IV. PHOTOEMISSION SPECTROSCOPY

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1. ELECTRONIC AND MAGNETIC STRUCTURE OF SOLID SURFACES USING PHOTOELECTRON SPECTROSCOPY

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As this is a recently initiated project, our efforts have been primarily devoted to the design and construction of the experimental apparatus that is to be used. Some preliminary results have already been obtained, however, for some theoretical work on photoemission processes which we have been pursuing in collaboration with the Semiconductor Surface Studies Group of Professor John D. Joannopoulos.

We have under construction an ultrahigh vacuum probe system that will operate in conjunction with the Hewlett-Packard 5950A photoelectron spectrometer in the Department of Chemistry, M. I. T. We hope this probe will be completed by March 1977. We shall use this system to study single crystals using high-energy ($h\nu$ = 1486.6 eV) angle-resolved photoemission spectroscopy. In this project we hope first to settle a controversy concerning the proper interpretation of these spectra. We then plan to extend these techniques by modifying the spectrometer to provide higher angular resolution. This will allow us to perform photoemission experiments that will yield densities of initial (valence band) states in selected regions of the Brillouin zone, and to study orbital symmetry effects. We are confident that this will prove to be a new and important form of band-structure spectroscopy for both metals and semiconductors.

In theoretical studies performed in collaboration with Professor Joannopoulos we have been examining the nature of the final states involved in high-energy photoemission experiments. Although, at the present time, the calculations are incomplete, there is an indication that the high-energy photoelectrons are much less effectively screened by the valence electrons from the ion cores of the solid. This indicates that a simple free-electron model will be inadequate to explain the spectra. We hope that these calculations, when completed, will serve to put the analysis of such photoemission spectra on a much more solid theoretical footing.

Final design work for our new spectrometer, designed primarily for surface studies, is being finished and construction should soon begin. Two first-year chemistry graduate

students have joined the group and are working on the photon sources to be used in our experiments. Michael R. McClellan, who came to M. I. T. from the University of California at Santa Barbara is designing a rotatable multiple reflection polarizer for He I and He II radiation. The use of polarization will be extremely valuable in the study of angular distribution of molecules on surfaces. This will allow us to obtain detailed information on the molecular nature of the oxidation properties of metal and semiconductor surfaces. Peter K. Smith, of St. Mary's University, Nova Scotia, is designing the x-ray source to provide Y Mξ x-rays. These x-rays will be very useful in the study of surfaces, since they produce valence band photoelectrons with escape depths that are near the minimum value attainable for many crystals.