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Photoemission Properties of Cesiated Copper: Theory

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Abstract: Here we report the photoemission properties of cesiated copper. The theoretical Photoemission (PES) spectrum at ħw = 6.5eV shows 4 distinct structures but we have 2 peaks in the energy range-4.0 to-2.6eV. On increasing the photon energy, the left-hand peak fades away, then makes a comeback. At ħw = 7.1eV, there is a single broad pieces of structure which splits into a doublet on going to ħw = 8.2eV. The behaviour of the structure obtained on varying the photon energy is characteristics of direct transitions.

Key words: Photoemission, band structure, Energy Distribution Curve (EDC), photon energy, symmetry points and valence bands

INTRODUCTION

Photoemission Spectroscopy (PES) is based on the phenomenon of photoemission which was detected by Hertz (1887). Photoemission spectroscopy probes the kinetic energy E_k of photoelectrons emitted from inner levels of a solid or from the outermost Occupied Band (OB) as a result of the interaction of the solid with incoming Ultra-violet (UPS) radiation of energy ħw. Therefore, the initial state is the ground state of the system whereas there is a hole in the final state. The photoemission process involves three successive steps: The excitation of the photoelectron, Its travel through the sample and the ejection of the photoelectron into the vacuum.

The results of photoemission investigation of metals especially Cu and Ag by Berglund and Spicer (Berglund *et al*., 1964) could not be reconciled with conventional theory of direct transitions. Direct transitions, it was argued (Berglund *et al*., 1964) should give rise to structure which moves in a peculiar way on varying ħw; in addition, peaks in the EDC might be expected to vary markedly in strength and to disappear and reappear in a rather abrupt fashion because of the gaps between the bands.

It was found that the behaviour of structure in the photoelectron Energy-Distribution Curves (EDC's) on varying the photon energy, ħw. The structure was found to remain stationary or to move in energy with increments in ħw. The failure of Berglund and Spicer to reconcile their result with the conventional theory of direct transition necessitated this present study.

Calculations on Cu, however (Smith *et al*., 1969), have indicated that the equal-increment behaviour is not inconsistent with direct transitions, at least for clean Cu in the range ħw≤11eV. The same calculations indicated that the characteristic behaviour peculiar to direct transitions was expected to occur at energies below the vacuum level of clean Cu. In other words, it is necessary to lower the work function, for example by cesiation, in order to see these effects.

In this research, we have investigated theoretically photoemission properties of cesiated copper and the results obtained which are reported here revealed that some of these transitions from the Cu d bands can be identified as direct even on the basis of experiment.

METHOD OF CALCULATION

We use the three-step model (Berglund *et al*., 1964) (or formulation) of photoemission to obtained the Photoemission Spectroscopy (PES) spectrum. In the three-step model or formulation of photoemission, photoemission is treated as a sequence of optical excitation of an electron, its transport through the solid which includes the possibility for inelastic scattering by the other electrons and finally, the escape through the sample surface into the vacuum. The Energy Distribution Curve (EDC) of photoemitted electrons I(E, ħw) is consequently a sum of a primary distribution of electrons I_p(E, ħw) that have not suffered an inelastic collision and a background of secondary electrons I_s (E, ħw), have suffered an energy loss in one or more collisions.

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$$I(E, \hbar w) = I_p(E, \hbar w) + I_s(E, \hbar w) \quad (1)$$

The primary distribution is factorized according to the three-step model into a distribution of photoexcited electrons D(E, ħw), a transmission function T(E) and an escape function C(E).

$$I_p(E, \hbar w) = D(E, \hbar w) \times T(E) \times C(E) \quad (2)$$

$I_p(E, \hbar w)$ is thus the fraction of electrons that escapes from the solid without energy loss.

We obtained the Energy Distribution of the Joint Density of States (EDJDOS) which is defined by

$$D(E, \hbar w) = (2\pi)^{-3} \Sigma \int^1 d^3k \delta(E_f(k) - E_i(k) - \hbar w) \, \delta(E - E_i(k)) \quad (3)$$

Where $E_i(k)$ and $E_f(k)$ denote the energies in an initial band i and a final band f.

The prime on the integral denotes that the integration is to be performed only over those portions of k-space for which $E_i < \epsilon_f < E_f$, where ϵ_f is the Fermi energy. In a constant-matrix-element approximation, the Energy Distribution of the Joint Density of States (EDJDOS) represents the energy distribution of photoexcited electrons referred to initial-state energy.

The Energy Distribution of the Joint Density of States (EDJDOS) obtained was then converted to an Energy Distribution Curve (EDC) of photoemitted electron I(E, ħw) by multiplying by appropriate threshold and escape factors.

RESULTS AND DISCUSSION

Theoretical calculations of the EDC's have been performed assuming direct transitions and constant matrix elements. When optical transitions are direct, the initial and final states lie at the same point in K space in the reduced-zone scheme. If $E_i(k)$ and $E(k_f)$ denote the energies in an initial band i and a final band f, then the transitions at photon energy ħw are restricted to lie on the surface given by

$$\Omega_{fi}(k) = E_f(k) - E_i(k) - \hbar w = 0 \quad (4)$$

The relevant property of the band structure for our present purpose is the Energy Distribution of the Joint Density of States (EDJDOS) defined by

$$D(E, \hbar w) = (2\pi)^{-3} \Sigma \int^1 d^3k \delta(\Omega_{fi}(k)) \, \delta(E - E_i(k)) \quad (5)$$

The prime on the integral denotes that the integration is to be performed only over those portions of k space for which $E_i < \varepsilon_f < E_f$ where ε_f is the fermi energy. In a constant-matrix-element approximation, the EDJDOS represents the energy distribution of photoexcited electrons referred to initial-state energy.

The EDJDOS has been calculated analytically for Cu from Eq. 5 by sampling k space at more than 10^5 points in the primitive 1/48 of the zone. Calculations of this kind were first performed by Brust (1965). The band structure used here was the combined interpolation scheme of Hodges *et al.* (1966) with its parameters fitted to the augmented plane-wave calculation of Burdick (1963). The EDJDOS was then converted to an EDC by multiplying by appropriate threshold and escape factors[1]. The curves were also broadened by convolving them with a Lorentzian whose width at half-maximum was 0.3eV.

The theoretical EDC's calculated in this way for photon energies between 6.5 and 8.2eV are shown in

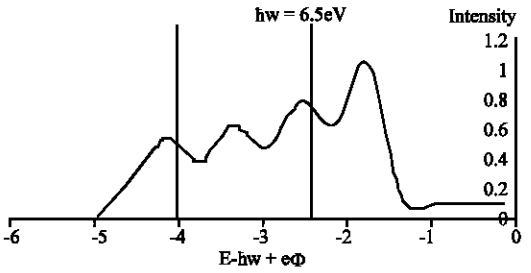

Fig.1: Theoretical EDC measured at ħw = 6.5eV

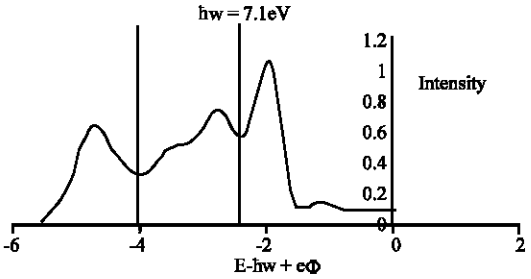

Fig. 2: Theoretical EDC measured at ħw = 7.1eV

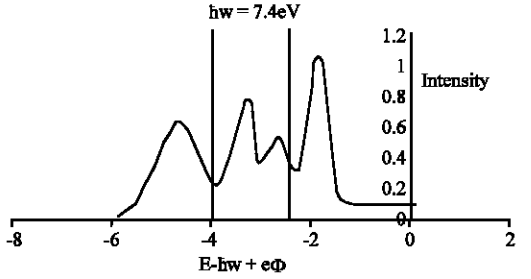

Fig. 3: Theoretical EDC measured at ħw = 7.4eV

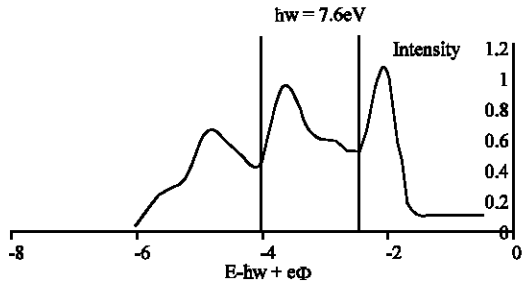

Fig. 4: Theoretical EDC measured at ħw = 7.6eV

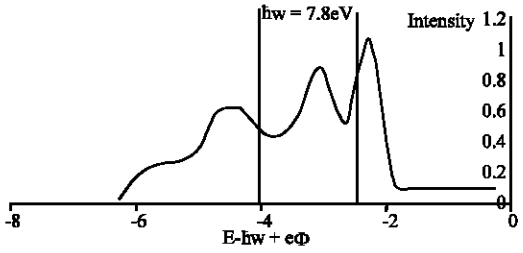

Fig. 5: Theoretical EDC measured at ħw = 7.8eV

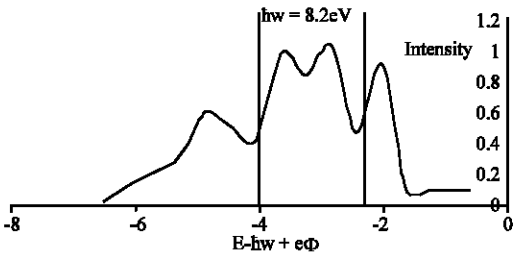

Fig. 6: Theoretical EDC measured at ħw = 8.2eV

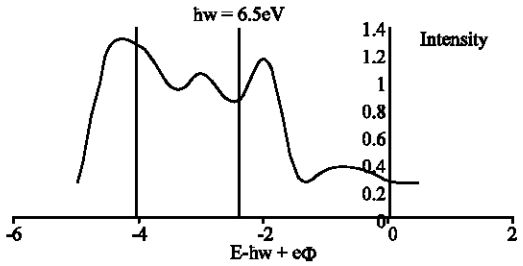

Fig. 7: Experimental EDC measured at ħw = 6.5eV

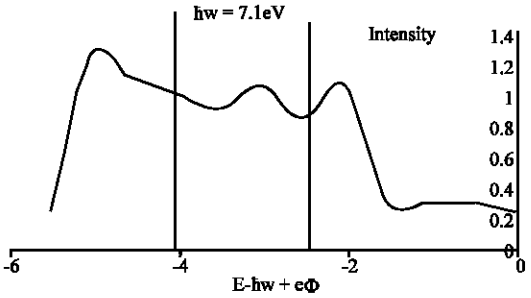

Fig. 8: Experimental EDC measured at ħw = 7.1eV

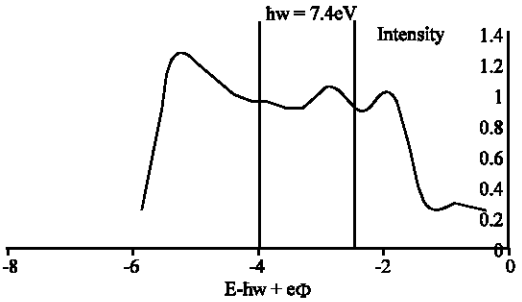

Fig. 9: Experimental EDC measured at ħw = 7.4eV

Fig. 1-6. In arriving at the graph of Fig. 1-6, transitions involving bands 3,4,5,6 and 7, i.e (3,4) → (5,6,7) only are used.

The new and most note worthy information has been obtained in the photon energy range 6.5-8.2eV and so we will concentrate our discussion on this region. The theoretical EDC's of photoemitted electrons are shown in Fig. 1-6 for photon energies between 6.5 and 8.2eV. We notice at about-2.3eV a peak due to transitions from the uppermost d band. There is additional structure at lower energies associated with the lower lying bands. Here lies the main difference between the present work and that of Berglund and Spicer. Their research revealed a broad peak in this lower d-band region which did not change on varying the photon energy.

A significant feature of the new structure seen in the present data is the way the profile of the EDC changes with photon energy. Let us examine the trends in the energy range-4.0--2.6eV indicated by vertical lines. At ħw = 6.5eV we have 2 peaks. On increasing the photon energy, the left-hand peak fades away, then makes a comeback. At ħw = 7.8eV, there is a single broad piece of structure which splits into a doublet on going to ħw = 8.2eV. This kind of qualitative behaviour is characteristic of direct transitions. Infact, Berglund and Spicer searched specifically for such effects in just this energy region. Since their research did not exhibit these effects, they were led to propose a nondirect model which has been quite successful in Cu and other materials (Spicer, 1967; Blodgett *et al*., 1966).

Theoretical Photoelectron energy-distribution curves for cesiated Cu calculated on the basis of direct transitions. The curves are plotted against initial-state energy with the zero of energy taken at the Fermi level.

The experimental energy-distribution curves is shown in Fig. 7-12. Let us focus attention on the behaviour in the energy range-4.0-2.6eV, indicated by vertical lines in Fig. 7-12. At ħw = 6.5eV we have two peaks I this region

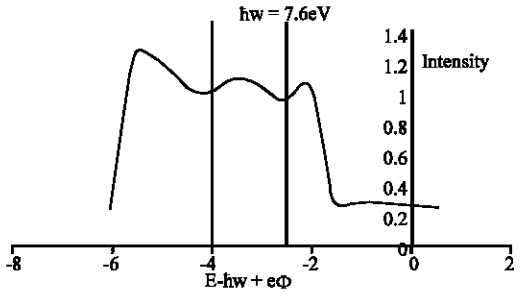

Fig. 10: Experimental EDC measured at ħw = 7.6eV

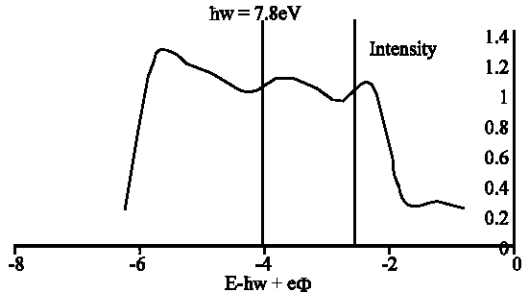

Fig. 11: Experimental EDC measured at ħw = 7.8eV

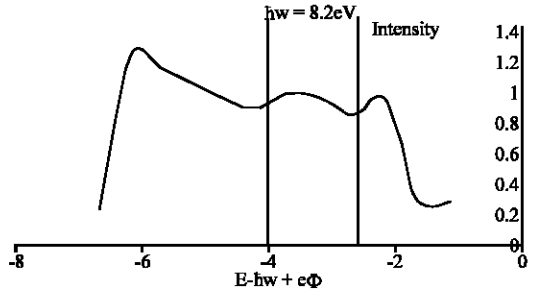

Fig. 12: Experimental EDC measured at ħw = 8.2eV

As the photon energy is increased the left-hand peak fades away. While this is happening, the right-hand peak broadens with shifting its low-energy edge downwards, until at ħw = 7.8eV , there is one broad piece of structure filling the whole range. On going to ħw = 8.2eV this broad peak then splits into a doublet. The similarity of the trends in theoretical EDC in Fig. 1-6 to those shown by the experimental data in Fig. 7-12 is striking and would seem to lend further support to a direct-transition interpretation.

Experimental Photoelectron energy-distribution curves for cesiated Cu calculated on the basis of direct transitions. The curves are plotted against initial-state energy with the zero of energy taken at the Fermi level.

CONCLUSION

It has been found that direct-transition calculations work quite well for some of the transitions from the Cu d bands and other transitions.

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