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## A study of the $\text{Cu}_2\text{MnAl}$ Heusler alloy using ultraviolet photoemission spectroscopy

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**Abstract.** Ultraviolet photoemission spectroscopy has been employed to provide information on the valence band of the  $\text{Cu}_2\text{MnAl}$  Heusler alloy. The contribution of the d bands of Mn and Cu to the density of states has been investigated by means of 3p to 3d resonant enhancement. The valence band extends to 6 eV below the Fermi level, with a main peak at a binding energy of 3.2 eV and a shoulder extending to the Fermi edge. Resonant photoemission indicates that the Mn 3d character extends across the full width of the band. An experimental photoemission spectrum obtained at a photon energy of 40 eV has been compared with a calculated spectrum derived from a theoretical band structure. The main difference occurs in the region 1–2 eV below the Fermi level. The calculated spectrum exhibits a peak at a binding energy of 1.5 eV, comprising contributions from both the Cu and Mn 3d bands. There is no evidence of a similar feature in the experimental spectrum.

### 1. Introduction

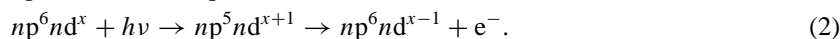
Heusler alloys are ternary magnetic alloys of composition  $\text{X}_2\text{YZ}$  that possess the  $\text{L}_{21}$  structure [1]. This consists of four interpenetrating face-centred cubic sublattices, two occupied by atoms of element X and one each by atoms of elements Y and Z. Generally,  $\text{X} = \text{Co}, \text{Ni}, \text{Cu}$  or  $\text{Pd}$ ,  $\text{Y} = \text{Mn}$  and  $\text{Z} = \text{Al}, \text{Sn}, \text{In}$  or  $\text{Sb}$ . The magnetic order in these systems is known to be strongly dependent on the conduction electron concentration [2].  $\text{Cu}_2\text{MnAl}$  is a ferromagnetic Heusler alloy with a Curie temperature of 630 K and a magnetic moment of  $4.12 \mu_B$  confined to the Mn sublattice [3]. Band-structure calculations for this material [4, 5] have indicated that the Mn 3d majority-spin states are mostly occupied and form a delocalized band together with the Cu 3d states. By contrast, the Mn 3d minority-spin states were indicated to be mostly unoccupied. Therefore, the localized magnetization has been explained in terms of the exclusion of minority-spin electrons from Mn sites. However, there is a need to confirm such theoretical predictions by direct experimental investigation of the electronic structure.

Ultraviolet photoemission spectroscopy is a powerful technique for the investigation of the occupied electronic states of metals and their alloys [6]. In particular, information on the contribution of constituent elements to the valence band spectra can be obtained by employing resonant photoemission [7, 8]. This involves an enhancement of the

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photoemission signal when two separate paths connect a given initial and final state. In the case of photoemission from d bands, this will occur whenever the photon energy is tuned to excite a p to d transition. The process can be described as follows:



Path (1) corresponds to direct photoemission from a d state, whilst path (2) corresponds to excitation of a p electron to an unoccupied d state, followed by autoionization. The interference of the autoionization and direct photoemission channels gives rise to a characteristic variation in photoemission intensity with photon energy. This characteristic line shape is described theoretically by Fano [9].

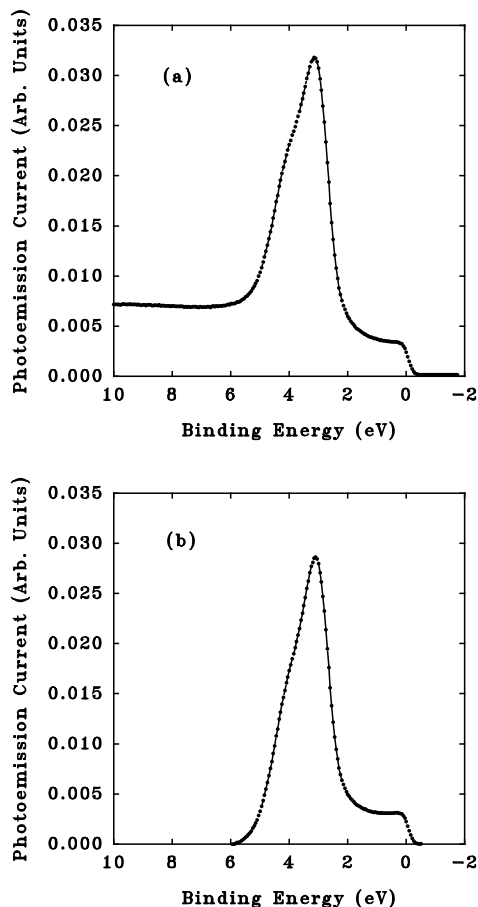
In this study, we have employed ultraviolet photoemission spectroscopy with synchrotron radiation to obtain information on the valence band structure of  $\text{Cu}_2\text{MnAl}$ . In particular, 3p to 3d resonances have been utilized to probe the contribution of the Cu and Mn 3d bands to the density of states. The experimental results have been compared with a theoretical band-structure calculation.

## 2. Experimental details

The  $\text{Cu}_2\text{MnAl}$  sample, supplied by the Institute Laue–Langevin in Grenoble, was investigated by ultraviolet photoemission spectroscopy in the photon energy range 15–100 eV. The alloy was cut to shape using spark erosion to form an ingot of approximate dimensions  $14 \times 3 \times 1$  mm and the front face polished with diamond paste to a final grade of  $1 \mu\text{m}$ . The sample was then mounted on a stainless steel platen and held in place with spot-welded tabs. Before being attached to the sample manipulator all components were cleaned ultrasonically in a degreasing solvent bath.

All experimental measurements were performed on station 6.2 at the Daresbury synchrotron radiation source. Station 6.2 is an ultrahigh-vacuum beamline equipped with a toroidal grating monochromator with two gratings [10]. The first grating has a line density of 710 lines  $\text{mm}^{-1}$  giving an effective photon energy range of 15–60 eV. The second grating has 1800 lines  $\text{mm}^{-1}$  and has an effective range of 40–140 eV. The beamline has two Pt-coated SiC mirrors and a Au-coated post-focusing mirror delivering approximately  $10^{11}$  photons per second. Photon flux was monitored by measuring the drain current from a tungsten grid. Electron energy analysis was performed using a Physical Electronics double-pass cylindrical mirror analyser (CMA) aligned at  $90^\circ$  to the photon beam. Pumping was maintained by rotary backed turbomolecular pumps and titanium sublimation pumps. A base pressure of  $5 \times 10^{-11}$  mbar was achieved following a  $180^\circ\text{C}$  bakeout for 24 hours and the use of liquid-nitrogen-cooled traps.

*In situ* cleaning of the alloy sample was achieved by mechanical abrasion of the surface using a tungsten brush mounted on a wobble stick. The as-loaded sample was initially brushed vigorously for about 15 minutes to remove surface oxide. Subsequently, the sample was brushed for about two minutes every two to three hours to remove any contamination due to adsorption of residual gases. Sample cleanliness was verified by Auger electron spectroscopy. Photoemission spectra were recorded with the sample at an angle of  $45^\circ$  between the photon beam and energy analyser. The CMA was operated with a pass energy of 10 eV.

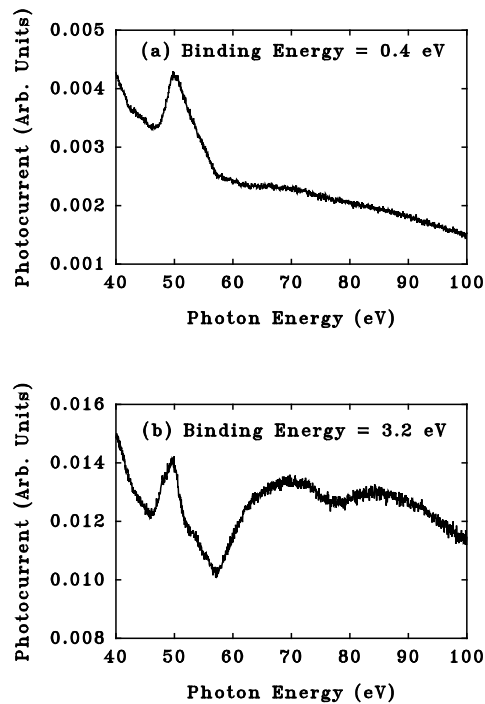


**Figure 1.** Electron energy distribution curves for  $\text{Cu}_2\text{MnAl}$  obtained at a photon energy of 45 eV showing (a) the spectrum before background subtraction and (b) the spectrum after background subtraction.

### 3. Results and discussion

Electron energy distribution curves (EDCs) were obtained at photon energies between 15 and 100 eV in order to identify any features of interest in the valence band spectra. EDCs were normalized to the photon flux and the Fermi edges aligned to zero binding energy. Since the photoionization cross-sections for the s and p bands are comparatively low, the spectra will be dominated by transitions from the 3d bands of Cu and Mn [11]. Figure 1(a) shows a typical electron energy distribution curve for  $\text{Cu}_2\text{MnAl}$  obtained at a photon energy of 45 eV. Figure 1(b) shows the same spectrum, but with the inelastic background removed using a Shirley algorithm [12]. The valence band extends to approximately 6 eV below the Fermi level, exhibiting a main peak with a maximum at about 3.2 eV and a shoulder extending to the Fermi edge. This is similar to an earlier photoemission study of  $\text{Cu}_2\text{MnAl}$  using a He I (21.2 eV) source [13]. In this study, a strong maximum was observed in the spectrum at about 3.1 eV and attributed to the Cu d band.

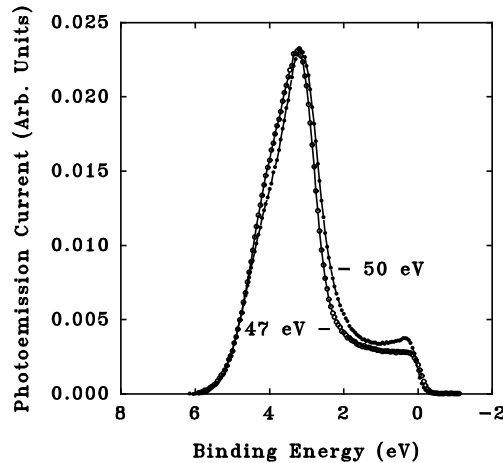
Figure 2 shows constant-initial-state (CIS) spectra for  $\text{Cu}_2\text{MnAl}$  at binding energies of



**Figure 2.** Constant-initial-state spectra for  $\text{Cu}_2\text{MnAl}$  for photon energies between 40 and 100 eV at binding energies of (a) 0.4 eV and (b) 3.2 eV.

(a) 0.4 eV and (b) 3.2 eV between 40 and 100 eV photon energy. These spectra exhibit several prominent features. At a binding energy of 0.4 eV, there is a strong increase in the photoelectron signal commencing at a photon energy of about 48 eV with a maximum at approximately 50 eV. In addition, there is a very weak enhancement of the photocurrent in the region 60–100 eV. At a binding energy of 3.2 eV, the feature at 50 eV is still present but the enhancement of the photocurrent over the energy range 60–100 eV is considerably more intense. There are two peaks, one with a maximum at 70 eV, the other with a maximum at 84 eV photon energy. Also, there are what appear to be anti-resonant features at 57 and 77 eV. Further CIS spectra, with coarse photon energy increments, were obtained at 0.5 eV intervals across the width of the valence band. These spectra indicated that the feature centred at 50 eV is present across the full width of the band. However, the features above 60 eV are most intense between binding energies of about 2–6 eV and are very weak at the Fermi edge. The peak at 50 eV is consistent with a Mn 3p to 3d resonant enhancement, since the binding energy of the 3p state in metallic Mn is at 47.2 eV [14]. In addition, resonant enhancement due to a coherent Mn 3p to 3d transition has also been observed at a photon energy of 50 eV in a photoemission study of  $\text{Ni}_2\text{MnSb}$  [15].

Figure 3 shows background-subtracted EDCs obtained just before the resonance (47 eV) and at the resonance maximum (50 eV). In this figure, the total intensity of the spectra is not as important as the variation in spectral shape with photon energy. For this reason, the spectra have been normalized such that the difference between the maximum and minimum photoemission signal is the same in each case. It can be seen that the two spectra are very similar except for a small relative enhancement in the 50 eV spectrum immediately below the Fermi edge. The presence of resonant enhancement attributable to Mn in all the CIS



**Figure 3.** Background-subtracted electron energy distribution curves obtained just below the Mn 3p to 3d resonance (47 eV) and at the resonance maximum (50 eV). The spectra are scaled such that the difference between the maximum and minimum photoemission signal is the same in each case.

spectra indicates that Mn 3d character extends across the full width of the valence band. A possible explanation for the variation in spectral shape between EDCs obtained ‘on’ and ‘off’ resonance would be that there is a slightly larger concentration of localized Mn 3d states near the Fermi edge. Band-structure calculations indicate that the largest contribution of Mn 3d electrons to the density of states should lie 1–2 eV below the Fermi level [4, 5].

The enhancement of photocurrent above 60 eV is not so clearly attributable. The  $3p_{3/2}$  and  $3p_{1/2}$  binding energies of metallic Cu are at 75.1 and 77.3 eV [14] and so any enhancement of photoelectron signal arising from a Cu resonance will be observed in this region. Resonant enhancement in the region of the Cu 3p binding energy has been observed in several studies of Cu and its compounds [16, 17]. However, these so-called two-electron resonances have been confined to shake-up satellites and involve an excited 4s electron and a  $3d^8$  final state. These satellite peaks are generally observed some 8–12 eV below the main Cu 3d emission peak. The increase in photocurrent observed in our CIS spectra coincides with the Cu 3d emission peak [4, 13]. The enhancement of photocurrent between photon energies of 80–100 eV could be the result of a one-electron 3p to 3d resonance, but this would indicate that the Cu d band is not completely full. Also, since this feature is very weak in CIS spectra between binding energies of 0–2 eV, this would suggest that Cu 3d character is mainly confined to the 2–6 eV region of the valence band. Although this interpretation is highly speculative, a similar resonant enhancement attributed to a partly full Pd 4d band has been reported for the  $\text{Pd}_2\text{TiAl}$  alloy [18]. However, this would not account for the increase in photocurrent in the region 60–75 eV, since this lies below the Cu 3p threshold.

A resonant feature in a CIS spectrum,  $S_{CIS}(h\nu)$ , can be described in terms of the resonant and nonresonant components [19], so

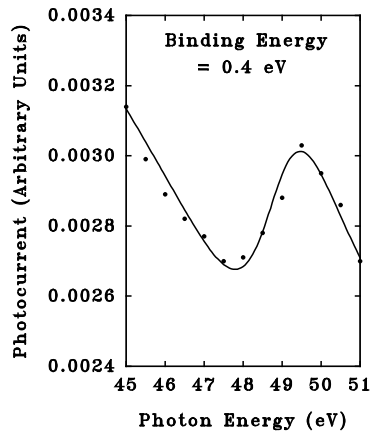
$$S_{CIS}(h\nu) = I_R(h\nu)f(\varepsilon) + I_{NR}(h\nu).$$

$I_R(h\nu)$  and  $I_{NR}(h\nu)$  represent the intensities due to direct photoemission from valence band electrons that do and do not contribute to the resonance respectively. The function  $f(\varepsilon)$

can be described by a Fano line shape [9], where

$$f(\varepsilon) = \frac{(q + \varepsilon)^2}{1 + \varepsilon^2} \quad \text{and} \quad \varepsilon = \frac{2(h\nu - h\nu_0)}{\Gamma}.$$

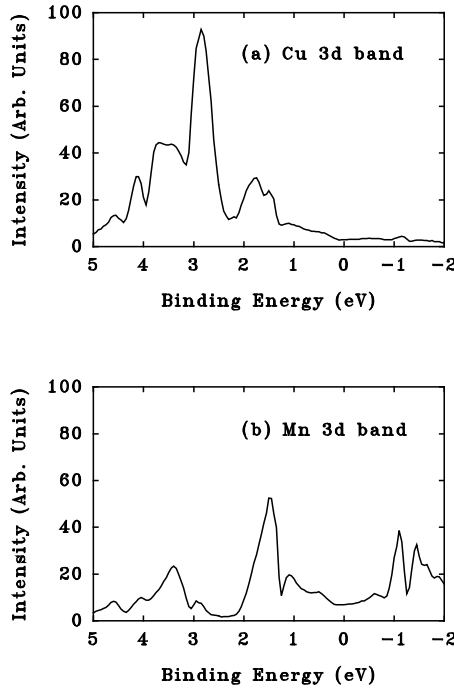
The important Fano parameters that characterize a resonance are the asymmetry parameter ( $q$ ), the resonance energy ( $h\nu_0$ ) and the spectral width ( $\Gamma$ ). The shape and magnitude of a resonance can be affected by the degree of initial-state hybridization [20, 21]. Therefore, Fano parameters can be useful in providing some information on the degree of localization of states within the valence band.



**Figure 4.** The constant-initial-state spectrum at a binding energy of 0.4 eV in the region of the Mn 3p to 3d resonance. Data points represent the photoemission intensity obtained following subtraction of the inelastic background. The solid curve represents a fit of the data to a Fano line shape.

In order to obtain quantitative information on the Mn 3p to 3d resonance, a Fano line shape was fitted to the experimental data at a binding energy of 0.4 eV. No attempt was made to fit a profile to the Mn resonance at 3.2 eV binding energy since, in this case, overlap with the broad feature at photon energies above 60 eV may have significantly distorted the natural line shape. The results of the fit are shown in figure 4. Individual EDCs were obtained at photon energies across the region of the resonant feature in 0.5 eV intervals. Each EDC was then normalized so that the photoemission intensity at a binding energy of 0.4 eV was consistent with the CIS spectrum of figure 2(a). The inelastic background was then removed using a Shirley algorithm. The experimental data points in figure 4 represent the resulting photoemission intensities. A smooth nonresonant background was modelled using a fourth-order polynomial and the solid curve in figure 4 represents the resulting fit of a Fano line shape to the data. The corresponding Fano parameters were  $h\nu_0 = 48.9$  eV,  $q = 1.4$  and  $\Gamma = 2.6$  eV. The value obtained for  $q$  can be compared with values of about 2 obtained in a resonant photoemission study of MnTe [22] and values between 0.5–2.4 obtained for Ni<sub>2</sub>MnSb [15]. For resonances in the partial cross-sections of the <sup>6</sup>S–<sup>6</sup>P transition in atomic Mn, the value of  $q$  ranged from 2.1–2.5 [23]. In a study of the Mn resonance in Ni<sub>2</sub>MnSb, it was suggested that the extent to which  $q$  differs from the value for atomic Mn may indicate the degree of hybridization of the Mn d states [15]. The value of  $q = 1.4$  obtained for the resonance at 0.4 eV binding energy may, therefore, suggest some hybridization of the Mn 3d states close to the Fermi edge in Cu<sub>2</sub>MnAl. However, such a conclusion would be speculative, since the values for the Fano parameters will be

affected by the details of the fitting procedure and other factors may also affect the shape and intensity of a resonance.



**Figure 5.** The contribution of (a) the Cu 3d band and (b) the Mn 3d band to the density of states of  $\text{Cu}_2\text{MnAl}$  calculated using the symmetrized augmented-plane-wave method. The results are adapted with permission from [4].

Energy band calculations have been performed for  $\text{Cu}_2\text{MnAl}$  by Ishida *et al* [4] using the symmetrized augmented-plane-wave (SAPW) method [24]. The electronic configurations of the constituent atoms were taken as  $3d^{10}4s^1$  for Cu,  $3d^64s^1$  for Mn and  $3s^23p^1$  for Al. The resulting theoretically derived partial density of states for (a) the Cu 3d band and (b) the Mn 3d band are shown in figure 5. Since the photoemission process creates a hole that can interact with other electrons, photoemission spectroscopy probes an excited rather than a ground state. Depending on the degree of screening and localization, this can result in the measured initial-state energy being shifted by a substantial fraction of an eV. This must be considered when comparing experimental photoemission results with theoretical band structures. However, the overall shape of the spectrum should still reflect the density of states.

The valence band photoemission spectrum for  $\text{Cu}_2\text{MnAl}$ ,  $S(h\nu, E_B)$ , can be calculated for a particular photon energy using the expression

$$S(h\nu, E_B) = C(h\nu) [N_{Cu}\sigma_{Cu}(h\nu)D_{Cu}(E_B)^* + N_{Mn}\sigma_{Mn}(h\nu)D_{Mn}(E_B)^*].$$

$C(h\nu)$  is an instrumental factor representing the variation in total spectral intensity with photon energy; it does not affect the overall shape of the spectrum.  $N_{Cu}$  and  $N_{Mn}$  are the fractional contributions of Cu and Mn 3d electrons to the valence band. The respective photoionization cross-sections are given by  $\sigma_{Cu}(h\nu)$  and  $\sigma_{Mn}(h\nu)$ .  $D_{Cu}(E_B)^*$  and  $D_{Mn}(E_B)^*$  represent the calculated partial density of states for the Cu and Mn 3d bands



broadened to account for lifetime effects and instrumental resolution. Consequently, the theoretical partial densities of states for the Cu and Mn 3d bands shown in figure 5 were broadened by convolution with Lorentzians of half-width at half-maximum (HWHM) given by

$$\text{HWHM} = \Gamma_0 \frac{(E_B - E_F)^2}{(E_F - E_0)^2}.$$

$E_F$  and  $E_0$  represent the energies of the Fermi level and the bottom of the valence band respectively.  $\Gamma_0$  is the HWHM at the bottom of the band. Similar functions have been used previously to represent lifetime broadening in  $\text{Cu}_3\text{Pd}$  [25, 26].  $\Gamma_0$  was taken to be 0.6 eV, since this value has been used previously for  $\text{Pd}_2\text{TiAl}$  [27]. To represent instrumental broadening, this result was convoluted again with a Gaussian of HWHM equal to 0.2 eV. This represents broadening due to the finite instrumental resolution of both the monochromator and the electron energy analyser.

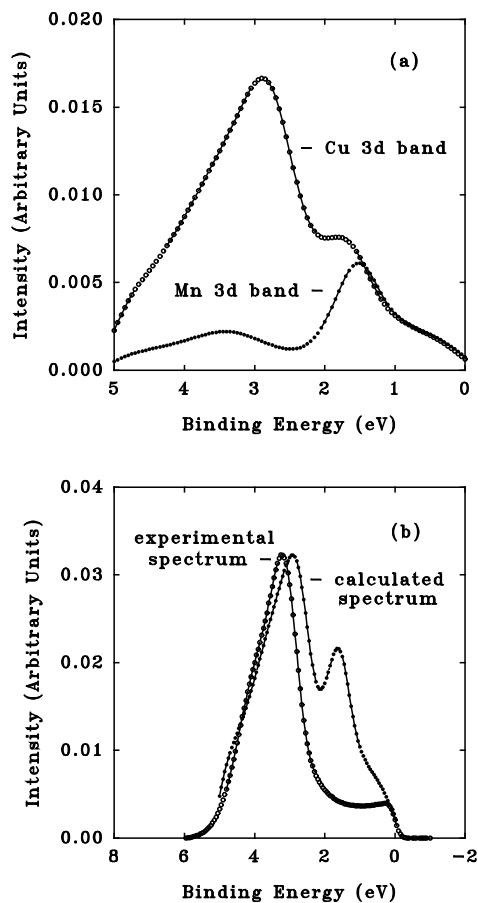
Figure 6(a) shows the broadened partial density of states for both the Cu and Mn 3d bands. In each case, the partial density of states has been normalized to account for the fractional contributions of Cu and Mn 3d electrons to the valence band, so that

$$\sum_{E_B} D_{\text{Cu}}(E_B)^* = 0.7692 \quad \text{and} \quad \sum_{E_B} D_{\text{Mn}}(E_B)^* = 0.2308.$$

Figure 6(b) shows a spectrum calculated for a photon energy of 40 eV using the broadened partial density of states from figure 6(a) and the photoionization cross-sections for the Cu and Mn 3d bands taken from Yeh and Lindau [11]. This calculated spectrum is compared with a background-subtracted spectrum obtained experimentally at a photon energy of 40 eV. At this photon energy  $\sigma_{\text{Cu}}/\sigma_{\text{Mn}}$  is equal to 1.2. The calculated spectrum has been arbitrarily normalized to be on approximately the same scale as the experimental spectrum. The calculated and experimental spectra provide good agreement in terms of the width of the valence band. In addition, a peak at approximately 3 eV binding energy is observed in both spectra. Reference to figure 6(a) shows that the theoretical results predict that this feature will be dominated by transitions from the Cu 3d band. However, the calculated and experimental spectra differ markedly in the region 1–2 eV below the Fermi edge. In this region, the theoretical spectrum shows a second major peak at about 1.5 eV binding energy. According to figure 6(a), this comprises contributions from both the Cu and Mn 3d bands. In the latter case, the largest contribution to the density of states is located in this region. A very weak maximum at a binding energy of 1.2 eV has been observed in a photoemission spectrum of  $\text{Cu}_2\text{MnAl}$  obtained with a He I source [13]. This was attributed to the Mn 3d band. However, in contrast, we can find no evidence to support the existence of this feature in our photoemission spectra. In summary, therefore, the spectrum derived from the calculated band structure is in qualitative agreement with the experimental spectrum in terms of the width of the valence band and the presence of a peak at about 3 eV binding energy. However, agreement is poor in the region up to 2 eV below the Fermi level.

#### 4. Conclusion

The ternary magnetic alloy  $\text{Cu}_2\text{MnAl}$  has been studied using ultraviolet photoemission spectroscopy with a tunable synchrotron radiation source. The valence band extends to 6 eV below the Fermi level. Photoemission measurements in the region of the Mn 3p to 3d resonance indicate that the Mn 3d contribution to the density of states extends across the full width of the valence band. Enhancement of photocurrent in the region



**Figure 6.** (a) Comparison of the theoretical partial density of states for the 3d bands of  $\text{Cu}_2\text{MnAl}$  following convolution with Lorentzians (varying HWHM) and a Gaussian (HWHM = 0.2 eV) to represent lifetime and instrumental broadening respectively. The partial density of states for each metal has been normalized to account for the fractional contributions of Cu and Mn 3d electrons to the valence band. (b) Comparison of the background-subtracted valence band photoemission spectrum of  $\text{Cu}_2\text{MnAl}$  obtained at a photon energy of 40 eV with a spectrum calculated from the theoretical partial density of states shown in figure 6(a). The calculated spectrum has been arbitrarily normalized to be on approximately the same scale as the experimental spectrum.

of the Cu 3p threshold has also been observed, most noticeably in CIS spectra obtained at binding energies 2–6 eV below the Fermi level. If this feature is attributable to a Cu 3p to 3d resonance, then this would indicate that the Cu d band is not completely full. A valence band spectrum calculated from a theoretical band structure has been compared with a representative photoemission spectrum obtained at a photon energy of 40 eV. Experiment and theory provide good agreement in terms of the width of the valence band and the presence of a peak at approximately 3 eV binding energy. Theory predicts that this feature will be dominated by contributions from the Cu 3d band. However, the calculated spectrum exhibits a second major peak at 1.5 eV binding energy, comprising contributions from both Cu and Mn 3d states. This feature is not observed in the experimental spectrum.

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