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Diffraction of Photoelectrons Emitted from Core Levels of Te and Na Atoms Adsorbed on Ni(001)

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Azimuthal anisotropies in the photoemission from the Te 4*d* and Na 2*p* core levels have been measured for these atoms adsorbed in the $c(2\times2)$ configuration on Ni(001). The observed variations with photoelectron kinetic energy, polar angle of emission, and adsorbate species indicate that this is a very promising technique for surface-structure determination. Preliminary multiple-scattering calculations show encouraging agreement with experiments.

The availability of synchrotron radiation in the photon energy range $\hbar\omega > 30$ eV has led to proposals by Liebsch[1] and others[2,3] that measurements of the anisotropy of photoemission from the core levels of adsorbed atoms could be used to determine their positions relative to the surface. The wave function of the excited photoelectron is envisaged as a wave emanating from the atom of origin. This wave will scatter against substrate atoms, and the resulting electron interference pattern should be observable with an external detector. The theoretical prospects for a technique based on this effect appear quite good.[1,3-5] In contrast, the experimental situation has been less hopeful. Observations at low energy ($\hbar\omega = 24$ eV) of the emission from the 5*p* levels of Cs adsorbed on W(001) showed only weak anisotropies.[2] More recently, x-ray ($\hbar\omega = 1487$ eV) photoemission measurements of the 1*s* level of O adsorbed on Cu(001) showed somewhat larger anisotropies,[6] but such high-energy work appears to be restricted to grazing angles of emission presumably because of Debye-Waller effects and the weakness of all but forward scattering.[7]

Ideally, in such experiments, one would wish to tune $\hbar\omega$ so that the photoelectrons emerge with kinetic energies, E, in the range 30–200 eV appropriate to the conventional structural technique of low-energy electron diffraction (LEED). Synchrotron radiation is therefore essential. This would allow the extensive theoretical expertise accumulated in LEED studies to be transferred to the photoemission problem. It would also ensure strong backscattering amplitudes with only limited Debye-Waller degradation at room temperature.[7] Moreover, as in

LEED itself, it is probably essential to collect data over a reasonable range of experimental variables if a unique structural determination is to be obtained.[8] For example, if the azimuthal anisotropy is to be studied, measurements should be made for a range of polar emission angles θ and a number of emergent kinetic energies E. Finally, for preliminary studies, it is desirable to work on adsorbate systems whose structure have already been investigated by LEED. In this Letter we report what appear to be the first experimental measurements which satisfy all these requirements. Azimuthal anisotropies are observed which are quite strong and which vary appreciably with E, θ, and adsorbate species. We argue that a unique structural determination should prove possible. We present also the preliminary results of some multiple-scattering calculations which offer further encouragement.

The experiments were performed on the (001) surface of Ni with Na or Te atoms adsorbed in the $c(2\times2)$ configuration. Both of these systems have been analyzed previously by LEED.[8-10] Surface order was checked by means of medium-energy (4.5 keV) grazing-incidence electron diffraction. The spectrometer system has been described elsewhere.[11] An electron-energy analyzer samples photoelectrons propagating in the plane of incidence. The radiation was incident at $-45°$ to the surface normal and was p polarized. The light source was the Tantalus I storage ring, and the radiation was monochromatized by a plane-grating grazing-incidence monochromator which provided useful photon flux in the 60–120-eV range.[12]

We will concentrate here on data obtained for the azimuthal dependence of the core-level photoemission intensity. In these experiments, θ is kept fixed and the intensity is monitored as the sample is rotated about its surface normal. As discussed earlier,[2] this approach has the virtue of eliminating those anisotropies in the core-state emission which would arise even for free atoms, and isolates those anisotropies associated with photoelectron diffraction effects involving the structural surroundings of the emitter.

A group of azimuthal plots at $\theta=30°$ is shown in Fig. 1 for emission at photon energies 80, 90, and 100 eV from the 4d level of Te (binding energy 41 eV relative to the Fermi level) in a Ni(001)-Te$c(2\times2)$ surface, and from the 2p level of Na (binding energy 31 eV) in a Ni(001)-Na$c(2\times2)$ surface. The data points have been subjected to a fourfold symmetrization which enhances the

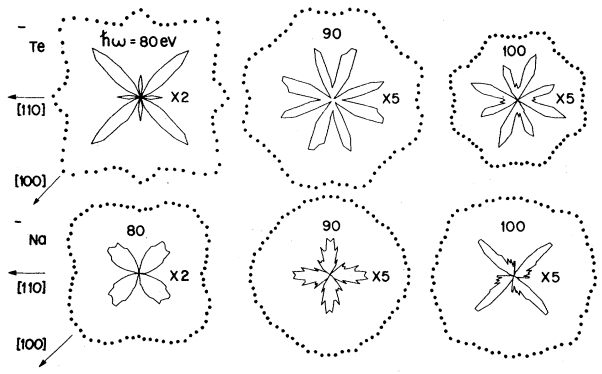

FIG. 1. Radial plots of the azimuthal dependence of adsorbate core level photoemission at the photon energies 80, 90, and 100 eV. The upper sets of data were obtained on Ni(001)-Te$c(2\times2)$ and the lower on Ni(001)-Na$c(2\times2)$. The inner full curves are enhanced data plots obtained by subtracting the minimum value from all others. The polar angle was $\theta=30°$ in all cases.

statistics and removes small spurious variations which occur from quadrant to quadrant.[2] (Note that this procedure does not introduce mirror symmetry; the observed asymmetries in Fig. 1 are indicative of residual statistical noise and provide a measure of the reliability of the data.) The anisotropies are strongest at $\hbar\omega=80$ eV, amounting to a maximum/minimum ratio of 1.43 in the case of Te and 1.31 in the case of Na. The data points of Fig. 1 have had a background subtracted. This background was determined by measuring the electron flux at a kinetic energy 5–7 eV higher than the relevant core-level photoemission peak; it is therefore a slight underestimate of the true background. Also shown in Fig. 1 are enhanced azimuthal distributions obtained by subtracting the minimum intensity from all other values.[6] While this method of data presentation is somewhat misleading, since it tends to overdramatize the actual variations, it does reveal more clearly the way in which the anisotropies vary with E. It is seen in Fig. 1 that variations with E are quite strong. In the case of Na, for example, the 2p emission is preferentially along ⟨100⟩ azimuths for $\hbar\omega=80$ and 100 eV but along ⟨110⟩ azimuths at the intermediate energy $\hbar\omega=90$ eV. Since the lobes change their orientations with E, it immediately follows that any simplistic shadowing-type interpretation attempting to relate lobe directions to spaces between nearest-neighbor atoms will be inadequate.

It is also seen in Fig. 1 that the observed anisotropies are quite different for Te and Na even though they are believed to occupy the same co-

ordination sites. This is not simply related to differences in kinetic energy E. At $\hbar\omega = 80$, 90, and 100 eV, the values of E for Te $4d$ emission are approximately 33, 43, and 53 eV, respectively, and for Na $2p$ emission 46, 56, and 66 eV, respectively. The latter two kinetic-energy values for Te lie close to the first two values for Na, and yet the azimuthal patterns are quite different. This species difference is attributed to differences in the adsorbate z spacings relative to the outermost Ni layer [2.23 Å in the case of Na (Refs. 8, 9) and 1.90 Å in the case of Te (Ref. 10)]. Further differences should arise through the angular momentum symmetry of the initial core states. If we represent the outgoing photoelectron wave function in terms of a wave emanating from the atom of origin, then Na $2p$ states will couple to $l = 0$ and $l = 2$ components of that wave, and Te $4d$ states will couple to $l = 1$ and $l = 3$ components.

The azimuthal anisotropy also varies with polar angle θ, and this is illustrated in Fig. 2 where we show results on Ni(001)-Tec(2×2) at $\hbar\omega = 80$ eV. Data are shown for $\theta = 30°$, 45°, and 60° corresponding, respectively, to $k_{\parallel} = 1.47$, 2.08, and 2.55 Å^{-1}. The range of $k_{\parallel}$ is somewhat larger than that obtained by varying E, as in the results of Fig. 1. The qualitative changes in the azimuthal anisotropy, however, appear to differ from those obtained by varying E, indicating that the θ dependence represents additional, rather than redundant information.

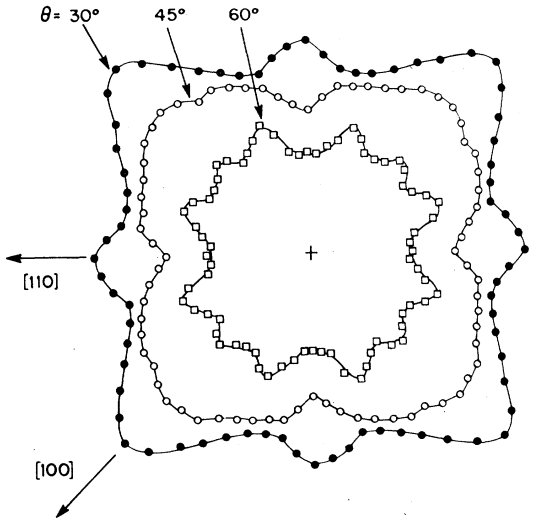

FIG. 2. Radial plots of the azimuthal dependence of emission at $\hbar\omega = 80$ eV from the Te $4d$ levels from Ni(001)-Tec(2×2) at various polar angles.

While the measurements presented above seem likely to be an adequate data base for a unique structural determination, the success of such an approach relies upon our ability to model the data by theoretical calculations. We have therefore initiated a project to perform such calculations, using a scheme described elsewhere.[13] Preliminary calculations have been done so far for the Na $2p$ emission from a $c(2\times2)$ overlayer. The calculations include full multiple scattering.[14] The details of the Ni and Na phase shifts, the complex inner potential, and the structural parameters will be presented in a future publication. The important point as far as this discussion is concerned is that these parameters are nonadjustable, and are determined by previous LEED investigations.[9,10,15]

The results of the calculations for Na at $\hbar\omega = 80$ eV and $\theta = 30°$ are compared with the experimental data in Fig. 3. The overall agreement is quite good. Not only are the main lobes along the ⟨100⟩ azimuths predicted, but the secondary substructure within these lobes is also well reproduced. This level of agreement is clearly encouraging, and further calculations are in progress on both Na and Te on Ni(001) to assess the sensitivity of the model to both structural and nonstructural parameters.

In summary, we have demonstrated, both ex-

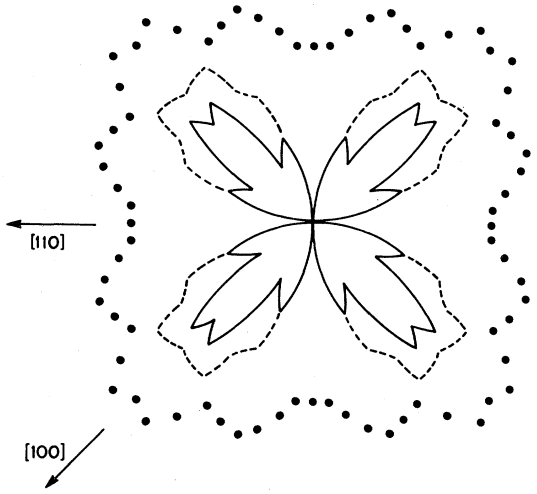

FIG. 3. Comparison between theory and experiment for the azimuthal dependence of emission from the Na $2p$ levels for Ni(001)-Nac(2×2) at $\hbar\omega = 80$ eV and $\theta = 30°$. The full circles are the calculated intensities. The full curve represent the same data with a minimum value subtracted. The dashed curve is the corresponding mirror-symmetrized experimental data.

perimentally and theoretically, strong prospects for a new technique, photoelectron diffraction, in the determination of surface structures.

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Coexistence of Antiferromagnetism and Superconductivity: A Neutron Diffraction Study of $DyMo_6S_8$

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Although $DyMo_6S_8$ is a superconductor below $T_c = 2.05$ K previous studies of the resistivity, susceptibility, and upper critical field strongly suggest the development of magnetic order at $T_M = 0.4$ K. The present neutron study shows conclusively that this superconducting compound also develops coexistent long-range (greater than 300 Å) antiferromagnetic order at T_M. The Dy atoms form a simple cubic sublattice (with a slight rhombohedral distortion) in which the observed magnetic structure consists of (100) planes with moments of $8.77\mu_B$ alternately parallel and antiparallel to the [111] direction.

Two classes of ternary compounds are known to become superconducting in spite of the fact that the compounds have a rare earth with a large magnetic moment as one of their constituent elements.[1-3] More dramatically two materials,[4,5] $ErRh_4B_4$ and $HoMo_6S_8$, undergo phase transitions below T_c in which they resume normal conductivity and develop magnetic order. Neutron scattering experiments[6,7] have (1) demonstrated that both materials are ferromagnets with long-range order, (2) identified the spin direction, and (3) measured the temperature-dependent spontaneous magnetization. Although these studies showed some evidence of a small temperature interval

