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Angle-Dependent Photoionization Cross Sections of Cu

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It is shown that the positions of the peaks in the angle-resolved photoemission spectra from a Cu(111) surface for $h\nu = 11.6$–40.8 eV are predicted reasonably well by the initial-state band structure and a single-plane-wave final state, but the strengths of the peaks are described by atomiclike dipole selection rules.

The free-electron final-state (FEFS) model predicts the positions of the peaks in the angle-resolved photoemission spectra of the noble metals reasonably well for $h\nu = 11$–200 eV,[1-4] but it does not predict correctly the observed strengths of the peaks.[1,5] Constant matrix elements appear to explain the peak strenghts better than plane-wave matrix elements,[1,6,7] but there has been no theoretical justification for them. It has been suggested recently[8] that since the photoionization matrix element is predominantly due to the spherically symmetric atomic potential,[5] its angular behavior ought to be governed by atomiclike dipole selection rules.

In this Letter, we show that the angle-resolved photoemission spectra from a Cu(111) surface for photon energies ranging from 11 to 40 eV can be explained by a FEFS model in which the atomic photoionization cross sections calculated by plane waves are replaced by those based upon atomic dipole selection rules.

In the angle-resolved photoemission experiment, the magnitude of the component of the momentum of the photoelectron parallel to the smooth surface, $k_{\parallel}$, which is conserved as the electron passes from the solid into the vacuum, is given by[9]

$$k_{\parallel} = (2mE/\hbar^2)^{1/2} \sin\theta_e, \tag{1}$$

where E is the measured kinetic energy of the photoelectron, θ_e is the polar angle of emission, and m is the free-electron mass.

Inside the solid, the energy dispersion of the photoelectron with momentum $\vec{k}_f$ is

$$E_f(\vec{k}_f) = \hbar^2 k_f^2/2m^* = E + W, \tag{2}$$

which yields, in terms of $k_{\parallel}$, the component of the momentum perpendicular to the surface

$$k_{\perp} = \{[2m^*(E+W)/\hbar^2] - k_{\parallel}^2\}^{1/2}, \tag{3}$$

where W is the inner potential and m^* is the effective mass of the internal photoelectron, which is close to, but not necessarily equal to, the mass of the free electron.

Including the finite mean free path of the photoelectron, the photoemission spectrum according to the free-electron final-state model is[10]

$$I(E, \vec{k}_{\parallel}, \vec{\epsilon}) \propto \sum_n \int_{-\infty}^{\infty} \sigma_n(\vec{k}, \vec{\epsilon})\, \delta(E_f(\vec{k}_f) - E_n(\vec{k}) - \hbar\omega)[\Gamma^2 + (k_{\perp}' - k_{\perp})^2]^{-1} dk_{\perp}', \tag{4}$$

where $\vec{k} = \vec{k}_{\parallel} + \vec{k}_{\perp}'$, $\Gamma = (l \cos\theta_i)^{-1}$, l is the mean free path of the photoelectron, θ_i is the angle between $\vec{k}_f$ and the normal to the surface, $\vec{\epsilon}$ is the direction of the electric field of the photon, and $\sigma_n(\vec{k}, \vec{\epsilon})$ is the photoionization cross section of the atomic orbital corresponding to band n, and n extends over all of the filled valence states. The Lorentzian factor in Eq. (4) accounts for the weakening of the conservation of the component of the photoelectron momentum perpendicular to the surface due to the finite mean free path of the photoelectron.[9,10] The energy dispersion of the initial state, $E_n(\vec{k})$, we take to be periodic in $\vec{k}$ space, while the energy dispersion of the photoelectron is given by Eq. (2). The initial-state energies and eigenfunctions were computed in a tight-binding two-centered approximation using five d orbitals and one s orbital. The interaction parameters were adjusted to obtain good agreement with the results of Smith and Mattheiss,[11] and Janak, Williams, and Moruzzi.[6]

The plane-wave final-state model predicts the photoionization cross section of the atomic orbital, $\varphi_{n,\vec{k}_i}(r)$, to be[10]

$$\sigma_n(\vec{k},\vec{\epsilon}) = (\vec{k}\cdot\vec{\epsilon})^2 |\tilde{\varphi}_n(\vec{k})|^2, \tag{5}$$

where

$$\tilde{\varphi}_n(\vec{k}) = \int \varphi_{n,\vec{k}_i}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}\, d^3r. \tag{6}$$

As discussed by Bethe and Salpeter,[12] the plane-wave final-state model fails to give the correct angular dependence of the photoionization cross section for a single atomic potential; inspection of Eqs. (5) and (6) shows that only initial atomic orbitals having projections of angular momentum $m=0$ with respect to the direction of propagation of the photoelectron can contribute to the spectra. It has been suggested that since the primary contribution to the photoionization cross section comes from regions of the wave in the vicinity of the atomic cores,[5,8] where the true final-state wave function has spherical rather than planar symmetry, atomiclike dipole selection rules[13] (i.e., $\Delta l = \pm 1$, $\Delta m = 0, \pm 1$) ought to govern the angular behavior of the photoionization cross sections in the solid. When the true final state is approximated well by a single orthogonalized plane wave (OPW) or an augmented plane wave (APW), it contains only spherical harmonics for which $m=0$ with respect to the direction of propagation.[14] The atomic dipole selection rules tell us that initial states having $m = 0, \pm 1$ can couple to the final state, in contrast to the prediction of the plane-wave final-state model for which the $m = \pm 1$ initial states cannot be photoexcited. Using the atomic selection rule on m, we find that the general form of the polarization and directional dependence of the atomic matrix element for d orbitals must be[15]

$$\sigma_n(\vec{k},\vec{\epsilon}) \propto |\vec{\epsilon}\cdot\vec{P}_n(\vec{k})|^2, \tag{7}$$

where $\vec{P}_n(\vec{k})$ is a "polarization vector" of the d orbital given by

$$\vec{P}_n(\vec{k}) = \hat{x} C_{zx}{}^n(\vec{k}) + \hat{y} C_{zy}{}^n(\vec{k}) + \hat{z}\xi C_{z^2}{}^n(\vec{k}), \tag{8}$$

where the $C^n(\vec{k})$'s are the coefficients of the five atomic d orbitals defined in the following coordinate system. The z axis is taken to be in the direction of the momentum $\vec{k}$. The y axis is perpendicular to the z axis but lies in the plane containing $\vec{k}$ and the Poynting vector of the incident photons. The remaining x axis is perpendicular to both the z and y axes. The z component of $\vec{P}_n(\vec{k})$ corresponds to optical transitions for which $\Delta m = 0$, and the x and y components correspond to the transitions for which $\Delta m = \pm 1$. The quantity ξ, the ratio of the $m=0$ to $|m|=1$ photoionization matrix elements, depends upon the relative importance of the $l \to l+1$ and $l \to l-1$ optical transition channels. When only one channel dominates, its value is close to one.[13] For the present case in which the $d \to p$ channel was assumed to dominate, $\xi = 2/\sqrt{3}$.[13] For the unpolarized light used in our experiments, the angular dependence of the photoionization cross section as determined from Eq. (8) is given by

$$\langle \sigma_n(\vec{k},\vec{\epsilon})\rangle \propto [\xi C_{z^2}{}^n(\vec{k}) \sin\beta + C_{zy}{}^n(\vec{k}) \cos\beta]^2 + |C_{zx}{}^n(\vec{k})|^2, \tag{9}$$

where β is the angle between $\vec{k}$ and the Poynting vector. We have also assumed that the photoionization cross section of the s orbital is negligible compared to those of the d orbitals.

Angle-resolved photoemission spectra were taken on a single-crystal Cu(111) surface using photons of energies 11.8, 16.9, 21.2, 26.9 and 40.8 eV incident upon the sample at an angle of 45° with respect to the surface normal. The spectrometer had an energy resolution of 0.15 eV and an angular acceptance of ± 2°.

We show in Figs. 1 and 2 the experimental data as the solid lines for several photon energies and polar angles adjusted so that the magnitude of $\vec{k}_{\parallel}$ as given by Eq. (1) for initial states with a 3-eV binding energy remains the same for all

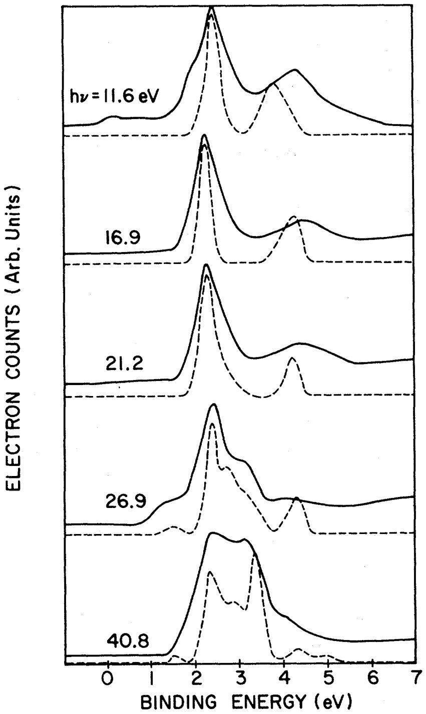

FIG. 1. Experimental (solid line) and theoretical (dashed line) photoemission spectra from a Cu(111) surface for several photon energies indicated. The *K* point in the Brillouin zone lies closest to the analyzer.

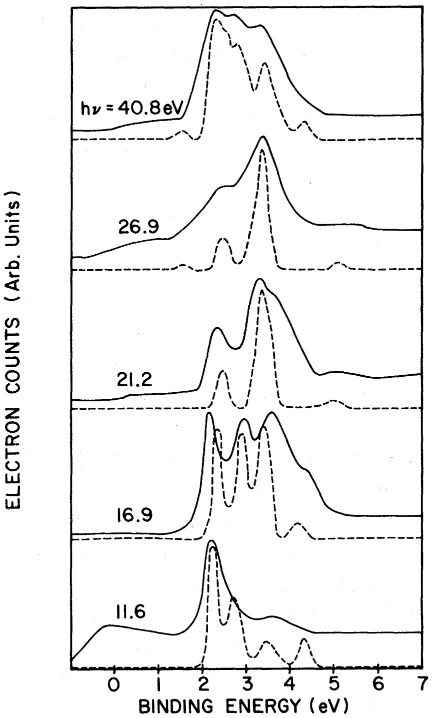

FIG. 2. Experimental (solid line) and theoretical (dashed line) photoemission spectra from a Cu(111) surface for several photon energies indicated. The *U* point in the Brillouin zone lies closest to the analyzer.

spectra. The two azimuthal orientations of $\vec{k}_\parallel$ were chosen so that $\vec{k}_\perp$ must lie on a line connecting the *U* and *K* points lying on opposite hexagonal faces of the Brillouin zone. The spectra have been plotted in a sequence in which the $\vec{k}_\perp$, as given by Eq. (2), moves from near the *U* point at the top of Fig. 1 to the *K* point at the bottom of Fig. 2. We observed that if the one-dimensional density-of-states model were valid and all points with the same $\vec{k}_\parallel$ were allowed to contribute at the same photon energy,[16,17] then all of the spectra in Figs. 1 and 2 would be essentially the same, aside for variations in the photon-energy and directional dependence of the atomic photoionization cross sections. Clearly, the experimental data show that this model does not apply to Cu.

The spectra computed from the model described above are shown as the dashed lines in Figs. 1 and 2. They have been broadened by 0.3 eV to simulate instrumental resolution and lifetime effects. In locating $\vec{k}$ for the spectra, the effective mass of the photoelectron was taken to be 8% less than the free-electron value in order to simulate the effects of exchange and correlation computed by Janak, Williams, and Moruzzi.[6] The value for *W* of 14.7 eV found from the position of the bottom of the *s* band as calculated in Ref. 6 was used initially in our computations. However, we found that a value of the inner potential of 12.2 eV used in low-energy electron-diffraction (LEED) studies[18] gave better agreement between theory and experiment. This change in the inner potential which resulted in a change in $\vec{k}_\perp$ of about 10% at low photon energies had an appreciable effect on the spectra obtained for $h\nu = 26.9$ eV in Fig. 1 and $h\nu = 11.6$ and 16.9 eV in Fig. 2. The contributions to these spectra were found to originate from regions in the Brillouin zone where the initial band structure was varying very rapidly with $k_\perp$. We can offer no insight into why the inner-potential estimate from LEED studies gives better results than those estimated from band theory.

Considering that our simple initial-state band structure has limited accuracy and that the energy of the final electron state might be perturbed by the crystal potential away from the free-electron energy dispersion, particularly at low-photon energies, the basic agreement between theory and experiment is quite good. Spectra computed with plane-wave and constant matrix elements gave poor agreement with experiment. We note that agreement with experiment would be improved if the theoretical spectra were convoluted with an asymmetric energy-broadening function.

One notable success of the present model is the predicted strength of the peak near 5 eV of binding energy occurring in Fig. 2. We find that this peak is 80% d like, but it occurs weakly since it has mostly $m=2$ character. The relative strength of this peak should increase when the photon energy and angle of emission are chosen so that $\vec{k}_i$ and $\vec{k}_f$ are perpendicular to each other.

We have thus demonstrated that the details of the final-state band structure are not terribly important and that a simple model based upon the free-electron–like energy dispersion and atomic-like dipole selection rules provides a good description for the angle-resolved photoemission spectra of Cu and possibly of other noble and transition metals. Complications due to many-body effects, the surface potential, multiple scattering, and surface bands seem to be unimportant for describing the spectra.[17] The success of the model introduced here opens the possibility of using experimental peak positions to map out the energy bands, and the experimental peak strengths and the polarization dependence to determine the orbital composition of the initial states.

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Voltage Measurements within the Nonequilibrium Region near Phase-Slip Centers

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We have used complementary sets of normal and superconducting probes to study the nonequilibrium region near phase-slip centers in narrow superconducting strips. An exponentially decaying branch imbalance potential, μ_Q, is observed and the decay length, the quasiparticle diffusion length, is measured directly and compared to the phase-slip resistance.

In recent studies[1-5] of the current-voltage (I-V) characteristics of narrow superconducting strips and microbridges, a significant role is attributed to the quasiparticles generated at localized resistive regions or "phase-slip centers" in the superconductor. It is concluded that R_D, the differential resistance of a phase-slip center above the critical current, and the range of phase-slip center interactions are determined by the quasiparticle diffusion length. This length is $\lambda_Q \cong (v\tau_Q l)^{1/2}$,