B 11, 3535 (1975).
[10a]N. Gupta and B. Sutherland, Phys. Rev. A 14, 1790 (1976).
[10b]J. F. Currie, M. B. Fogel, and F. L. Palmer, Phys. Rev. A 16, 796 (1977).
[10c]R. A. Guyer and M. D. Miller, Phys. Rev. B 11, 3535 (1978).
[11]J. V. José, Phys. Rev. B 14, 2180 (1976).
[12]R. Hirota, J. Phys. Soc. Jpn. 33, 1459 (1972).
[13]E. Stoll, T. Schneider, and A. R. Bishop, Phys. Rev. Lett. 42, 937 (1979).
[14]J. Rubinstein, J. Math. Phys. 11, 258 (1970).
[15]T. Schneider and E. Stoll, Phys. Rev. Lett. 41, 1429 (1978), and to be published.
[16]In a recent paper by J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger (to be published), it was shown that the $(m_p K)^{1/2}$ coefficient arises from the phase-shift interaction of solitons with the harmonic models. It is possible to think that the extra power of $\frac{1}{2}$ in Eq. (14) comes from the interaction of the solitons with the nonlinear magnons in the system.
[17]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegum (U. S. GPO, Washington, D.C., 1964), Ch. 20, Eq. 20.2.31.

E vs $\vec{k}$ and Inverse Lifetime of Cu(110)

P. Thiry
Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, Orsay, France, and Laboratoire de Physique des Solides, Université Pierre et Marie Curie, 75230 Paris Cédex 05, France

and

D. Chandesris, J. Lecante, and C. Guillot
Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, Orsay, France, and Service de Physique Atomique, Commissariat à l'Energie Atomique, 91190 Gif-sur-Yvette, France

and

R. Pinchaux and Y. Pétroff
Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, Orsay, France, and Laboratoire de Physique des Solides, Université Pierre et Marie Curie, 75230 Paris Cédex 05, France

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We present a very accurate determination of the valence bands of copper along ΓKX. This is obtained with high-resolution angle-resolved photoemission spectroscopy, using synchrotron radiation in the $15 \leq \hbar\omega \leq 100$ eV photon energy range. In addition the data yield inverse lifetime measurements for the $3d$ hole at the top and the bottom of the d band which have a value much smaller (< 50 and 250 meV) than recently reported.

Angle-resolved photoemission spectroscopy (ARPES) measurements on copper using variable photon energy and attempting to derive E vs $\vec{k}$ for the valence band have been already reported by different groups.[1-3] However, in the previous attempts it was not possible to reach all the bands along the symmetry directions, because of either lack of high angular resolution[1] or the small photon energy range used.[2,3] In this Letter we report data obtained for photon energies of $15 \leq \hbar\omega \leq 100$ eV. This large energy range permits covering completely the direction ΓKX in normal emission and to observe all the bands (d and sp). Since photoemission involves both the initial and the final states, an analysis of such data requires an accurate model for the final-state bands. For this it is possible to use either an existing band[2] structure or a free-electron approach.[1] In the present work, we have found that the last one gives excellent results. The experimental valence band shows a very good agreement (± 100 meV) with the augmented-plane-wave (APW) calculation of Burdick.[4] In particular, the bottom of the sp band at Γ is in better agreement with these calculations than with the self-consistent bands of Janak, Williams, and Moruzzi.[5,6] The measurement of the hole inverse lifetime at the bottom and the top of the d band gives values much smaller than recently reported.[2]

The measurements were performed at Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, the Orsay Synchrotron Radiation Center. The use of a new high-flux monochromator[7] (> 4×10^{12} photons/Å sec at 100 eV) allowed

us to work with an energy resolution for monochromator and analyzer that varied between 130 meV at low photon energy and 170 meV at 100 eV. The angular resolution is of the order of $\pm 0.5°$. The importance of such angular resolution is illustrated on Fig. 1, which shows energy distributions obtained for Cu(100) at $\hbar\omega = 30$ eV for three polar angles: $\theta = 18°$, 18.5°, and 19° that are markedly different. This resolution permits working easily up to 140 eV, keeping a low instrumental Δk broadening.[8] The energy distribution curves were obtained with either s or p polarizations; it is then possible to draw conclusions about the symmetry of the initial state.[9] The analyzer is a 127° cylindrical one and the count rate for the Cu d bands, with the experimental conditions previously described, was of the order of 20 000 counts/sec. The Cu crystals were prepared by argon bombardment and annealing at 500°C; the cleanliness of the surface was checked by Auger-electron spectroscopy. The vacuum was less than 3×10^{-10} Torr and no contamination was observed, even after several hours.

All the results that we discuss now have been obtained at normal emission ($k_{\parallel}=0$). If we use a free-electron model for the final state we have a simple relation between $k_{\perp}$ in the solid and the kinetic energy outside

$$\hbar^2 k_{\perp}^2/2m = E_{\mathrm{kin}} + U_0, \qquad (1)$$

where E_{kin} is the kinetic energy of the photoelectron and U_0 is the inner potential.

To be able to plot $\vec{E}$ vs k we suppose that we are in a direct-transition model. The zero of the free-electron scale was taken to be the bottom of the sp band at Γ (– 8.6 eV). This value was extracted from our data and it is in excellent agreement with the bottom of the free-electron–like band in the band structure (– 8.9 eV) of Burdick.

The results for Cu(110) are summarized in Fig. 2: The experimental points are indicated by small rectangles; the open symbols correspond to weak structures or shoulders, the filled symbols to well-defined peaks in the energy distributions. The solid curves are the APW bands of Burdick[4]; the agreement between theory and experiment is very good for both the sp and the d

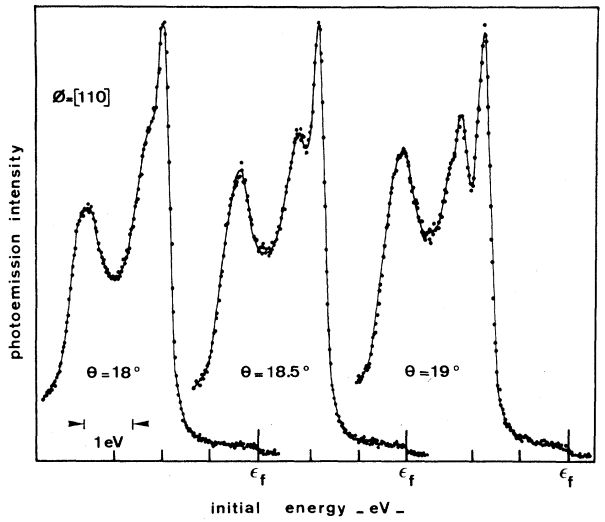

FIG. 1. Normal-emission distribution curves obtained from Cu(100) at $\hbar\omega = 39$ eV for three polar angles: $\theta = 18°$, 18.5°, and 19°.

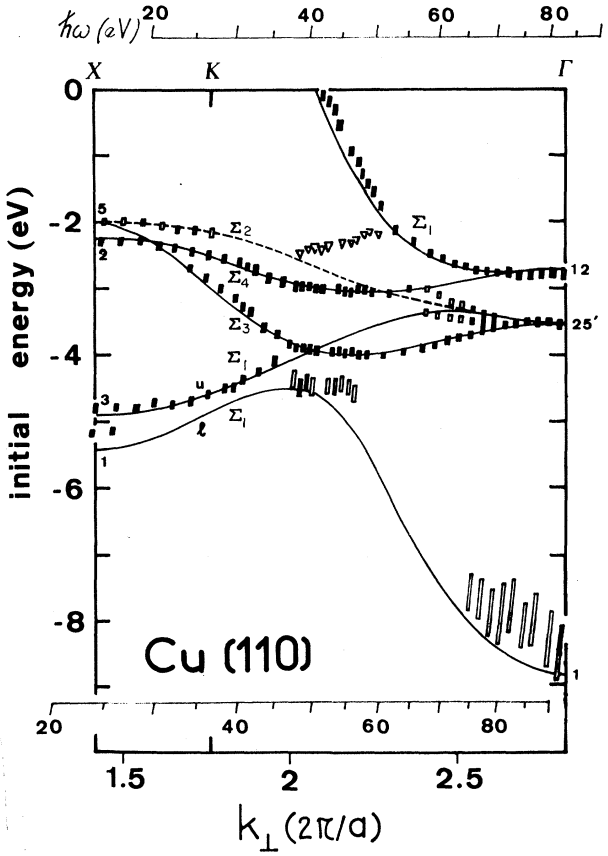

FIG. 2. Experimentally determined valence band for copper along the ΓKX line. The full curves correspond to the Burdick's band-structure calculation (Ref. 4). The dashed curve (level Σ_2) is forbidden in both polarizations (s and p) for normal emission. The few points indicated along this line are obtained by moving the analyzer by a few degrees. The height of the rectangles gives the experimental uncertainty.

bands with typical deviations $\leq \pm 0.1$ eV. The self-consistent calculation by Janak, Williams, and Moruzzi[5,6] gives also a very good agreement for the d bands and the upper sp at Γ is off by about 1.4 eV. Table I summarizes the values of the different experimental symmetry points and those given by the calculations of Burdick[4] and Janak, Williams, and Moruzzi.[5,6]

There are also several other points that we would like to emphasize in connection with the analysis of Fig. 2:

(1) It is clear that even at Γ around 80 eV we do not observe the density of states and that the direct-transitions model still applies: only two sharp structures corresponding at Γ_{12} and $\Gamma_{25'}$ and one very weak to Γ_1 are observed.

(2) Transitions from the Σ_2 band (dashed line) are forbidden[9] at normal emission for both s and p polarizations. Thus the few points that we have indicated are obtained by moving the detector off normal by 3°.

(3) For a final energy $14 < E < 22$ eV (above the Fermi level) there is a band gap in the conduction band, which gives some surface photoemission[3] into evanescent final states; two weak structures not represented in Fig. 2 are in this case observed at -3 and -4 eV.

(4) For $42 < \hbar\omega < 52$ eV a strong structure indicated by triangles on Fig. 2 is observed. It corresponds to an umklapp processs involving the reciprocal-lattice vector $\vec{G} = (1\bar{1}1)$. This is the only case where we need to introduce it.

(5) The large error bar at the bottom of the valence sp band around Γ is due to the fact that the structures are weak and broadened by Auger processes.

As predicted by Pendry and Titterington[10] and shown recently by Knapp, Himpsel, and Eastman,[2,11] ARPES can be used to obtain information on electron and hole lifetimes. This is done by measuring the full width at half maximum intensity (FWHM) of the experimental peaks and using a relationship between the inverse lifetimes Γ_h (hole) and Γ_e (electron) and the group velocity along the normal in the initial and the final states. Following Spanjaard and Jepsen,[12] the full width at half maximum ΔE is then given by

$$\Delta E \simeq |V_h|\,\Gamma_e/|V_e - \bar{V}_h| + V_e\Gamma_h/|V_e - \bar{V}_h|, \qquad (2)$$

where $\bar{V}_h$ and $\bar{V}_e$ are the algebraic values.[13]

V_e and V_h can be calculated accurately. Then by measuring ΔE it is possible to obtain the value of Γ_h and Γ_e for some simple cases:

(1) At the crossing point of the sp band with the Fermi level $\Gamma_h \sim 0$. This allows one to measure Γ_e and the mean free path $l(E) = V_e/\Gamma_e$ and has been used by Eastman, Knapp, and Himpsel.[11] However, there is only one crossing point at normal emission and therefore the possibility to obtain only one $l(E)$. The method can be improved by working off normal, changing $\hbar\omega$ and θ, and it allows one to obtain the mean free path[14] $l(E)$ between $\hbar\omega = 10$ and 70 eV.[14]

(2) For very flat bands $V_e \gg V_h$ and $\Gamma_h \ll \Gamma_e$,

$$\Delta E \simeq \Gamma_h + (|V_h|/V_e)\Gamma_e. \qquad (3)$$

For Cu, an inverse lifetime Γ_h of 0.2 to 0.5 eV for d bands energies from 2 to 5 eV below E_F has

TABLE I. Energy values for the valence band of copper at X, K, and Γ taken from our experiments and two theoretical calculations. All energies are given in eV relative to the Fermi level.

Irreducible representation	Our results	Burdick (Ref. 3)	Janak, Williams, Moruzzi (Ref. 5)
X_5	−2.00	−1.95	−1.95
X_2	−2.30	−2.12	−2.20
X_3	−4.80	−4.83	−5.02
X_1	−5.15	−5.33	−5.50
K_2	−2.15	−2.16	−2.19
K_4	−2.50	−2.56	−2.59
K_3	−2.95	−3.10	−3.24
K_1	−4.60	−4.45	−4.61
K_1	···	−4.76	−4.82
Γ_{12}	−2.80	−2.69	−2.75
$\Gamma_{25'}$	−3.50	−3.48	−3.57
Γ_1	−8.60	−8.91	−10.0

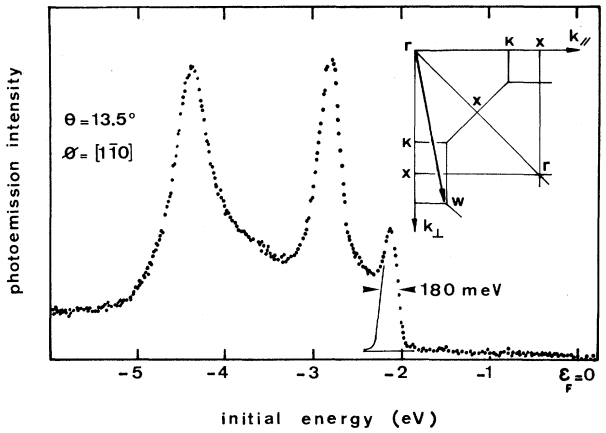

FIG. 3. Energy distribution curve of Cu(110) obtained off normal ($\theta = 13.5°$) at $\hbar\omega = 30$ eV. The structure located at -2.15 eV corresponds to the top of the d band around the W point in the Brillouin zone.

been reported by Knapp, Himpsel, and Eastman.[2]

We have also performed such inverse-lifetime measurements, but the value that we obtain at the top of the d band is much smaller. Figure 3 shows an energy distribution curve of Cu(110) obtained with off-normal emission ($\theta = 13.5°$) at $\hbar\omega = 30$ eV. At this photon energy and for the azimuth [110] the origin of the first structure at -2.15 eV is the W critical point. At that point, the d band is very flat and the ratio V_h/V_e negligible, which means that $\Delta E \sim \Gamma_h$. Taking account of our experimental energy resolution ΔE_{expt} and using the relationship

$$\Delta E_{\text{meas}} = (\Delta E^2 + \Delta E^2{}_{\text{expt}})^{1/2}, \quad (4)$$

where ΔE_{meas} is the measured experimental full width at half maximum, we obtain $\Gamma_h \leq 50$ meV. This value is in good agreement with the one quoted by Pendry and Titterington.[10]

Other measurements made around X_5 (top of the d band at X) gives $\Gamma_h \leq 100$ meV. However, it should be noted that these values are an upper limit because they are strongly dependent of the angular resolution which is very difficult to introduce properly.

Similar results have been obtained for the bottom of the d band: Γ_h varying between 250 and 350 meV have been measured at -4.4 eV below the Fermi level at different points of the Brillouin zone.

In conclusion we have shown that high-angular-resolution ARPES permits very accurate mapping of the bands along $k_\perp$ and that the direct-transition model with a free-electron final state works very well for Cu(110) up to 95 eV. As expected we do not observe any surfaces states [contrarily to cases for the (111) and (100) faces[15]]. These measurements also have permitted more accurate inverse-lifetime determination.

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[1]P. S. Wehner, G. A. Apai, R. S. Williams, J. Stöhr, and D. A. Shirley, in *Proceedings of the Fifth International Conference on Vacuum Ultraviolet Radiation Physics, Montpellier, France, 1977*, edited by M. C. Castex, M. Poney, and N. Poney (Centre National de la Recherche Scientifique, Meudon, France, 1977), extended abstract 67.

[2]J. A. Knapp, F. H. Himpsel, and D. E. Eastman, Phys. Rev. B 19, 4952 (1979).

[3]E. Dietz and F. J. Himpsel, Solid State Commun. 30, 235 (1979); E. Dietz and D. E. Eastman, Phys. Rev. Lett. 41, 1674 (1978).

[4]G. A. Burdick, Phys. Rev. 129, 138 (1963).

[5]J. F. Janak, A. R. Williams, and V. L. Moruzzi, Phys. Rev. B 6, 4367 (1972).

[6]J. F. Janak, A. R. Williams, and M. L. Moruzzi, Phys. Rev. B 11, 1522 (1975).

[7]C. Depautex, P. Thiry, R. Pinchaux, Y. Pétroff, D. Lepére, G. Passereau, and J. Flamand, Nucl. Instrum. Methods 152, 101 (1978).

[8]For an angular resolution of 1°, at $\hbar\omega = 140$ eV, $\Delta k_{||} = 0.1$ Å^{-1} by comparison with the radius of the Brillouin zone along $\Gamma KX = 1.4$ Å^{-1}.

[9]J. Hermanson, Solid State Commun. 22, 9 (1977). For example, on the (110) face among the four irreducible representations Σ_1, Σ_2, Σ_3, and Σ_4 only three are allowed at normal emission: Σ_1 in p polarization, Σ_3 and Σ_4 in s.

[10]J. B. Pendry and D. J. Titterington, Commun. Phys. 2, 31 (1977).

[11]D. E. Eastman, J. A. Knapp, and F. J. Himpsel, Phys. Rev. Lett. 41, 825 (1978).

[12]D. Spanjaard and D. Jepsen, unpublished.

[13]This expression is different from the one used by Knapp *et al.* (Refs. 2 and 11): $\Delta E \sim \Gamma_h + \Gamma_e V_h/V_e$, valid only for a flat $3d$ band.

[14]P. Thiry, D. Chandesris, J. Lecante, C. Guillot, R. Pinchaux, and Y. Pétroff, unpublished.

[15]P. Thiry, D. Chandesris, J. Lecante, C. Guillot, R. Pinchaux, and Y. Pétroff, unpublished.