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ANGULAR-RESOLVED ELECTRON EMISSION STUDIES OF MICROWAVE MATERIA--ETC(U)

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(10) Author: Gerald J. Lapeyre
Principal Investigator
Professor
Physics Department
Montana State University
Bozeman, Montana 59717

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B. Description of Grant Effort and Results

a. Introduction

The purpose of our program is to investigate the electronic properties of bulk solids, surfaces of solids, and adsorbed molecules on solid surfaces using the newly-developed method of polarization-dependent angle-resolved ultraviolet photoemission spectroscopy (PARUPS).

The program utilizes the unique properties of synchrotron radiation available at the University of Wisconsin Synchrotron Radiation Center, and we are one of the user groups at that center. The radiation emitted from the Wisconsin storage ring, ^{which} forms an intense continuum which extends well past 200 eV in energy. The portion of this continuum we have used depends on our monochromator and extends from 6 eV to about 40 eV. It is possible to take data at any selected photon energy in this range, as well as to do so while varying the photon energy continuously. The radiation is linearly polarized so it is possible to study photoemission effects which depend on the orientation of the polarization vector with respect to the crystal axes of the sample. Such data allows one to draw inferences about the electronic structure, wave function symmetry and, in certain cases, the orientation of adsorbed molecules.

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b. Materials and Systems Studied

The materials we have studied have been semiconductors, metals, and chemisorbed gases and the information we have sought has been concerned with bulk band structure, intrinsic surface states, chemisorption states, excitonic effect, and wave function symmetry. A detailed description of all the results are not presented here, however, detailed information can be obtained from our publications which are listed in Section C. We will present an overview of all the results which are organized as follows. In itemized form - a very brief description of the experiments and some of the results are given for each of the systems studied. Table I shows a list of the material systems that were studied. Then, for selected systems, which exemplify the nature and scope of our work, we give a more detailed presentation of the results. Concurrent with the experimental studies, theoretical investigations of the electronic structure for some of the systems measured, as well as other systems of interest, have been carried out and those results are summarized in the last section of the narrative.

Table I: Materials and Systems Investigated

<u>Semiconductors</u>		<u>Metals</u>	
Gallium Arsenide	(110) surface	Tungsten	(001) surface
Gallium Phosphide	"	Nickel	(001) & (110) surface
Indium Phosphide	"		
Zinc Selenide	"		
Tin Oxide	(001) surface		
<u>Chemisorbed Gases</u>			
Hydrogen on Tungsten	(001) surface		
Oxygen on Nickel	"		
Carbon monoxide on Ni	"		

c. Brief Description of Experiments on Each System

1. Semiconductors

III-IV Semiconductors: Fairly complete data sets were taken for the (110) cleavage face of GaAs, and these were analyzed for a determination of bulk-band structure and critical points along certain symmetry lines in the Brillouin Zone (B.Z.), as well as surface states. Based on the experience gained in all the early angle-resolved experiments, selected experiments were performed on other III-IV-s, i.e. InP and GaP. The data analysis for the InP bulk electronic structure was essentially completed. Excitonic effects were studied for GaAs and similar data collected on InP and GaP. The intrinsic occupied surface states on the (110) surface of GaAs were discovered in this effort and studied. Surface state data on InP were also collected. The data collected on InP and GaP forms the initial phase of a program to be continued in our follow-on efforts, to study selected band structure features in all of the III-IV semiconductors. For the purposes of examining the systematics of semiconductor properties, data were also collected for the II-VI ZnSe, since ZnSe is isoelectronic with GaAs.

SnO₂: Ion sputter etching and heat cleaning techniques were used to prepare the (001) surface of SnO₂ cut from a small single crystal. Data were taken from the samples and their analysis allowed a determination of the valence band width and the location of bands derived from the tin and oxygen orbitals. Unexpected features in this data led us to propose that the states near the bottom of the conduction band (e.g. 14eV below the vacuum level) are composed of Sn d-derived orbitals.

2. Metals

Tungsten (001) surface: Data were taken and analyzed for comparison with, and a check on, existing band structure calculations. Agreement with those calculations was good. Detailed studies were made of polarization effects related to wave function symmetry. This system also served as a prototype for exploring and developing necessary experimental and data analysis techniques necessary in PARUPS.

Nickel (001) and (011) surfaces: Emission from the bottom of the d-bands was observed at 4.3 eV below the Fermi level. This result cleared up a long standing controversy in the d-band width. Emission at -6 eV was determined to be due to the s-p bands, not to many-body effects as had been proposed.

3. Chemisorbed Systems

Hydrogen on Tungsten (001): Polarization effects were very pronounced in this system. Their analysis resulted in a determination of the symmetry of the chemisorption wave functions, providing support for certain model calculations. Strong umklapp, or diffraction, effects were seen, having quite general implications for chemisorption systems where the surface symmetry is altered.

CO on Nickel (001): The angular and polarization dependence of the photoemission spectra, analyzed in the context of theoretical calculations performed elsewhere, provided the first direct experimental determination of the orientation of the chemisorbed CO molecules. A photoemission feature was observed which was probably due to the theoretically predicted, but hitherto undetected, back-bonding orbital derived from the $2\pi^*$ CO orbital. The observed band is about 1 eV wide centered about 1.6 eV below E_F .

Oxygen on Nickel (001): The amplitude and position of the oxygen peak (6 eV binding energy) due to the oxygen p-like orbitals were studied as a function of emission direction, polarization, and photon energy. The polarization properties showed that the p_z -like and $p_{x,y}$ -like components were split and that the splitting has wave vector dependence. The results were in good agreement with theoretical calculations performed elsewhere.¹

d. Detailed Description of the Results of Selected Experiments

1. Introduction

During the period which this report covers, particularly the earlier part, angle resolved photoemission was a largely unexplored territory. It was necessary to determine just what information was available from such experiments and work out experimental approaches and data analysis methods to obtain the information most efficiently. For instance, the importance of band structure determination along symmetry lines in the Brillouin Zone and of polarization effects relating to wave function symmetry were appreciated only during this period. The program has profited a great deal from the study of several rather dissimilar systems. Experimental results from representative systems, GaAs, W (001) and W (001) + H, and Ni (001) + CO, illustrate this point quite effectively.

2. GaAs

One of the central problems in photoemission spectroscopy is to locate, in the Brillouin zone, the initial and final states for the transition observed in the spectra. A very useful partial solution to this problem evolves out of the fact that $\vec{k}_{||}$, the component of electron momentum (or wavevector) $\vec{k}$, parallel to the sample surface is conserved in the photo-absorption and emission process. In PARUPS one can determine $\vec{k}_{||}$ and thus locate $\vec{k}_i$ and $\vec{k}_f$, the initial and final state wave vectors, on the locus of points for which $\vec{k}_{||} = \text{constant}$: a single line in the B.Z. and which is perpendicular to the surface. Experimentally, one holds $\vec{k}_{||}$ constant by measuring emission at a fixed angle and fixed kinetic energy while varying the photon energy: the angle-resolved constant final-state energy (ARCFSE) mode of photoemission. Assuming direct inter-band transitions permits a

more precise location of $\vec{k}_i$ and $\vec{k}_f$ with the help of band structure calculations and in turn allows a check on those calculations. Generally $\vec{k}_{||}$ is chosen to coincide with a symmetry element (line, point) of the B.Z. for which bands are usually calculated. In the limiting case of normal emission, $\vec{k}_{||} = 0$ irrespective of kinetic energy, a fact which confers substantial simplification in performing the experiments and analyzing the results.

GaAs, as the first semiconductor we studied, was the subject of rather detailed investigation, and a great deal of information was obtained concerning its electronic structure. The energy positions of a number of critical points in the valence bands and in the conduction bands were determined. These positions were generally in good agreement with theoretical calculations;² the agreement constituted a good check on the accuracy of the calculations. Observed polarization effects served as an additional check on the calculated bands by allowing symmetry properties of certain bands to be inferred. How this inference is made is described later in this section.

Two occupied surface states at 1 and 7 eV below the Fermi level were observed that had been predicted to exist on theoretical grounds.³ These states had not been detected before in angle-integrated spectra (photoelectrons collected over a large solid angle) because in much of the Brillouin Zone they are degenerate with the valence band continuum. The dispersions (energy as a function of $\vec{k}_{||}$) of these states were measured and found to be in qualitative agreement with the calculations, although the band width was found to be larger than predicted.

3. W (001) and W (001) + H

The major emphasis in the study of these systems was on polarization effects. Early in the program it was observed that certain photoemission features (peaks) were strongly enhanced or suppressed depending only on the

direction of the vector potential $\vec{A}$ in the surface of the sample crystal. A correct understanding of this effect⁴ was found to involve the following selection rule. If the initial and final states have the same parity with respect to reflection in a mirror plane (symmetry under reflection), then the transition is forbidden for $\vec{A}$ perpendicular to that mirror plane and not forbidden otherwise. If they have opposite parity the transition is forbidden for $\vec{A}$ parallel to the mirror plane. The potentialities for determining band symmetry have since been applied routinely to the several systems we have studied. The surface of GaAs has only one symmetry element - a single mirror plane - while tungsten, with a 4-fold symmetric surface has four distinct mirror planes. A comparison between the two surfaces has been of considerable help in elucidating the nature of the polarization dependence and rather general group-theoretical rules have been derived for such effects.

The utility of such polarization dependence extends to a determination of which among several adjacent initial state bands contribute to a photo-emission peak. In the case of tungsten, one band could be selected from three possible candidates on the basis of its measured parity.

The parity of electron states resulting from chemisorption can also in certain cases be determined. For W (001) + H, chemisorption states were found, some with even and some with odd parity. This result placed severe restrictions on possible models of this chemisorption system and favored an existing model⁵ which assumed there were two hydrogen atoms per unit mesh on the surface, and in an antisymmetric combination of 1s orbitals.

4. Ni (001) + CO

In this experiment, the important result was the determination of the orientation of the CO molecule on the nickel surface. The observed photo-emission depended on the direction of emission and on the orientation of $\vec{A}$

with respect to the surface. In contrast to previous discussion, however, the polarization dependence was on the existence of a component of $\vec{A}$ perpendicular to the surface. Calculations existed⁶ for the directional photoemission from a free oriented CO molecule. Adapting these calculations to the chemisorbed case, the experimental results were consistent with a CO molecule standing vertically on the surface with the carbon end down. These results marked the first time that photoemission spectroscopy had been applied to a problem of surface atom or molecule geometry.

e. Theoretical Studies

The formalism, involving a semi-infinite tight-binding model using a resolvent method, was developed for the computation, layer by layer, of the local density of states for the transition metal surfaces W (001), MO (110), and W (111), and for the (110) surfaces of zinc blende semiconductors. Results include the existence of surface states or resonances in hybridization gaps as well as important modifications of the density of states near band edges, due to the surface potential. A rigorous group-theoretical analysis of polarization effects observed in photoemission was carried out. It was shown that for normal emission, or emission in a mirror plane, the allowed initial state must have the symmetry of the dipole operator and that the allowed final state must have even parity. The analysis, applied to clean and hydrogen-saturated W (001) surfaces supports the conclusions that both the Fermi peak on the former and the "hydrogen peak" on the latter correspond to symmetric initial states, composed of atomic sp_d^2 orbitals.

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C. Publications Resulting from AFOSR Support

a. Research Journal Articles

1. "Angle-Resolved Photoemission Studies of Surface State on (110) GaAs," J. A. Knapp and G. J. Lapeyre, J. Vac. Sci. Tech. 13, 757 (1976).
2. "Chemisorption-Induced Surface Umklapp Process in Angle-Resolved Photoemission from W (001)," J. Anderson and G. J. Lapeyre, Phys. Rev. Lett. 36, 376 (1976).
3. "Study of W Bulk Bands with Normal (001) Photoemission Using Synchrotron Radiation," R. J. Smith, J. Anderson, J. Hermanson, and G. J. Lapeyre, Solid State Commun. 19, 975 (1976).
4. "Adsorbate Orientation Using Angle-Resolved Polarization-Dependent Photoemission," R. J. Smith, J. Anderson, and G. J. Lapeyre, Phys. Rev. Lett. 37, 1081 (1976).
5. "Synchrotron Photoemission Studies of Single Crystal Tin Oxide," P. L. Gobby and G. J. Lapeyre, Proceedings of the 13th International Conference on the Physics of Semiconductors, Rome (1976).
6. "New Experimental Band Width for Ni," R. J. Smith, J. Anderson, J. Hermanson, and G. J. Lapeyre, Solid State Commun. 21, 459 (1977).
7. "Angle-Resolved Synchrotron Photoemission Studies of Clean and Chemisorbed Surfaces," G. J. Lapeyre, R. J. Smith, and J. Anderson, J. Vac. Sci. Technol. 14, 3841 (1977).
8. "Surface Density of States for Directional Photoemission Spectroscopy of W (001)," J. Hermanson, M. Kawajiri, and W. Schwalm, Solid State Commun. 21, 327 (1977).
9. "Final State Symmetry and Polarization Effects in Angle-Resolved Photoemission Spectroscopy," J. Hermanson, Solid State Commun. 22, 9 (1977).
10. "Surface Densities of States for Normal Photoemission from Mo (110) and W (111)," J. Hermanson, M. Kawajiri, and W. Schwalm, Solid State Commun., in press.
11. "Symmetry-Related Polarization Effects in Angle-Resolved Synchrotron Photoemission from W (001) and W(001) + H," J. Anderson, G. J. Lapeyre, and R. J. Smith, in preparation for submission to Phys. Rev.

C. Publications (cont.)

b. Conference Papers

Invited Conference Papers

1. "Three Modes of Photoemission Spectroscopy Using the Synchrotron Radiation Continuum," G. J. Lapeyre, Annual New York American Physical Society Meeting, 3-6 February 1976.
2. "Angle-Resolved Photoemission Studies of Surface States on (110) GaAs," J. A. Knapp and G. J. Lapeyre, Third Annual Conference on "The Physics of Compound Semiconductor Interfaces," 3-5 February 1976, Naval Electronics Laboratory Center, San Diego.
3. "Angle Resolved Photoemission from W Using Synchrotron Radiation," G. J. Lapeyre and J. Anderson, 36th Annual Conference on Physical Electronics, University of Wisconsin, 7-9 June 1976.
4. "Discussion of General and Shared VUV Instrumentation at Synchrotron Radiation Facilities," G. J. Lapeyre, Synchrotron Radiation Facilities Quebec Summer Workshop, Laval University, 15-18 June 1976.
5. "Study of Solids and Surfaces with Polarization Dependent Angle-Resolved Photoemission," G. J. Lapeyre, Conference on Recent Developments in Optical Spectroscopy of Solids, Taormina, Italy, 6-9 September 1976.
6. "Angle-Resolved Synchrotron Photoemission Studies of Clean and Chemisorbed Surfaces," G. J. Lapeyre, 23rd American Vacuum Society Symposium, Chicago, 21-24 September 1976.

Contributed Conference Papers

1. "Energy Band Analysis Along Symmetry Lines with Angle-Resolved Photoemission Constant Final-State Spectroscopy," R. J. Smith, J. Anderson, G. J. Lapeyre, and J. Hermanson, March 1976 Amer. Physical Soc. Meeting, Bull. Amer. Phys. Soc. 21, 431 (1976).
2. "Surface States in Angle-Resolved Synchrotron Photoemission from (110) GaAs," J. A. Knapp and G. J. Lapeyre, 36th Annual Conference on Physical Electronics, University of Wisconsin, June 7-9, 1976, Bull. Amer. Phys. Soc. 21, 938 (1976). J. A. Knapp won the W. B. Nattingham Prize for the best student paper presented.
3. "Angle-Resolved, Polarization Dependent Photoemission from W (001), W (001) + H, and Ni (001) + CO," G. J. Lapeyre, J. Anderson, and R. J. Smith, ESRO-Sponsored Conference on "Photoemission from Surfaces", Noordwijk, Holland, 13-16 September 1976.
4. "GaAs and InP Energy Band Measurements by Directional Photoemission," J. A. Knapp and G. J. Lapeyre, March Meeting of the American Physical Society, San Diego, Bull. Amer. Phys. Soc. 22, 363 (1977).

C. Publications (cont.)

5. "Angle-Resolved Photoemission Evidence for d-like Valence Bands in Tin Oxide," P. L. Gobby and G. J. Lapeyre, *ibid*, p. 363.
6. "Ni (001) + CO: The Chemisorption Band as Studied by Angle-Resolved Photoemission," R. J. Smith, J. Anderson, and G. J. Lapeyre, *ibid*, p. 413.
7. "Symmetry-Related Polarization Effects in Angle-Resolved Synchrotron Photoemission from W (001) and W (001) + H," G. J. Lapeyre and J. Anderson, *ibid*, p. 415
8. "Final-State Symmetry and Polarization Effects in Angle-Resolved Photoemission Spectroscopy," J. Hermanson, *ibid*, p. 253.
9. "Angle-Resolved Photoemission Study of Oxygen Chemisorption on Ni (001)," J. Anderson, G. J. Lapeyre, and R. J. Smith, 37th Annual Conference on Physical Electronics, Stanford, California, June 20-22, 1977.

c. Theses

1. "Angle-Resolved Photoemission Spectroscopy of Gallium Arsenide Using Synchrotron Radiation," J. A. Knapp, Doctoral Dissertation, November, 1976

Portions of this thesis formed the basis for a paper presented at the 36th Annual Conference on Physical Electronics, for which J. A. Knapp won the W. B. Nottingham Prize for the best student paper.
2. "Angle-Resolved Photoemission of Single Crystal SnO₂ Using Synchrotron Radiation," P. L. Gobby, Doctoral Dissertation, June, 1977.

D. Professional Personnel

Principal Investigator

Gerald J. Lapeyre
Professor of Physics

Theoretical Associate

John C. Hermanson
Associate Professor of Physics

Research Associates (post-doctoral)

Richard J. Smith
James R. Anderson
Gwyn P. Williams

Research Assistants

Peter L. Gobby, Ph.D., completed 1977
James A. Knapp, Ph.D., completed 1976
William A. Schwalm, Ph.D. student
John Seffens, M.S. student

E. Coupling

- a) Presented paper at the 1975 and the 1976 "Annual Synchrotron Radiation Users' Meeting" at the University of Wisconsin, Synchrotron Radiation Center in Stoughton, Wisconsin.
- b) Seminars given at the following laboratories:

Bell Laboratories, Murray Hill, September 9, 1975
University of Pennsylvania, September 11, 1975
Bell Laboratories, Murray Hill, February 4, 1976
National Bureau of Standards, Washington, February 5, 1976
Washington State University, March 16, 1976
University of Washington, March 17, 1976
University of Illinois, April 2, 1976
Stanford University, February 2, 1977
Lawrence Radiation Labs, University of California, February 3, 1977
Xerox Research Laboratory, Palo Alto, February 4, 1977
General Motors Research Laboratory, Warren, Michigan, March, 1977

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Methods were developed for performing polarization-dependent, angle-resolved photoemission experiments and of analyzing the results. The methods were applied to investigating the bulk and surface properties of the semiconductors GaAs, GaP, InP, ZnSe, and SnO₂; the metals W and Ni, and the chemisorption systems W+H, Ni+CO, and Ni+O. Energy positions of critical points in the valence band (VB) of GaAs were in eV below the VB maximum: L₃, 1.15; X₅, 2.9; ₁min, 4.1; X₃, 6.8. Conduction band critical points were in eV above the VB maximum: ₁2, 10.6; ₁5, 12.8; ₁, 14.9; ₁C⁸(min), 7.0; ₁C⁹(min), 9.2; ₂C¹⁰(min), 8.6; ₁C¹²(min), 9.8. VB critical points for InP were: X₅, 1.8; ₁min, 3.5; X₃, 5.5. GaAs surface states at 1 eV and 7 eV below the VB maximum were observed and their dispersions measured. The VB width of SnO₂ was measured to be 9 eV, the upper portion being derived from the O-2p orbitals, the lower portion from the Sn 4d orbitals. The conduction bands above 10 eV were identified with the Sn 4f states. Emission from the bottom of the Ni VB was observed for the first time; the d-band width was measured to be 4.3 eV, resolving an apparent anomaly in the experimental data. Polarization effects were exploited to determine wave function parity for the systems investigated and to infer the orientation of the CO molecule adsorbed on the Ni (001) surface: its axis is normal to the surface with the carbon end down.

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