### REPORT DOCUMENTATION PAGE

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<td>Nicholas Winograd</td>
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| 16. SUPPLEMENTARY NOTATION | |
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| 19. ABSTRACT (Continue on reverse if necessary and identify by block number) | |
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<td>(202) 767-4960</td>
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This project was aimed toward increasing our fundamental knowledge of the details of the interaction of energetic particles with solid surfaces. These studies included the measurement of the angular and energy contributions of the yield of desorbed ions by secondary ion mass spectrometry (SIMS). In addition, we developed a novel angle and energy resolved detector capable of measuring for the first time the yield of neutral particles desorbed from monolayers. This detector utilized multi-photon resonance ionization of the ejected atoms which occur at efficiencies approaching 100%. The results of the experimental measurements were coupled to classical dynamics calculations of the ion impact event.

This approach has been pursued to utilize ion beams to examine the structure of surface layers through anisotropies observed in the angular distributions. A variety of materials including alloys, semi-conductors and organic monolayers on metals were candidates as model system. The experiments have opened new avenues for using ion beam methods for the trace analysis of important electronic materials at unprecedented sensitivity limits.
COMPLETED PROJECT SUMMARY

TITLE: Studies of Ions and Neutrals Desorbed From Solid Surfaces by Ion and Electron Bombardment

PRINCIPAL INVESTIGATOR: Professor Nicholas Winograd
Department of Chemistry
The Pennsylvania State University
University Park, PA 16802

INCLUSIVE DATES: November 1, 1984 to October 31, 1988

CONTRACT/GRANT NUMBER: AFOSR-85-0028

SENIOR RESEARCH PERSONNEL:

Curt Reimann
Rajender Trehan
Kerry Walzl

JUNIOR RESEARCH PERSONNEL:

Jim Baxter
Che-Chen Chang
Susan Donner
Matthew Ervin
Mohamed El-Maazawi
William Kay
Robert Levis
Geoffrey Malafsky
Dave Pappas
Brad Weaver

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ABSTRACT OF OBJECTIVES AND ACCOMPLISHMENTS

This project was aimed toward increasing our fundamental knowledge of the details of the interaction of energetic particles with solid surfaces. These studies included the measurement of the angular and energy contributions of the yield of desorbed ions by secondary ion mass spectrometry (SIMS). In addition, we developed a novel angle and energy resolved detector capable of measuring for the first time the yield of neutral particles desorbed from monolayers. This detector utilized multi-photon resonance ionization of the ejected atoms which occur at efficiencies approaching 100%. The results of the experimental measurements were coupled to classical dynamics calculations of the ion impact event.

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Cumulative List of Publications Since 1984 Acknowledging AFOSR Support


7. L. A. DeLouise, E. White and N. Winograd, "Characterization of CO Binding Sites on Rh(111) and Rh(331) Surfaces by XPS and LEED: Comparison to EELS Results", Surface Sci. 147, 252 (1984).


Publications continued


Publications continued


FINAL SCIENTIFIC REPORT

for

Period Ending 31 October 1988

*Studies of Ions and Neutrals Desorbed From Solid Surfaces by Ion and Electron Bombardment*

*Grant No. AFOSR-85-0028*

*Principal Investigator*

Nicholas Winograd
Department of Chemistry
The Pennsylvania State University
University Park, Pennsylvania 16802

Submitted to:

Air Force Office of Scientific Research
Bolling Air Force Base
Washington, D.C. 20332

Approved for public release; distribution unlimited.
ABSTRACT

This project is aimed toward increasing our fundamental knowledge of the details of the interaction of energetic particles with solid surfaces. These studies will include the measurement of the angular and energy contributions of the yield of desorbed ions by secondary ion mass spectrometry (SIMS). In addition, we have developed a novel angle and energy resolved detector capable of measuring for the first time the yield of neutral particles desorbed from monolayers. This detector utilizes multi-photon resonance ionization of the ejected atoms which occurs at efficiencies approaching 100%. The results of the experimental measurements will be coupled to classical dynamics calculations of the ion impact event.

This approach is being pursued to utilize ion beams to examine the structure of surface layers through anisotropies observed in the angular distributions. A variety of materials including alloys, semi-conductors and organic monolayers on metals are candidates as model system. The experiments should also open new avenues for using ion beam methods for the trace analysis of important electronic materials at unprecedented sensitivity limits.
I. SUMMARY OF PROGRESS

Our efforts have been aimed toward experimental and theoretical investigations into the fundamental aspects of the interaction of energetic particles with solids. There have been 5 major phases to our work.


In this study, molecular dynamics calculations of 100 eV to 6 keV incident particles scattering from single crystal surfaces are performed using three particle interaction models. We find that for some incident conditions, a more extended interaction model is needed to produce accurate trajectory simulations than the binary collision model. This extended model takes into account the simultaneous interactions among the primary particle and all the other atoms in the system but not the ones among the substrate atoms. A fair agreement between the calculated results of this extended interaction model and that of the full dynamics model is observed for nearly the entire energy regime studied. The range of primary energies where the binary collision model is adequate is discussed.


Energy and angular distributions of Rh atoms ejected from a Rh{111} surface due to keV ion bombardment are predicted from classical dynamics calculations and are compared to those measured using a multiphoton resonance ionization scheme. The comparison is generally quite favorable. For example, the calculated distributions reproduce the changes in azimuthal anisotropy which occur over an ejected-particle kinetic energy range of 5-50 eV. The new detailed experimental data do, however,
expose deficiencies in the pair potential, which we believe can be overcome with a many-body potential.


We have shown for the first time that many-body interactions are important for describing the energy- and angle-resolved distributions of neutral Rh atoms ejected from keV-ion-bombarded Rh\{111\}. We compare separate classical-dynamics simulations of the sputtering process assuming either a many-body potential or a pairwise additive potential. The most dramatic difference between the many-body potential and the pair-potential is in the predicted kinetic energy distributions. The pair-potential kinetic energy distribution peaks at \(-2\) eV, whereas the many body-potential predicts a broader peak at \(-4\) eV, giving much better agreement with experiment. A specific set of parameters has been found which leads to excellent agreement with recent experimental trajectory measurements of desorbed Rh atoms.


The shadow-cone created by an incident keV bombarding ion is observed to enhance the yield of secondary ions sputtered from the target. This effect may be utilized to determine the bonding configuration of surface atoms in a manner similar to that reported for impact-collision ion scattering spectrometry (ICISS). This new method is utilized to study the bonding of Cl to Ag\{110\} as the coverage is increased from near
zero to the p(2x1) low-energy electron diffraction structure. The results show that the Ag-Cl bond length is extended by 0.4 Å in the isolated atom limit when compared to the p(2x1) coverage due to a large amount of charge transfer between the Ag substrate and the adsorbed Cl atom. This bond length becomes shorter as the coverage increases due to dipole-dipole repulsions.


A temporally sensitive ionization scheme is used in conjunction with a position-sensitive detector to measure simultaneously energy- and angle-resolved distributions of sputtered neutral atoms. We report results for 5-keV Ar⁺ ion-bombarded Rh(111) single-crystal surfaces, both clean and with a p(2x2) overlayer of oxygen atoms. The angular distributions and their variation with ejection kinetic energy are shown to give information about simple collision sequences that produce directionally preferential atom ejection. The changes that occur in the ejection distributions upon O atom adsorption suggest that O atoms occupy the "expected" sites, the sites that would be occupied by Rh atoms in a new monolayer.
II. Cumulative List of Publications Since 1984 Acknowledging AFOSR Support


7. L. A. DeLouise, E. White and N. Winograd, "Characterization of CO Binding Sites on Rh(111) and Rh(331) Surfaces by XPS and LEED: Comparison to EELS Results", *Surface Sci.* 147, 252 (1984).


Publications continued


Publications continued


III. Recent Invited Talks by Nicholas Winograd


145. Chemistry Departmental Colloquium, University of Cincinnati, Cincinnati, OH, "Ion Beam Spectroscopy of Solids and Surfaces", September 26, 1984

Invited Talks continued


155. 3rd Annual Texas A&M Chemistry Department Industry-University Cooperative Chemistry Program Symposium, College Station, TX, "Ion Beam Techniques", April 1, 1985.


157. Texas Instruments' Foundation, Dallas, TX, "Ion Beam Studies of Solids and Surfaces", May 17, 1985


Invited Talks continued


166. First International Laser Science Conference, Dallas, TX, "Multiphoton Resonance Ionization of Atoms Desorbed from Surfaces by Energetic Particle Bombardment", November 21, 1985.


168. Chemistry Department Colloquium, Texas A&M University, College Station, TX, "Ion Beam Spectroscopy of Solids and Surfaces", December 10, 1985.


Invited Talks continued


Invited Talks continued


Invited Talks continued


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V. Awards and Prizes - Nicholas Winograd

1. Texas Instruments Foundation 1984 Founders Prize

This prize consisting of a cash award of $50,000 (tax free) recognizes Winograd's work in fundamental studies of the bombardment of solids with energetic particles. The award is presented each year to a single individual to recognize achievement in the fields of physical science, health science, management science, engineering or mathematics. According to the Foundation, the award is made "for past achievement that would indicate even greater potential for accomplishment in the future".

2. Penn State Faculty Scholar Medal

This Medal is awarded for outstanding achievement in recognition of a single contribution or series of related contributions to a Professor in the Physical Sciences or Engineering. The recipient's contribution must have occurred within the last three years of the nomination.

3. Evan Pugh Professorship

In 1985 Winograd was named an Evan Pugh Professor, the highest honor that Penn State bestowes on a faculty member. Evan Pugh Professorships are awarded to faculty members whose "research publications or creative work or both have been of the highest quality over a period of time". The award has been given to 33 faculty members during the history of Penn State. There are currently 17 Evan Pugh Professors in residence.