Aspects of Reaction Dynamics at Metal Surfaces," Fourth International Conference on Solid Surfaces, Cannes, France, September, 1980.
- Girvin, S. M., "Electron-phonon Dynamics and Transport Anomalies in Random Metal Alloys," University of Virginia, Charlottesville, VA, September, 1979.
- Girvin, S. M., "Transport in Random Metal Alloys," American Physical Society, New York, NY, March, 1980.
- Girvin, S. M., "Theory of Transport Anomalies in Random Metals," University of Maryland, College Park, MD, May, 1980.
- Goodman, D. W., "The Kinetics of Carbon Deposition From CO on Ru(110) and Ni(100)," 26th AVS Symposium, New York, NY, October, 1979.
- Goodman, D. W., "Surface Science and Catalysis," Auburn University, Auburn, AL, November, 1979.
- Goodman, D. W., "Methanation Over Single Crystal Catalysts," Columbia University, New York, NY, November, 1979.
- Goodman, D. W., "Hydrogenation of CO over Single Crystal Catalysts," Exxon Research and Engineering, Linden, NY, November, 1979.
- Goodman, D. W., "Methanation over Single Crystal Catalysts," Sandia Laboratories, Albuquerque, NM, December, 1979.
- Goodman, D. W., "Hydrogenation of CO over Single Crystal Catalysts," Ninth Symposium, American Vacuum Society, Tampa, Florida, February, 1980.
- Goodman, D. W., "Single Crystals as Models for Catalytic Studies," 16th American Vacuum Society Symposium, Santa Fe, New Mexico, May, 1980.
- Goodman, D. W., "Single Crystals as Models for Catalytic Studies," Bell Telephone Labs, Murray Hill, NJ, May, 1980.
- Griffin, G. L., "Combined Temperature Programmed Desorption and IR Study of H₂ Adsorption on ZnO," 180th American Chemical Society Meeting, San Francisco, CA, August, 1980.

- Jach, T., "Dependence of Auger-Electron Lineshapes on Incident Electron Energy near Threshold," American Physical Society Meeting, New York, NY, March, 1980.
- Jach, T., " $L_{2,3}VV$ Auger Electron Lineshapes and Peak Positions for Near-Threshold Electron Excitation in Nickel and Copper," Gordon Conference on Electron Spectroscopy, Wolfeboro, NY, July, 1980.
- Kelley, R. D., "Catalytic Methanation over Single Crystal Nickel and Ruthenium: Reaction Kinetics on Different Crystal Planes," Symposium on Catalytic Reactions Involving Synthesis Gas and 179th American Chemical Society Meeting, Houston, TX, March, 1980.
- Kelley, R. D., "Synthesis Gas Reactions over Single Crystal Ni and Ru: Effect of Pressure and H_2/CO Ratio on Kinetics, Product Distribution, and Surface Carbon Concentration," New England Catalysis Society, M.I.T., Cambridge, MA, May, 1980.
- Kelley, R. D., "Neutron Inelastic Scattering (NIS) from Molecular Species Chemisorbed on a Catalyst Surface: Potential for NIS in Catalysis," Joint Chemistry-Physics Colloquium, University of Rhode Island, Kingston, RI, May, 1980.
- Kelley, R. D., "Synthesis Gas Reaction Over Single Crystal Nickel and Ruthenium: Effect of Pressure and H_2/CO Ratio on Kinetics, Product Distribution, and Surface Carbon Concentration," 19th Annual Spring Symposium, Pittsburgh Catalysis Society, Monroeville, PA, May, 1980.
- Kelley, R. D., "Inelastic Neutron Scattering as a Probe of Catalytic Reactions on Raney Nickel," Solid State Seminar, Brookhaven National Laboratory, Upton, NY, June, 1980.
- Madey, T. E., "Electron Stimulated Desorption Phenomena: Relationship to the Structure of Surface Molecules," Surface Physics Dept., Bell Laboratories, Murray Hill, NJ, November, 1979.
- Madey, T. E., "An Overview of Surface Science and Vacuum Technology in the Soviet Union," Rocky Mountain Chapter of American Vacuum Society, Denver, CO, December, 1979.
- Madey, T. E., "Use of Electron Stimulated Desorption for Determining Structures of Adsorbed Molecules," Electrical Engineering Department, University of Minnesota, Minneapolis, MN, January, 1980.
- Madey, T. E., "Use of Electron Stimulated Desorption for Determining Structures of Adsorbed Molecules," Dept. of Chemistry, Brown University, Providence, RI, February, 1980.

- Madey, T. E., "Electron Stimulated Desorption and its Relation to Surface Molecular Structure," Florida Chapter of the American Vacuum Society, Tampa, FL, February, 1980.
- Madey, T. E., "Electron Stimulated Desorption, Relation to Surface Molecular Structure," American Physical Society Meeting, New York, NY, March, 1980.
- Madey, T. E., "Electron and Photon Stimulated Desorption," National Research Council, Ottawa, Canada, April, 1980.
- Madey, T. E., "Structure of Molecules and Molecular Complexes at Surfaces," International Seminar on Catalysis and Catalytic Phenomena, Instituto Mexicano del Petroleo, Mexico City, Mexico, May, 1980.
- Madey, T. E., "Catalytic Processes as Studied by Modern Kinetic & Spectroscopic Methods," International Seminar on Catalysis and Catalytic Phenomena, Instituto Mexicano del Petroleo, Mexico City, Mexico, May, 1980.
- Madey, T. E., "Catalyst Characterization Using Electron Spectroscopies," International Seminar on Catalysis and Catalytic Phenomena, Instituto Mexicano del Petroleo, Mexico City, Mexico, May, 1980.
- Madey, T. E., "Angle Resolved Electron and Photon Stimulated Desorption: Relation to Surface Structure," Physics Department Colloquium, University of Wisconsin, Milwaukee, WI, May, 1980.
- Madey, T. E., "Surface Characterization Using Angle Resolved Electron and Photon Stimulated Desorption," Department of Physics, University of Wisconsin, Milwaukee, WI, May, 1980.
- Madey, T. E., "Determination of Surface Molecular Geometry Using Angle Resolved Electron and Photon Stimulated Desorption," IBM, Yorktown Heights, NY, June, 1980.
- Madey, T. E., "Electron and Photon Stimulated Desorption," University of Wroclaw, Wroclaw, Poland, September, 1980.
- Madey, T. E., "Physical Principles of Electron and Photon Stimulated Desorption," Conference on Inelastic Ion-Solid Collisions, Munich, W. Germany, September, 1980.
- Madey, T. E., "Bonding Geometry of CO on Planar and Stepped Single Crystal Surfaces," 4th International Conference on Solid Surfaces, Cannes, France, September, 1980.

- Melmed, A. J., (co-authors: R. Blaszczyzyn, M. Blaszczyzyn, R. Meclowski, and T. E. Madey, "Interactions of Sulfur and Nickel: Preliminary Observations," Fifth Seminar on Surface Physics, Karpacz, Poland, April, 1980.
- Melmed, A. J., (co-authors: R. T. Tung, and W. R. Graham) "Evidence for Reconstructed (001)W and (001)Mo Obtained by FIM," 40th Conference on Physical Electronics, Cornell University, Ithaca, NY, June, 1980.
- Melmed, A. J., "A History of Field Emission Microscopy," 27th International Field Emission Symposium, Tokyo, Japan, July, 1980.
- Melmed, A. J., (co-authors: M. Blaszczyzyn, R. Blaszczyzyn, R. Meclowski, and T. E. Madey) "Interactions of Sulfur and Nickel: Preliminary FEM Observations," 27th International Field Emission Symposium, Tokyo, Japan, July, 1980.
- Melmed, A. J., (co-authors: M. Martinka, T. Sakurai, and Y. Kuk), "Analysis of High Resistivity Silicon in an Energy-Compensated ToF Atom-Probe," 27th International Field Emission Symposium, Tokyo, Japan, July, 1980.
- Powell, C. J., "Progress of the ASTM Committee E-42 on Surface Analysis," International Conference on Quantitative Surface Analysis, National Physical Laboratory, London, England, October, 1979.
- Powell, C. J., "Shapes and Shifts of Auger Lines," Physics Department, Technical University of Munich, West Germany, October, 1979.
- Powell, C. J., "Quantitative Surface Analysis by Auger-Electron Spectroscopy and X-ray Photoelectron Spectroscopy," Institute of Interface Science and Vacuum Physics, Kernforschungsanlage, Julich, Germany, October, 1979.
- Powell, C. J., "Quantification of X-ray Photoelectron Spectroscopy and Auger-electron Spectroscopy," Eighteenth Eastern Analytical Symposium, New York, NY, November, 1979.
- Powell, C. J., "Introduction to Surface Analysis," "X-ray Photoelectron Spectroscopy," "Auger-Electron Spectroscopy," and "Comparisons of Surface-Analysis Techniques," Surface Analysis Course, NBS, February, 1980.
- Powell, C. J., "Recent Progress in Quantification of Surface Analysis Techniques," Symposium on Modern Spectroscopies in Surface and Solid-State Chemistry, Chemistry Dept., Case Western Reserve University, Cleveland, OH, May, 1980.

- Powell, C. J., "Angular Resolved Electron and Photon Stimulated Desorption: Work in the Surface Science Division," Contractors and Staff of the Office of Naval Research, Case Western Reserve University, Cleveland, OH, May, 1980.
- Powell, C. J., "Application of X-Ray Photoelectron Spectroscopy and Auger-Electron Spectroscopy for the Surface Characterization of Pollutant Particles," (co-author T. J. Jach) Program Review on the Physics & Chemistry of Atmospheric Pollution, Harpers Ferry, W.Va., May, 1980.
- Powell, C. J., "Comparative Observation of the 2p and 3p Electron Energy Loss Features in Nickel, Copper, and Gallium," (co-authors: T. J. Jach, J. Fine, and T. Andreadis), Physical Electronics Conference, Cornell University, Ithaca, NY, June, 1980.
- Powell, C. J., "Recent Progress in the Quantification of Surface Analysis Techniques," Aspen Symposium of the Rocky Mountain Chapter of the American Vacuum Society, Aspen, CO, June, 1980.
- Powell, C. J., "Comparison of the ESCA with other Surface-Analysis Techniques," Seventh Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Philadelphia, PA, Sept., 1980.
- Stockbauer, R. L., "Shape Resonance and Autoionization Effects in Molecular Photoionization. Results from the Triply Differential Photoelectron Experiment at SURF II," Center for Thermodynamics and Molecular Science Seminar, NBS, January, 1980.
- Stockbauer, R. L., "Shape Resonance and Autoionization Effects in Molecular Photoionization," Joint Physics-Chemistry Seminar, Polytechnic Institute of Brooklyn, Brooklyn, NY, May, 1980.
- Stockbauer, R. L., (co-authors: H. M. Rosenstock and A. C. Parr), "Photoelectron-Photoion Coincidence Study of the Bromobenzene Ion," Twenty-eighth Annual Conference on Mass Spectrometry and Allied Topics, New York, NY, May, 1980.
- Stockbauer, R. L., (co-authors: A. C. Parr, J. L. Dehmer, B. E. Cole, D. L. Ederer, and J. B. West), "Triply Differential Photoionization Studies of Small Molecules," Twenty-eighth Annual Conference on Mass Spectrometry and Allied Topics, New York, NY, May, 1980.
- Stockbauer, R. L., (co-authors: H. M. Rosenstock and A. C. Parr), "Recent Photoelectron-Photoion Coincidence Studies on Benzonitrile and Pyridine Fragmentation," Twenty-eighth Annual Conference on Mass Spectrometry and Allied Topics, New York, NY, May, 1980.

- Stockbauer, R. L., (co-authors: A. C. Parr, J. L. Dehmer, B. E. Cole, D. L. Ederer and J. B. West), "An Angle Resolved Photoelectron Spectrometer for Triply Differential Photoionization Studies," Sixth International Conference on Vacuum Ultraviolet Radiation Physics, Charlottesville, VA, June, 1980.
- Stockbauer, R. L., (co-authors: A. C. Parr, J. L. Dehmer, B. E. Cole, D. L. Ederer, J. B. West, and K. Codling), "Perturbation of Vibrational Intensity and Angular Distributions by Autoionization in Molecular Photoionization," Sixth International Conference on Vacuum Ultraviolet Radiation Physics, Charlottesville, VA, June, 1980.
- Stockbauer, R. L., (co-authors: K. Codling, J. B. West, A. C. Parr, J. L. Dehmer, B. E. Cole, D. L. Ederer), "Partial Cross Sections, Vibrational Branching Ratios, and Angular Distributions in the 570-600 Å Window Resonances in O_2 ," Sixth International Conference on Vacuum Ultraviolet Radiation Physics, Charlottesville, VA, June, 1980.
- Stockbauer, R. L., (co-authors: J. L. Dehmer, A. C. Parr, J. B. West, K. Codling, D. L. Ederer, B. E. Cole, E. D. Poliakoff), "Effects of Shape Resonances on Vibrational Branching Ratios and Photoelectron Angular Distributions in Molecular Photoionization," Sixth International Conference on Vacuum Ultraviolet Radiation Physics, Charlottesville, VA, June, 1980.
- Stockbauer, R. L., (co-authors: H. M. Rosenstock and A. C. Parr), "Photoelectron-Photoion Coincidence Studies of Chlorobenzene and Bromobenzene," Sixth International Conference on Vacuum Ultraviolet Radiation Physics, Charlottesville, VA, June, 1980.
- Stockbauer, R. L., (co-authors: T. E. Madey, J. F. van der Veen, and D. E. Eastman), "Angle Resolved Photon Stimulated Desorption of Oxygen Ions from a W(111) Surface," Sixth International Conference on Vacuum Ultraviolet Radiation Physics, Charlottesville, VA, June, 1980.
- Yates, J. T., Jr., "Spectroscopic Correlations in Catalytic Chemistry on Single Crystal and on Dispersed Metal Substrates," Advances in Catalytic Chemistry Symposium, University of Utah, Snowbird, Utah, October, 1979.
- Yates, J. T., Jr., "Spectroscopic and Other Structural Studies of Chemisorbed Species on Metal Single Crystals and on Dispersed Metal Substrates," 3M Research Center, St. Paul, MN, January, 1980.

- Yates, J. T., Jr., "Spectroscopic Correlations in Surface Chemistry," Dept. of Chemical Engineering, Stanford University, Palo Alto, CA, February, 1980.
- Yates, J. T., Jr., "Spectroscopic Correlations in Surface Chemistry," Department of Chemistry, University of California, Berkely, CA, February, 1980.
- Yates, J. T., Jr., "Spectroscopic and Other Structural Studies of Chemisorbed Species on Metal Single Crystals and on Dispersed Metal Substrates," Exxon Research and Development Laboratories, Baton Rouge, LA, March, 1980.
- Yates, J. T., Jr., "Spectroscopic Methods for Studying Chemisorption and Catalysis," Union Carbide Corporation, Charleston, W.VA., March, 1980.
- Yates, J. T., Jr., "Spectroscopic Correlation in Surface Chemistry on Single Crystal and Dispersed Metal Substrates," Joint Interdisciplinary Seminar, National Science Foundation, Washington, D.C., March, 1980.
- Yates, J. T., Jr., "Spectroscopic and Other Structural Studies of Chemisorbed Species on Metal Single Crystals and on Dispersed Metal Substrates," Southwest Texas Catalysis Symposium, Houston, TX, March, 1980.
- Yates, J. T., Jr., "The Rate of Isotopic Mixing Between CO Molecules on Ni(100)," 179th American Chemical Society Meeting, Houston, TX, March, 1980.
- Yates, J. T., Jr., "Spectroscopic Correlation in Surface Chemistry - Forging a Relationship between Chemisorption on Supported Metals, on Single Crystals, and to Bonding in Organometallic Chemistry," Tri State Catalysis Club, Charleston, W.VA., March, 1980.
- Yates, J. T., Jr., "Spectroscopic Methods for Studying Surface Species as a Means of Understanding Heterogeneous Catalysis at the Molecular Level," Frontiers in Chemistry Lecture Series, State University of New York, New Platz, NY, April, 1980.
- Yates, J. T., Jr., "Spectroscopic Methods for Studying Surface Species as a Means of Understanding Heterogeneous Catalysis at the Molecular Level," Philadelphia Catalysis Society, Philadelphia, PA, April, 1980.
- Yates, J. T., Jr., "Spectroscopic and Other Structural Studies of Chemisorbed Species on Metal Single Crystals and on Dispersed Metal Substrates," Pittsburgh Catalysis Symposium, Monroeville, PA, May, 1980.

- Yates, J. T., Jr., 1. "Kinetics of Chemical Processes on Single Crystal Surfaces;" 2. "The Vibration of Molecules in the Adsorbed Layer;" 3. "Molecular Dynamics and Fundamental Excitation in Surface Reactions;" International Seminar on Catalysis and Catalytic Phenomena, Instituto Mexicano del Petroleo, Mexico City, Mexico, May, 1980.
- Yates, J. T., Jr., "Vibrational Properties of Chemisorbed Molecules on Metal Surfaces," Department of Chemistry, Northwestern University, Evanston, IL, May, 1980.
- Yates, J. T., Jr., "Vibrational Properties of Chemisorbed Molecules on Metal Surfaces," Materials Science Colloquium, M.I.T., Cambridge, MA, May, 1980.
- Yates, J. T., Jr., "Spectroscopic Studies of CO Chemisorption on Transition Metals and Studies of the Kinetics of CH₄ Synthesis," Conference on Chemistry and Physics of Coal Utilization, University of West Virginia, Morgantown, W.VA., June, 1980.
- Yates, J. T., Jr., "Spectroscopic Correlation in Surface Chemistry - Forging a Relationship Between Chemisorption on Supported Metals, on Single Crystals and to Bonding in Organometallic Chemistry," 1st Whitney Symposium, General Electric Corporation, Schenectady, NY, June, 1980.
- Yates, J. T., Jr., "Electron Stimulated Desorption - A Review," 180th American Chemical Society Meeting, San Francisco, CA, August, 1980.
- Yates, J. T., Jr., "Vibrational Spectroscopy of Adsorbed Molecules on Metals," International Conference on Solid Surfaces, Cannes, France, September, 1980.

6. SURFACE SCIENCE DIVISION SEMINARS

- Brenner, A., Wayne State University, Detroit, MI, "Supported Organometallics: The Frontier between Traditional, Homogeneous and Heterogeneous Catalysts," April, 1980.
- Bryant, G. W., Washington State University, Pullman, WA, "Quadratic Shakeup Satellites in Core Level Spectroscopy," April, 1980.
- Cini, M., Lab Ricerche di Base, Snamprogetti, Rome, Italy, "Optical Properties of Small Particles," March, 1980.
- Cohen, G., Metallurgy Division, National Bureau of Standards, "Laboratory EXAFS and Surface EXAFS; NBS Plans for the Brookhaven Synchrotron," May, 1980.
- Cole, M., Penn State University, University Park, PA, "Bound State Resonances in Atomic Scattering from Surfaces," February, 1980.
- D'Andrea, A., C.N.R., Laboratory Metodologie, Avanzate Inorganiche-Roma, Italy, "The (e,2e) Reactions Near Surfaces," November, 1979.
- D'Andrea, A., C.N.R., Laboratory Metodologie, Avanzate Inorganiche-Roma, Italy, "Polaritons in Semi-infinite Crystals and in Thin Slabs: Microscopic Calculations," February, 1980.
- Davenport, J., Brookhaven National Laboratory, "Infrared Intensity and the CO Molecule," December, 1979.
- Dehmer, J., Argonne National Laboratory, Argonne, IL, "Connections between Electron-Molecule Scattering and Molecular Photoionization: Shape Resonances and Vibrational Effects," April, 1980.
- Egelhoff, W. F., Surface Science Division, NBS, "Photoemission Studies of Materials: Background and Planned Research," January, 1980.
- Einstein, T. L., University of Maryland, "Extended Appearance Potential Fine Structure: A New Probe of Interatomic Spacings at Surfaces," November, 1979.
- Fain, S. C., Jr., Physics Department, University of Washington, Seattle, Washington, "Low Energy Electron Diffraction Study of Physisorbed Monolayers on Graphite," March, 1980.
- Feldman, L. C., Bell Telephone Lab., Murray Hill, NJ, "Structural Studies of the W(001) and Si(001) Surfaces Using MeV Ion Scattering," April, 1980.

- Fink, J., Kernforschungszentrum Karlsruhe Institut für Angewandte Kernphysik, "The Layered Materials SnS_2 , SnSe_2 , NbS_2 and Intercalates: Investigation by High Energy Electron Loss Spectroscopy," June, 1980.
- Flodstrom, S. A., Linköping Institute of Technology, Sweden, "Oxidation of Simple Metals as Studied by Electron Spectroscopy," August, 1980.
- Girvin, S.M., Surface Science Division, National Bureau of Standards, "Orientational Order/Disorder Transitions in Surface Adlayers," January, 1980.
- Hecht, M. H., Stanford University, Palo Alto, CA, "Subshell Cross Sections for Synchrotron Radiation Studies in the Solid State," June, 1980.
- Herman, K., Institute für Theoretical Physik der Technischen, University of Clausthal, W. Germany, "Cluster Models for the Interpretation of Photoemission Spectra from Adsorbed Molecules," May, 1980.
- Houston, J. E., Sandia Laboratories, Albuquerque, NM, "Chemical Information in Auger Lineshapes," February, 1980.
- Jonson, M., Physics, Dept., Indiana University, Bloomington, IN, "The Dynamical Image Potential for Tunneling Electrons," April, 1980.
- Kiskinova, M., Surface Science Division, National Bureau of Standards, "Interaction of Oxygen and Alkali Metals with the Ni(100) Surface," July, 1980.
- Kolb, D. M., Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, Berlin, W. Germany, "Reflectance Spectroscopy in the Study of the Electrode-Electrolyte Interface," October, 1979.
- Lagally, M. G., Dept. of Metallurgical and Mineral Engineering, University of Wisconsin, Madison, WI, "Local Densities of States in Compound Semiconductor Surfaces from Auger Lineshapes," December, 1979.
- Larkins, F. P., Chemistry Dept., Monash University, Australia, "A Theoretical Study of Satellites in Atomic Photoelectron Spectra," July, 1980.
- Matthew, J.A.D., Physics Department, University of York, Heslington, York, England, "Relaxation Energies for Core Holes in Atoms, Vapours and Solids," July, 1980.
- Matthew, J.A.D., Physics Department, University of York, Heslington, York, England, "Autoionisation versus Auger Emission in Rare Earths," August, 1980.

- Matthew, J.A.D., Physics Department, University of York, Heslington, York, England, "Ion Excited Auger Spectra - A Critical Review," August, 1980.
- Metiu, H., Chemistry Department, University of California at Santa Barbara, "A Microscopic Theory of Thermal Desorption," July, 1980.
- Metiu, H., Chemistry Department, University of California at Santa Barbara, "Raman Spectroscopy at Metal Surfaces," July, 1980.
- Metiu, H., Chemistry Department, University of California at Santa Barbara, "Electrodynamics at Metal Surfaces," July, 1980.
- Monkenbusch, M., Kernforschungsanlage Julich GmbH, Julich, W. Germany, "Neutron Scattering Study on Benzene and Toluene on Graphite Basal Planes," June, 1980.
- Navinsek, B. J., Stefan Institute, University of Ljubljana, Ljubljana, Yugoslavia, "Surface Changes Induced by Medium Energy Ion Bombardment," May, 1980.
- Neiwenhuys, B. E., Gorlaeus Laboratories, State University at Leiden, Netherlands, "Adsorption and Catalysis on Metal and Alloy Surfaces," October, 1979.
- Ramaker, D., Naval Research Laboratory, Washington, D.C., "Hole-hole Correlation Effects on Auger Line Shapes and Electron Stimulated Desorption," June, 1980.
- Rowe, J., Bell Telephone Laboratories, Murray Hill, NJ, "Roughness and Coverage Dependence of Surface Enhanced Raman Scattering," December, 1979.
- Salaneck, W. R., Molecular and Organic Materials Area, Xerox Webster Research Center, Webster, NY, "Photoelectron Spectroscopy of Molecular Solids," March, 1980.
- Schonhammer, K., Institute for Theoretical Physics, University of Hamburg, Hamburg, W. Germany, "Deep-Level Spectroscopy from Adsorbates," July, 1980.
- Semancik, S., Physics Department, Brown University, Providence, RI, "CO Dissociation on Mo(100)," December, 1979.
- Thiel, P. A., Dept. of Chemical Engineering, California Institute of Technology, Pasadena, CA, "Vibrational Spectroscopy of H₂O Adsorbed on Ru(001)," April, 1980.

Tighe, N., Fracture and Deformation Division, National Bureau of Standards, "Scanning Transmission Electron Microscopy - An Overview," June, 1980.

Tolk, N., Bell Telephone Laboratories, Murray Hill, NJ, "Quantum Interference in Ion-Atom and Ion-Surface Collisions," May, 1980.

van der Veen, J. F., IBM, Thomas J. Watson Research Center, Yorktown Heights, NY, "Electronic and Geometrical Structure of Some Transition Metal Surfaces," March, 1979.

Walls, J. M., Physics Department, Loughborough University of Technology, England, "Composition-Depth Profiling in Surface Analysis," June, 1980.

7. TECHNICAL AND PROFESSIONAL COMMITTEE
PARTICIPATION AND LEADERSHIP

- W. F. Egelhoff, Jr.
Surface Science Division Safety Officer
- J. Fine
Chairman, ASTM Subcommittee E-42.09 on Standard Reference Materials
Member, NBS Metrology Users Group on Noise Policy
- J. W. Gadzuk
Treasurer, General Committee of the Physical Electronics Conference
Member, Program Committee for Nordic Institute for Theoretical Atomic Physics Conference "The Chemisorption Bond: Electronic Structure and Formation Mechanisms," Aspenasgarden, Sweden, 1979
Member, Local Committee for Second International Conference on Solid Films and Surfaces, College Park, MD., 1981
- D. W. Goodman
Treasurer, Division of Colloid and Surface Science of The American Chemical Society
- R. D. Kelley
Chairman, ASTM Subcommittee D-32.03 on Chemical Analysis
- T. E. Madey
U. S. Representative to Surface Science Division Steering Committee of the International Union of Vacuum Science, Techniques and Applications; Secretary of Committee
Member of Welch Scholarship Committee of the International Union of Vacuum Science, Techniques, and Applications
President-elect, American Vacuum Society
Member, ASTM Committee E-42 on Surface Analysis
- A. J. Melmed
Secretary, Steering Committee of the International Field Emission Symposium
- C. J. Powell
General-Chairman, Physical Electronics Conference
Chairman, ASTM Committee E-42 on Surface Analysis

Vice Chairman, 1980 Gordon Research Conference on Electron Spectroscopy

Member, NBS Radiation Safety Review Task Force

Member, Editorial Board, "Applications of Surface Science"

Member, Editorial Board, "Surface and Interface Analysis"

Invited Participant, Workshop on Basic Research Needs and Opportunities in Interfaces in Solar Materials, Solar Energy Research Institute, June 30-July 3, 1980

J. T. Yates, Jr.

Chairman, Division of Colloid and Surface Chemistry, American Chemical Society

Chairman, Steering Committee for the Industrial Fellowship Program in Surface Chemistry and Surface Physics, American Chemical Society

Member, ad hoc Surface Science Subcommittee, Committee on Planning for the Automobile of the Future, Department of Transportation

Member, Materials Research Division Evaluation Committee, Lawrence Berkeley Laboratory, University of California

Member, Board of Directors, Catalysis Society

Vice-Chairman, 1981 Gordon Research Conference on Dynamics of Surface Processes

Member, ASTM Committee D-32 on Catalysis

Member, ASTM Committee E-42 on Surface Analysis

Member, Solid State Sciences Committee, National Academy of Sciences

Chairman, NBS Research Advisory Committee

Vice-Chairman, CTMS Safety Committee

8. PROFESSIONAL INTERACTIONS, CONSULTING AND ADVISORY SERVICES

- (1) R. R. Cavanagh and J. T. Yates, Jr., are collaborating with J. Stephenson and D. King of the NBS Molecular Spectroscopy Division on laser fluorescence studies of the internal energy distribution of thermally desorbed molecules. This is a new measurement method for studying the details of the dynamics of gas-solid interactions.
- (2) R. R. Cavanagh, R. D. Kelley, and T. E. Madey are collaborating with J. J. Rush of the NBS Reactor Radiation Division on neutron inelastic scattering, measurements of hydrogen and hydrogenic species adsorbed on Raney nickel catalyst material.
- (3) S. T. Ceyer is collaborating with Prof. G. A. Somorjai and students at the University of California at Berkeley on surface-molecular beam scattering experiments.
- (4) W. F. Egelhoff, Jr. is collaborating with G. G. Tibbetts of the General Motors Research Laboratories and I. Lindau of the Stanford Radiation Laboratory on photoemission studies of rare-earth metals and alloys.
- (5) J. Fine is collaborating with Prof. M. Roush of the University of Maryland on computer simulations of ion bombardment and sputtering phenomena in which the effects of impurity concentration gradients as well as interfaces between layered materials are considered.
- (6) J. Fine is collaborating with Prof. B. Navinsek of the J. Stefan Institute, Ljubljana, Yugoslavia on the effect of surface topography on measurements of ion sputtering yields as well as on depth resolution at interfaces. This collaboration is conducted under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology.
- (7) J. Fine is collaborating with S. C. Hardy and J. Manning of the NBS Metallurgy Division on studies of surface impurities on liquid metals and the effect of ion beam bombardment mass transfer mechanisms for producing clean liquid metal surfaces.
- (8) J. Fine is collaborating with G. Candela of the NBS Electron Devices Division on a study of diffusion depths of metals in SiO_2 thin films on silicon.

- (9) J. Fine is collaborating with J. E. Houston of Sandia Laboratory, New Mexico (presently at NBS as a guest worker) on the analysis of the Auger spectra of liquid and solid gallium.
- (10) J. W. Gadzuk is collaborating with M. Sunjic of the Rudor Boskovic Institute and the University of Zagreb, Yugoslavia under the auspices of the U.S.-Yugoslavia Agreement for Cooperation in Science and Technology, on theories of electron spectroscopies of solids and surfaces.
- (11) J. W. Gadzuk is collaborating with theoretical and experimental physicists at Chalmers University, Gothenburg, Sweden, on theories of dynamical processes near surfaces under the auspices of a NORDITA (Nordic Institute of Theoretical Atomic Physics) visiting professorship.
- (12) J. W. Gadzuk is collaborating with Prof. Seb Doniach and a graduate student at Stanford University on theories of resonance lineshapes in photoelectron spectroscopy.
- (13) S. M. Girvin is collaborating with D. R. Penn of the NBS Electron Physics Group on theories of resonant photoemission satellites and other many body effects.
- (14) S. M. Girvin is collaborating with M. Jonson of Indiana University and Chalmers Tekniska Hagskola, Goteborg, Sweden, on studies of transport anomalies in highly disordered metal alloys and metallic glasses.
- (15) T. J. Jach is collaborating with W. Grant and R. Dehl of the NBS Polymer Science and Standards Division on studies of wear in dental materials using Auger-electron spectroscopy.
- (16) T. J. Jach is collaborating with J. Hamilton of the NBS Electron Physics Group on studies of the surface properties of magnetic materials near the Curie temperature.
- (17) T. E. Madey and R. Stockbauer are collaborating with D. E. Eastman and J. F. van der Veen of IBM on experiments to characterize the angle resolved photon stimulated desorption of ions from chemisorbed molecules on metal surfaces.
- (18) T. E. Madey is collaborating with R. Pollak of IBM, Yorktown Heights and J. Houston of Sandia Laboratories on experiments to compare electron and x-ray excited Auger spectra.

- (19) T. E. Madey and R. Stockbauer are collaborating with R. P. Madden of the NBS Radiation Physics Division and S. A. Flodstrom of Linkoping University, Sweden on photoelectron spectroscopy and photon stimulated desorption studies of adsorbed molecules on surfaces using the NBS SURF II facility.
- (20) T. E. Madey and A. J. Melmed are monitors of a PL-480 project between NBS and R. Meclowski and R. Blaszczyzyn of the University of Wroclaw, Poland concerning the diffusion of catalytic poisons on a nickel surface.
- (21) A. J. Melmed and M. Martinka are collaborating with S. Sakurai and Y. Kuk of the Pennsylvania State University on the analysis of high resistivity silicon in an electrically pulsed Energy-Compensated ToF atom-probe field-ion microscope.
- (22) A. J. Melmed and J. J. Carroll are collaborating with J. Kruger, J. J. Ritter, and J. R. Ambrose of the NBS Chemical Stability and Corrosion Division on stress-corrosion measurements, characterization of oxide films, and studies of electro plates.
- (23) A. J. Melmed is collaborating with Prof. W. R. Graham of the University of Pennsylvania on a project entitled, "High Resolution Microscopy of Surface Interactions" which has been funded (for 3 years) by NSF. A. J. Melmed is a co-principal investigator. We intend to use FIM to investigate the atomic structure of (001) crystal planes of Mo, Ta, Nb and V and (111) planes of Si and Ge, and to survey other major crystal planes of these materials for the occurrence of reconstruction.
- (24) C. J. Powell and T. J. Jach are collaborating with D. E. Newbury and J. E. Small of the NBS Gas and Particulate Science Division on surface and bulk characterizations of pollutant particles from the atmosphere.
- (25) R. Stockbauer is collaborating with A. C. Parr and D. L. Ederer, NBS Radiation Physics Division, J. L. Dehmer, Argonne National Laboratory, K. Codling, Reading University, U. K., and J. B. West, Daresbury Synchrotron Radiation Laboratory, U. K., on studies of gas-phase molecules using triply differential photoelectron spectroscopy with synchrotron radiation from the NBS SURF II facility.
- (26) R. Stockbauer is collaborating with P. M. Dehmer, E. D. Poliakoff and J. L. Dehmer of the Argonne National Laboratory on studies of cluster molecules using photoelectron-photoion coincidence techniques.

- (27) R. Stockbauer is collaborating with H. M. Rosenstock and A. C. Parr of the NBS Radiation Physics Division on measurements of the fragmentation of molecules using photoelectron-photoion coincidence techniques.
- (28) J. T. Yates, Jr. is collaborating with Profs. R. M. Martin and H. Metiu of the University of California at Santa Barbara on a study of the interaction of metastable inert gas atoms with surfaces under an NSF grant awarded jointly. This project is designed to explore a new measurement method for studying the electronic character of surfaces and adsorbed molecules on surfaces.

9. 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.

- (1) A. D'Andrea of the Consiglio Nazionale delle Ricerche, Rome, Italy has spent ten months at NBS as a guest worker studying (a) the $(e,2e)$ coincidence experiment with solid targets, (b) the spin-orbit splitting of surface resonances in the interaction of low-energy polarized electrons with surfaces, and (c) the use of more realistic surface potentials in describing the transport of optically-excited excitons in silicon.
- (2) T. D. Andreadis, a graduate student at the University of Maryland, has worked at NBS during the past year under a cooperative agreement (a) participating in laboratory measurements on sputtering phenomena and liquid-metal characterization, (b) developing and using a Monte Carlo program for studying sputtering phenomena in solids (c) interfacing two frequency counters with a small calculator for the NBS sputter-yield experiment, and (d) programming a microcomputer facility for Auger-electron spectroscopy.
- (3) D. K. Hoffman of Iowa State University has spent the equivalent of several weeks at NBS as a guest worker studying statistical mechanical effects in adsorbed layers while on assignment to the NSF.
- (4) J. E. Houston of Sandia Laboratories has spent a year at NBS as a guest worker and visiting scientist (a) applying the ESDIAD method to studies of adsorption on planar and stepped surfaces, (b) studying the enhancement of ion desorption yields for electron energies above core-electron excitation thresholds, (c) analyzing Auger-electron and electron energy-loss lineshapes in several experiments, and (d) making a critical comparison of various deconvolution schemes used in Auger lineshape analysis.
- (5) S. H. Kim of the National Industrial Research Institute, Seoul, Korea spent five weeks at NBS as a guest worker familiarizing himself with experimental methods used to deduce reaction mechanisms and kinetics in studies of the catalytic methanation reaction.
- (6) M. Kiskinova of the Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria has spent six months at NBS as a guest worker under the auspices of the International Research and Exchange Board studying (a) physisorption on zeolites and (b) the effects of poisons and promoters in the catalytic methanation reaction under controlled conditions.

- (7) J.A.D. Matthew of the University of York, England, is spending two months at NBS as a visiting scientist making a comparative study of the mechanisms of Auger-electron emission from surfaces under excitation by electrons, photons, and ions.
- (8) H. Metiu of the University of California at Santa Barbara is spending two months at NBS as a visiting scientist studying
 - (a) surface spectroscopies on rough metal surfaces and
 - (b) mechanisms of electron-stimulated desorption.
- (9) C. W. Seabury of Cornell University spent three weeks at NBS as a guest worker using ESDIAD to study the structure of ammonia on Ir(111) and Ni(111) surfaces.

10. SURFACE SCIENCE DIVISION STAFF

As of June 30, 1980, the Surface Science Division was staffed as follows:

C. J. Powell, Chief
S. K. Brereton, Administrative Aid
D. M. Keating, Secretary

J. J. Carroll
R. R. Cavanagh*
S. T. Ceyer
W. F. Egelhoff, Jr.
J. Fine
J. W. Gadzuk
S. M. Girvin
D. W. Goodman
G. L. Griffin*
T. J. Jach
R. D. Kelley
T. E. Madey
M. Martinka*
A. J. Melmed
A. Pararas
I. W. Price
R. Stockbauer
J. T. Yates, Jr.

*NBS-NRC Postdoctoral Research Associate

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET	1. PUBLICATION OR REPORT NO. NBSIR 80-2166	2. Gov't. Accession No.	3. Recipient's Accession No.
4. TITLE AND SUBTITLE Technical Activities 1980 Surface Science Division Reprinted from NBSIR 80-2132		5. Publication Date	6. Performing Organization Code
7. AUTHOR(S) C. J. Powell, editor	8. Performing Organ. Report No.		10. Project/Task/Work Unit No.
9. PERFORMING ORGANIZATION NAME AND ADDRESS NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, DC 20234		11. Contract/Grant No.	
12. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP)		13. Type of Report & Period Covered Final	
14. Sponsoring Agency Code			
15. SUPPLEMENTARY NOTES <input type="checkbox"/> Document describes a computer program; SF-185, FIPS Software Summary, is attached.			
16. 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 1980. These activities include experimental and theoretical research in surface science, the development of improved measurement methods, the provision of needed data, the development of reference materials, applications to important scientific and national problems, and surface-standards work. A listing is given of publications, talks, professional committee participation, and professional interactions by the Division staff.			
17. KEY WORDS (six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons) Surface chemistry; surface physics; surface science; surface standards			
18. AVAILABILITY <input checked="" type="checkbox"/> Unlimited <input type="checkbox"/> For Official Distribution. Do Not Release to NTIS <input type="checkbox"/> Order From Sup. of Doc., U.S. Government Printing Office, Washington, DC 20402, SD Stock No. SN003-003- <input type="checkbox"/> Order From National Technical Information Service (NTIS), Springfield, VA. 22161		19. SECURITY CLASS (THIS REPORT) UNCLASSIFIED	21. NO. OF PRINTED PAGES
		20. SECURITY CLASS (THIS PAGE) UNCLASSIFIED	22. Price

