was estimated from the elastic scattering above T_N by fits to (6) followed by estimates of the critical scattering using the scaling laws. After a few iterations, β converged at $\beta = 0.36 \pm 0.02$, in agreement with the theoretical value of $\beta \sim 0.38$ calculated to second order in ϵ.[4] The $(1-q, 0, 0)$ intensity is consistent with (5) $(2\beta = 1 \pm 0.3)$, but inconsistent with (6), thus confirming that the peak arises from a second-order coupling to the order parameter that only exists for the "triple-$\vec{q}$" structure. The possibility of multiple-scattering effects involving two magnetic satellites was ruled out by experimental tests and calculation.

The four parameters giving the magnitude and phase of the spins in the different layers, and the four parameters giving the corresponding lattice distortions still remain to be determined. Although intensities of approximately forty independent satellites are available this is a considerable numerical problem. Preliminary attempts indicate that $\mu_c \sim \mu_z \sim (10-20)\%$ of μ_h with $\theta \sim 180°$, and that the basal-plane lattice distortions are of the order of a few percent. The numerical problem may be somewhat reduced by deducing the ratio between the magnetic and the nonmagnetic contribution to each satellite from polarized-neutron data. A very interesting experiment would be to measure directly the lattice distortion by means of x-ray scattering.

We are indebted to S. M. Shapiro for communicating his unpublished elastic neutron diffraction data to us. These data agree quantitatively with ours. We acknowledge fruitful collaboration with P. Å. Hansen and B. D. Rainford, just as we are grateful to B. D. Rainford for the loan of one of the neodymium crystals.

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Effect of Refraction of *p*-Polarized Light on Angle-Resolved Photoemission from Surface States on Metals

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(Received 8 December 1977)

It is suggested that the suppression of normal photoemission from surface states on a W(100) surface near the plasma frequency is due to refraction effects. Two model calculations are presented which are expected to bracket the real situation, and they both exhibit this property. Possible additional effects of refraction on the photoemission cross section are discussed.

It was reported in two recent Letters[1,2] that the angle-resolved photoemission in the direction of the surface normal from the surface state(s) of W(100) is strongly suppressed in intensity when the light frequency is close to the plasma frequency of tungsten. We show in this Letter, with the help of two separate model calculations, that the experimental observation can be explained in a simple and natural way when one takes into account the refraction of p-polarized light at the metal surface. To our knowledge, this is the first time that the importance of the electric field distribution in the surface region has been recognized in computing the matrix element for photoemission *from surface states*. As an additional bonus, we find that our calculation can reproduce structures seen in the photoemission cross section from the low-lying (− 4.2 eV with respect to the Fermi energy) surface state[2] of W(100) at frequencies below the plasma frequency.

The importance of refraction of p-polarized light on the spatial distribution of the normal (i.e., z) component of the electric field is well known in classical electrodynamics.[3] This field component is believed to be responsible for normal photoemission from the surface states observed on W(100).[4] We report here two different model calculations on refraction which, between them, ought to bracket a realistic system such as the surface of tungsten. In the first model, the metal is represented by a semi-infinite square well confining its electrons, and its transverse dielectric response is studied exactly within the random-phase approximation (RPA). The model takes into account surface-induced nonlocality[5,6] and anisotropy[7,8] of the dielectric response, but it fails to describe the bulk in a realistic manner. In the second model, the metal is described in the bulk by a complex, frequency-dependent dielectric function $\epsilon(\omega)=\epsilon_1(\omega)+i\epsilon_2(\omega)$, where for ϵ_1 and ϵ_2 we use actual numbers obtained from optical measurements on tungsten.[9] But the dielectric function is assumed to remain local and vary linearly in an imagined surface region ($-a/2 \leq z \leq a/2$) to unity outside the surface. This model gives a reasonably good description of the bulk, including band-structure effects, but a poor description of the surface. In both cases we solve for the normal component of the *entire* electric field near the surface. Angle-resolved photoemission in the z direction from a well-localized surface state may be regarded as a way of monitoring the strength of this electric field. Our calculations show that the z component of the total electric field at the surface decreases dramatically in strength as ω approaches ω_p, thus explaining the experimental observation[1,2] on angle-resolved photoemission. We now discuss the models and their results in some detail.

Model I.—We picture the metal as a semi-infinite jellium with noninteracting electrons which move quantum mechanically in the potential $V(\vec{r}) = -V_0\theta(-z)$, where $\theta(x)$ is the step function. Physically this implies that we ignore crystallinity of the solid, impose the boundary condition of specular reflection of electrons at the surface, and treat the conductivity tensor in RPA. Electrons populate all states of the square well up to the Fermi energy $E_F = -\varphi$, where φ is the work function of the metal. The bulk electron density is $n_0 = k_F{}^3/3\pi^2$, expressed in terms of the Fermi momentum $k_F = [2m(E_F+V_0)/\hbar^2]^{1/2}$. We choose $V_0 = 10.7$ eV and $\varphi = 4.5$ eV for the sake of illustration.[8] The plasmon energy turns out to be $\hbar\omega_p = 9.813$ eV, while the Fermi momentum is $k_F = 1.275$ Å^{-1}. The nonlocal conductivity tensor $\overleftrightarrow{\sigma}_{\vec{Q},\omega}(z,z')$ for this problem is known[7,8] to be diagonal but anisotropic in the limit $Q \rightarrow 0$ where $\vec{Q}$ denotes a two-dimensional wave vector in the x-y plane. For light of wavelength λ and frequency ω incident at an angle θ_i on the surface, $Q=(\omega/c)\sin\theta_i$. Feibelman has solved numerically[6,7] for the z component of the vector potential $\vec{A}_\omega(z) = \vec{A}_{\vec{Q}\rightarrow 0,\omega}(z)$ produced by the refraction of p-polarized light in a similar model, choosing a gauge where the scalar potential is zero and the electric field is given by $\vec{E}_\omega(z) = (i\omega/c)\vec{A}_\omega(z)$. His calculations show that $|A_\omega{}^z(z)|$ has a strong surface peak for $\omega < \omega_p$, and the peak disappears above ω_p. To elucidate the physical origin of this result, we have solved the integral equation obeyed by the vector potential analytically within an effective local approximation, which is permissible in the neighborhood of $\omega = \omega_p$ where $A_\omega{}^z(z)$ is small and slowly varying over the range of nonlocality of $\sigma^{zz}(z,z')$. We find[10] that the surface peak in $|A_\omega{}^z(z)|$ can be explained easily as being a manifestation of the classical singularity[3] in the normal component of the electric field in refraction of p-polarized light by a medium whose dielectric constant vanishes locally. In the absence of symmetry restrictions of a compelling nature, the amplitude of photoemission in the direction of the surface normal will depend on the matrix element of the operator $p^z\tilde{A}_\omega(z)+\tilde{A}_\omega(z)p^z$ taken between the initial and final electronic-state wave functions. Here $\tilde{A}_\omega(z)=A_\omega{}^z(z)/A_0$, and A_0 is the amplitude of the vector potential associated with the incident wave. The surface peak in $A_\omega{}^z(z)$ is naturally reflected in $\tilde{A}_\omega(z)$ as well, and its height may be taken as a crude measure of the photoemission amplitude (i.e., the square root of the differential cross section) without using any detailed form of the relevant wave functions. Figure 1 shows the strength of the surface peak in $|\tilde{A}_\omega(z)|$, which we call $|\tilde{A}_\omega{}^{\text{peak}}|$, as a function of the frequency of light for $\theta_i = \pi/4$ and $\omega < \omega_p$. It is clear from the figure that the effect of refraction is to ensure that photoemission in the normal direction from a surface state will be very weak near the plasma frequency.[1,2]

Model II.—Here we imagine that the metal can

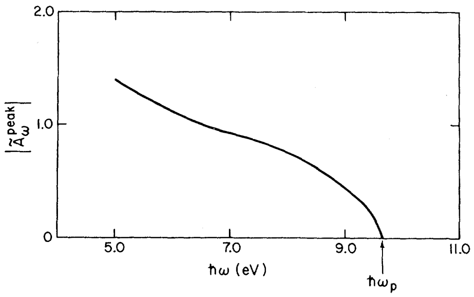

FIG. 1. Plot of $|\tilde{A}_\omega^{\text{peak}}|$, the strength of the surface peak in $|\tilde{A}_\omega(z)|$, as a function of the photon energy $\hbar\omega$ for $\omega < \omega_p$. $\tilde{A}_\omega(z)$ denotes the z component of the vector potential in the long-wavelength limit, normalized by the incident vector potential.

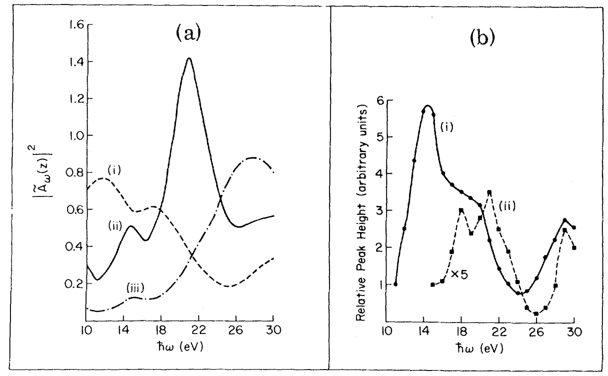

FIG. 2. (a) Theoretical calculations for $|\tilde{A}_\omega(z)|^2$ plotted against photon energy for three planes: (i) $z=a/2$, (ii) $z=0$ (nominal surface), (iii) $z=-a/2$. (b) Cross sections for normal photoemission from the two surface states on W(100): (i) high-lying state at $E_{ss}=-0.4$ eV (full circles are data points from Ref. 1); (ii) low-lying state at $E_{ss}=-4.2$ eV (full squares are data points from Ref. 1). Lines through data points have been drawn for comparison purposes. (Data of Ref. 1 used with permission of authors.)

be represented by a local, frequency-dependent, complex dielectric constant which goes over to the long-wavelength dielectric constant of tungsten in the bulk, and varies linearly in the surface region extending over $-a/2 \leq z \leq a/2$. We make no attempt to specify a except to note that physically it will be of the order of a few angstroms. The dielectric constant is

$$\epsilon_\omega(z) = \epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega), \quad z < -a/2,$$
$$\epsilon_\omega(z) = [1+\epsilon(\omega)]/2 + [1-\epsilon(\omega)](z/a), \quad |z| < a/2,$$
$$\epsilon_\omega(z) = 1, \quad z > a/2,$$

where for $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ we use the data of Weaver, Olson, and Lynch.[9] The problem of refraction of p-polarized light by such a medium is exactly solvable in the limit $a/\lambda \ll 1$, and the result is, for $|z| < a/2$,

$$\tilde{A}_\omega(z) = \frac{A_\omega^z(z)}{A_0} = -\frac{\sin 2\theta_i}{z/a + \frac{1}{2}[1+\epsilon(\omega)]/[1-\epsilon(\omega)]}\,\frac{\epsilon(\omega)/[1-\epsilon(\omega)]}{[\epsilon(\omega) - \sin^2\theta_i]^{1/2} + \epsilon(\omega)\cos\theta_i}. \quad (1)$$

The classical singularity mentioned earlier appears in the surface region if $\epsilon(\omega)$ is real and negative. In general, the modulus $|\tilde{A}_\omega(z)|$ shows a peak in the surface region, whose position is determined by the details of $\epsilon(\omega)$. It is more interesting, however, to consider the variation of $|\tilde{A}_\omega(z)|^2$—the quantity which is involved in photoemission cross-section calculations—with frequency for a fixed z, i.e., on a plane parallel to the surface. Three such curves are shown in Fig. 2(a)—curve (ii) for the nominal surface ($z=0$), and curves (i) and (iii) for the extremities of the surface region ($z=\pm a/2$). Once again we choose $\theta_i = \pi/4$. Insofar as the surface-state wave function is confined largely to the surface region (having a peak on or near $z=0$), is allowed by symmetry to couple to A^z for photoemission in the normal direction, and the final-state effects may be assumed to vary smoothly with energy, the variation of $|\tilde{A}_\omega(z)|^2$ with ω on the surface plane [curve (ii)] should mirror the frequency dependence of angle-resolved photoemission from the surface state. Curves (i) and (iii) are of importance to understand how the spatial extent of the initial-state wave function may affect this argument.

The most significant feature of curve (ii) of Fig. 2(a) is the pronounced minimum in the neighborhood of the plasmon energy of tungsten. Since a plasmon is not well characterized in a transition metal like tungsten, we have chosen to define plasma frequency as the frequency ω_p at which $\epsilon_1(\omega)$ vanishes. From the experimental data[9] used in computing the curves of Fig. 2(a), $\hbar\omega_p = 24.7$ eV and $\text{Im}[\epsilon^{-1}(\omega)]$ also has a (rather broad) peak at this energy. The experimental results[1] for normal photoemission from the surface states on W(100) are shown in Fig. 2(b) for comparison, and one observes a pronounced dip in the 24–26-eV range in both cases. Furthermore, the theoretical curve for $|\tilde{A}_\omega(z=0)|^2$ shows additional structures in the 14–18-eV range, including a dip around 16 eV, which correlate qualitatively with similar structures observed at slightly higher energies in the experimental curves. These correlations suggest that refraction effects are of importance in photoemission from tungsten surface states. They also indicate that the surface states are well localized in space, existing mostly near the $z=0$ plane. For a broad surface state, or a state whose wave function peaks at the edges of or outside the surface region, one would need an appropriate average of curves (i)–(iii) of Fig. 2(a), and this may render invalid conclusions regarding the photoemission cross section based solely on curve (ii) because curve (iii) differs from it qualitatively near $\omega = \omega_p$. It is interesting to note that the photoyield curve for the high-lying surface state resembles more closely the theoretical curve for $z=a/2$, leading one to speculate that the corresponding wave function may have more weight toward the vacuum side of the nominal surface. We are currently investigating in detail the effects of the location and spatial extent of the surface-state wave function on the cross section for normal photoemission.

The comparison of the experimental results of Fig. 2(b) with theoretical calculations for $|\tilde{A}_\omega(z)|^2$ is reasonable in view of the experimental fact[4] that normal photoemission from both surface states on W(100) is excited by A^z. According to Hermanson's arguments[11] based on symmetry considerations, this would imply that both the surface states are of Δ_1 character (Δ_6 if spin-orbit coupling is taken into account). Theoretical calculations on the unrelaxed tungsten surface[12] agree with this conclusion for the low-lying surface state, but are at variance with it for the high-lying one. Surface relaxation is known to push up the *sp-d* band-gap surface state Δ_1 symmetry to higher energies for both W[13] and Mo,[14] but the surface contraction necessary is considerably larger than that found experimentally for tungsten.[15] Thus, even though the theoretical situation remains unclear, we feel that our procedure is justified by experimental observations on photoemission. We therefore conclude that refraction of light can explain certain features of the normal photoemission data from surface states of W(100), although one must invoke final-state effects for a completely satisfactorily understanding of the entire data.

This research project was partially supported by the National Science Foundation under Grant No. DMR76-82128. One of the authors (A.B.) wishes to acknowledge a Faculty Research Award of the General Research Board of the University of Maryland for the period when the work was initiated. Thanks are due to the Computer Center of the University of Maryland for generously making their computing facilities available to us.

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