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[14]The unsymmetric error estimate quoted allows for the possibility that some e^+ might not escape from the surface as Ps at high temperatures. The Ps formation was also measured in a separate experiment which used a Ge(Li) detector. The relative intensities of the background-subtracted 511-keV photopeaks were found to be 0.466(5), 0.764(7), and 1.00(1) for (1) a Ge(111) target at 1000 K, 32-eV e^+, (2) the same target but with 1490-eV e^+ incident, and (3) an unclean Al target at 300 K, extrapolated to high-energy e^+ as $1/E$. This results means that 53% of the annihilations were via 3γ for low-energy e^+ on Ge at 1000 K and that the Ps fraction is not less than $\frac{4}{9}\times 53\% = 71\%$. The photopeak for 32-eV e^+ on Ge at 1000 K was found to be redshifted 100 ± 20 eV compared to the photopeak for 1490-eV e^+ on the same target. The shift is interpreted as a Doppler shift from $^1S_0$ Ps emitted from the target surface and receding from the detector as expected. The Ps energy is estimated to be about 1 eV. With such energies, it would not be unreasonable if one-quarter of the $^3S_1$ Ps annihilated via 2γ's because of wall collisions, thus accounting for the 53% 3γ yield at what appears to be $f = 98$.
[15]In the approximation that $dE/dx \propto 1/E$, the total path length S will be $S \propto \int_0^E E'\,dE' \propto E^2$. The mean penetration depth a will be less than S because the path is not a straight line. If the number N of collisions which significantly change the momentum direction is proportional to S, we then have $a \approx S/\sqrt{N} \propto E$.
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Azimuthal Anisotropy in Core-Level X-Ray Photoemission from $c(2\times2)$ Oxygen on Cu(001): Experiment and Single-Scattering Theory

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(Received 23 August 1978)

Azimuthal anisotropies in core-level x-ray photoemission from $c(2\times2)$O on Cu(001) have been found to show a strong dependence on polar emission angle. The anisotropies observed are $\Delta I/I_{max} \lesssim 24\%$ for O 1s emission, and $\lesssim 41\%$ for Cu $2p_{3/2}$ and Cu $3p$ emission. A single-scattering theoretical model is found to describe well both the O and Cu data, and suggests that O is present in fourfold coordination sites for which the O atoms are coplanar with the Cu surface atoms.

Kono, Fadley, Hall, and Hussain (KFHH)[1] have recently reported the first observation of azimuthal anisotropies in deep core-level x-ray photoemission from adsorbed atoms, specifically $c(2\times2)$O on Cu(001), and qualitatively discussed the utility of a single-scattering theoretical model for interpreting such data. In the present study, a higher-resolution and much-more-detailed set of azimuthal scans for both O and Cu levels at various polar angles is considered. The experimental data are found to compare favorably with quantitative theoretical calculations involving a single-scattering model, and the adsorbate bonding geometry is determined.

The experimental procedure has been discussed in KFHH.[1] Unpolarized Al $K\alpha$ radiation (1487 eV) was used for excitation. The polar emission angle θ is measured with respect to the surface, and the azimuthal angle φ with respect to the [100] crystal axis. A 1200-L (1 L = 10^{-6} Torr sec) exposure of oxygen was used to produce the $c(2\times2)$ structure (as verified by low-energy electron diffraction). Azimuthal scans were made for both the substrate peaks Cu $2p_{3/2}$ (E_{kin} = 551 eV) and Cu $3p$ (1408 eV) and the adsorbate O 1s peak (951 eV). Data processing involved the two-step procedure of fourfold averaging via $I = I(\varphi) + I(\varphi + 90°) + I(\varphi + 180°) + I(\varphi + 270°)$ and a subtraction of the minimum intensity. The resulting "flower patterns" amplify anisotropy and minimize spurious sources of nonfourfold anisotropy,[1] as shown for O 1s in Fig. 1.

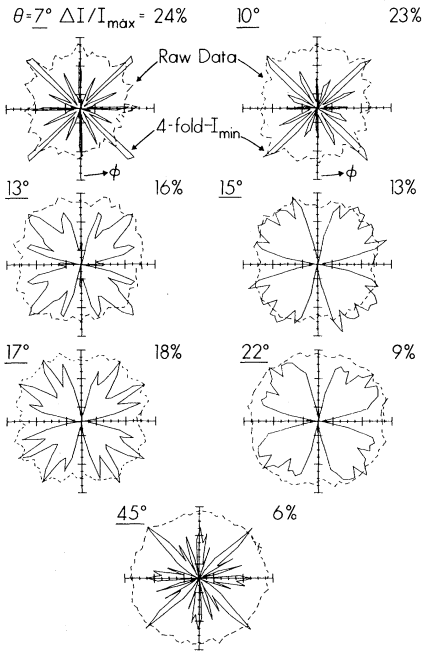

FIG. 1. Azimuthal distributions of O 1s photoelectron intensity for $c(2\times2)$O on Cu(001) at seven polar angles between 7° and 45°. θ is measured with respect to the surface. Both the raw data (dashed curves) and data subjected to a fourfold averaging and minimum subtraction (solid curves) are shown. The percentage anisotropy as determined from $\Delta I/I_{max}$ is indicated for each polar angle.

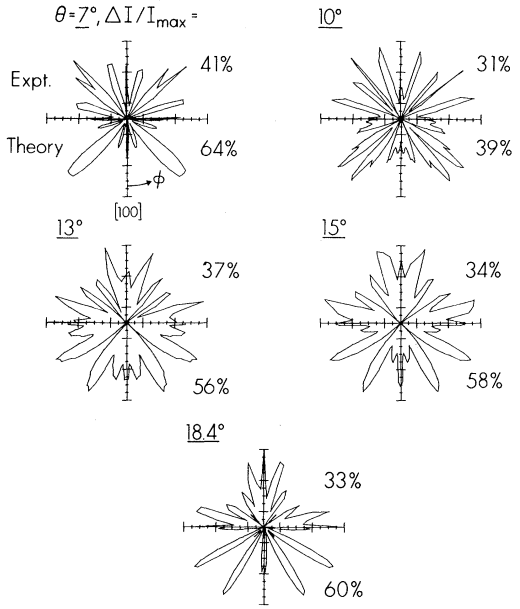

FIG. 2. Comparison of the fourfold-minus-I_{min} experimental and theoretical azimuthal distributions of Cu 3p intensity for a clean Cu(001) surface at five polar angles between 7° and 18.4°. Experiment is in the upper half of each figure, theory in the lower half. The percentage anisotropies are indicated for both experiment and theory. A full inner potential of 14.1 eV was used in all calculations.

The O 1s data in Fig. 1 exhibit several significant features. The resolution of fine structure is better than in KFHH[1] because of longer counting times and better near-surface crystalline order. Peak widths and positions change markedly with changes in polar angle. This sensitivity to θ was not noted in prior work[1] and suggests a strong dependence of the observed anisotropy on interference effects. It further indicates that an interpretation in terms of peaks pointing very nearly at neighboring atoms along the surface[1] is somewhat oversimplified. Finally, the marked decrease in anisotropy from $\Delta I/I_{max} = 24\%$ at $\theta = 7°$ to $\lesssim 6\%$ at $\theta = 45°$ confirms that small-angle-scattering events are primarily responsible for such effects.[1] In later comparisons with theory, attention will be limited to the range $7° \lesssim \theta \lesssim 18°$ for which anisotropies are $\gtrsim 15\%$.

In the upper halves of each plot in Fig. 2 are shown fourfold-minus-I_{min} azimuthal data for the Cu 3p intensity from a clean surface. The anisotropies here are as much as 1.7 times larger than those in O 1s at the lowest θ values and, furthermore, they are relatively constant with θ at 30–40%. Similar degrees of anisotropy and pattern sensitivity to θ are also found in Cu $2p_{3/2}$ azimuthal data over the same θ range.[2]

The basic features of the single-scattering model that we will now test against this experimental data have been discussed previously by McDonnell, Woodruff, and Holland[3] in connection with angle-resolved Auger emission and by Lee[4] in connection with angle-resolved photoemission, although a few additional modifications have been necessary to permit direct application to the cases at hand. The basic assumptions of the model are as follows: (1) The matrix elements describing the initial excitation step are assumed to have directional dependence as given by excitation from a filled core subshell to a plane-wave final state,[4,5] namely, $\hat{\epsilon}\cdot\hat{k}$, where $\hat{\epsilon}$ is the unit polarization vector of the radiation and $\hat{k}$ is a unit vector along the electron emission direction. (2) A single-scattering or kinematical approximation is used, with the scattering from the jth atom being described fully by a complex scattering factor $f_j(\theta_j) = |f_j(\theta_j)| \exp i\Psi_j(\theta_j)$ which is determined from 21 partial-wave phase shifts

as calculated by Pendry with an approximate allowance for the redistribution of valence electronic charge in bond formation.[6] However, the purely atomic scattering factors of Fink and Ingram[7] are found to yield essentially identical results. (3) Attenuation of the measured "no-loss" intensities by inelastic scattering is included by assuming an *isotropic* exponential decay of wave *amplitudes* along path length of $\exp(-\gamma L)$, where $\gamma = 1/(2\Lambda_e)$, Λ_e is the inelastic attenuation length for *intensities*, and L is the relevant path length from primary emitter to the surface or from emitter to scatterer j to the surface. Λ_e was taken to be 15.0 Å at 1482 eV and to scale as $(E_{\rm kin})^{1/2}$.[8] The surface cutoff of inelastic scattering was arbitrarily assumed to occur in a plane located at the Cu hard-sphere radius of 1.28 Å above the atomic centers in the (001) surface. Variations of Λ_e by $\pm 25\%$ were fortunately not found to influence significantly the predicted anisotropies. (4) The effects of vibrational motion are incorporated by inserting a Debye-Waller factor (DW) in each intensity term involving wave interference.[3] This DW factor is given by $\exp[-2k^2(1-\cos\theta_j)\overline{U_j^2}]$, with k equal to the magnitude of the electron wave vector $\vec{k}$ and $\overline{U_j^2}$ the mean-square displacement of the jth atom with respect to the emitter. The values used for $\overline{U_j^2}$ were 0.0108 Å^2 in the surface atomic layer (including adsorbate atoms) and 0.0065 Å^2 in below-surface Cu layers.[9] However, the values chosen for $\overline{U_j^2}$ could be increased by as much as a factor of 4 without significant effect on anisotropies, because $f_j(\theta_j)$ is large only at very low θ_j values for which the DW factor ≈ 1 as a result of the $(1-\cos\theta_j)$ factor in the exponential. (5) Only scattered waves emanating from a finite cluster of atoms were included, with the cluster size being increased until no important alterations in the predicted anisotropies were introduced by additional atoms. For O 1*s* emission, the O layer and two Cu layers totaling 119 atoms were used. For Cu $2p_{3/2}$ and Cu $3p$ emission, six Cu layers totaling 266 atoms were included. (6) The inner potential V_0 at the surface is assumed to cause only slight electron refraction. A reasonable V_0 for copper is 14.1 eV,[10] with which refraction is $\lesssim 4.5°$ for the cases considered here. For adsorbate emission, the full inner potential also may not be appropriate[6] and added calculations have thus been performed at the extreme limit of no refraction ($V_0 = 0$). (7) In order to approximate closely the actual experimental geometry, intensities have been summed over the various polarizations $\hat{\epsilon}$ in the unpolarized source and over five directions $\vec{k}$ within the spectrometer solid angle (a cone of 3.5° half-angle). The final expression for intensity $I(\vec{k})$ thus can be written

$$I(\vec{k}) = C\sum_{\vec{k}}\sum_{\hat{\epsilon}}\left(\left|\hat{\epsilon}\cdot\hat{k}\exp(-\gamma L) + \sum_j \hat{\epsilon}\circ\hat{r}_j \frac{|f_j(\theta_j)|}{r_j}\exp[ikr_j(1-\cos\theta_j)+i\Psi_j]\exp(-\gamma L_j)\exp[-2k^2(1-\cos\theta_j)\overline{U_j^2}]\right|^2 + \sum_j(\hat{\epsilon}\circ\hat{r}_j)^2\frac{|f_j(\theta_j)|^2}{r_j^2}\exp(-2\gamma L_j)\{1-\exp[-4k^2(1-\cos\theta_j)\overline{U_j^2}]\}\right),$$

where $\vec{r}_j$ is the coordinate of scatterer j relative to the primary emitter, $kr_j(1-\cos\theta_j)$ is the phase difference due to path-length difference, and the final summation over j allows for the fact that the DW factor is not needed in interference terms involving a single scattering center.[3]

The results of theoretical calculations based upon this model for Cu $3p$ emission from a clean (001) surface for which the atomic geometry is very well defined are shown in the lower halves of the plots in Fig. 2. There is, in general, very good agreement between experiment and theory as to peak positions and relative intensities, as well as to changes in fine structure with θ. Only for $\theta = 18.4°$ and directions equivalent to $\varphi \approx 13.8°$ are observed peaks missing in the theoretical curve, but even here, closer inspection shows that weak peaks are predicted at the correct angles. The theoretical anisotropies $\Delta I/I_{\rm max}$ are in all cases significantly higher than those observed, ranging from 1.3 to 1.8 times the experimental values. Such discrepancies could be due to deviations from ideal atomic geometry at a certain fraction of the emitting or scattering sites, nonisotropic *inelastic* scattering,[1] or finite cluster size. A similar comparison of experiment and theory for Cu $2p_{3/2}$ emission yields a corresponding degree of agreement.[2] Expanding or contracting the first atomic layer spacing by $\pm 5\%$ as might be consistent with prior LEED analyses of Cu(001)[11] gave no significant changes in either Cu $3p$ or Cu $2p_{3/2}$ patterns. From these and other comparisons,[2] we conclude that the single-scattering model provides a good first-

order description of the observed azimuthal anisotropies in XPS (x-ray photoemission spectroscopy) core-level emission from clean Cu(001) for $7° \lesssim \theta \lesssim 15°$, and the application of this model to adsorbate emission is encouraged.

The bonding geometry of $c(2\times2)$O on Cu(001) is not known for certain.[1,11] The two most plausible choices are coordination in fourfold holes in the (001) surface or a reconstruction with O atoms replacing every other Cu atom in the (001) surface.[11] Within either of these choices, the vertical or z position of the O atoms with respect to the Cu-atom centers constitutes the only geometric variable. Theoretical calculations of O 1s intensities have thus been performed for the full range of physically reasonable z positions in both the fourfold and reconstructed geometries.[2] The only geometry for which *all* major peaks and minima over the range $7° \lesssim \theta \lesssim 17°$ are correctly predicted is fourfold-hole coordination in which the O atoms are coplanar with the Cu atoms (that is, $z = 0.0$ Å), as shown in the comparison of Fig. 3. Even in the extreme limit of a zero inner potential (dotted curves), all major features are still correctly predicted. Although theory overestimates anisotropy by 2.7–4.6 times, this could be due to the same reasons discussed above for Cu emission. By contrast, positioning fourfold-coordinate O atoms *above* the Cu plane at a 1.0-Å distance consistent with prior LEED (low-energy electron diffraction) analyses of $c(2\times2)$O on Ni(001)[12] *or* typical Cu-O bond lengths of 1.9–2.1 Å[13] yields very poor agreement with experiment for $\theta = 10°$, 13°, and 15°. The optimum O position in the reconstructed geometry as judged by agreement with experiment is 0.2 Å *below* the Cu plane; theory in this case coincides well with experiment for $\theta = 7°$, 10°, and, to a lesser degree, 13°, and 17°, but there are serious discrepancies for $\theta = 15°$. For all cases studied, the predicted anisotropies furthermore were insensitive to reductions in the number of O atoms as long as all nearest neighbors to the emitter were retained. Thus, within the accuracy of this theoretical model, a clear choice of the coplanar fourfold geometry of Fig. 3 is possible and the optimum z position furthermore could be selected to $\sim \pm 0.1$ Å. The plausibility of this geometry is further enhanced by noting that it requires five Cu-O bond distances of 1.81 Å (four in the surface plane, one to the next plane below) that are not much shorter than the 1.84-Å distances in crystalline Cu_2O.[14] The use of such XPS data for a variety of surface-structure determinations thus seems possible, although it is still important to assess the influence of additional corrections due to surface nonidealities, cluster size, multiple-scattering effects, and nonisotropic inelastic scattering.

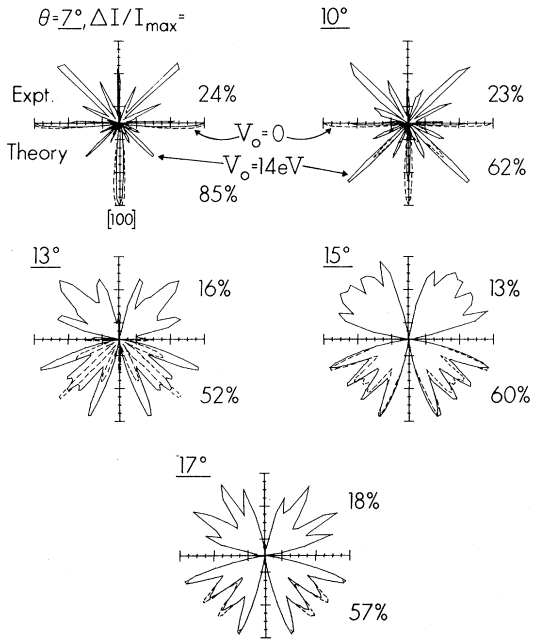

FIG. 3. Same as Fig. 2, but for O 1s emission from $c(2\times2)$O on Cu(001). Theoretical curves are for O atoms in fourfold holes at a z position coplanar with the surface Cu atoms. Solid curves correspond to full refraction ($V_0 = 14.1$ eV), dashed curves to no refraction ($V_0 = 0$).

We are indebted to J. B. Pendry for providing us with the phase shifts and Z. Hussain for preparing the single crystals. The support of the National Science Foundation (Grant No. CHE76-24506) and The Petroleum Research Fund of the American Chemical Society is also gratefully acknowledged.

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ERRATA

BÄCKLUND TRANSFORMATION FOR THE ERNST EQUATION OF GENERAL RELATIVITY. B. Kent Harrison [Phys. Rev. Lett. 41, 1197 (1978)].

In Eq. (19), the $\frac{1}{2}$ on the right-hand side should be replaced by $\frac{1}{4}$. In Eq. (22), both appearances of $\frac{1}{2}$ should be replaced by $\frac{1}{4}$.

K_S REGENERATION ON ELECTRONS FROM 30 TO 100 GeV/c: A MEASUREMENT OF THE K^0 CHARGE RADIUS. W. R. Molzon, J. Hoffnagle, J. Roehrig, V. L. Telegdi, B. Winstein, S. H. Aronson, G. J. Bock, D. Hedin, G. B. Thomson, and A. Gsponer [Phys. Rev. Lett. 41, 1213, 1523(E) (1978)].

The following should appear at the end of the Letter:

Note added.—See also the work of N. Isgur, Phys. Rev. D 17, 369 (1978), for a calculation of the mean-square K^0 charge radius.