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LETTER TO THE EDITOR

Quantum-well or bulklike behaviour of Cu layers on Co

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Abstract. Angle-resolved photoemission was employed to probe the quantum-well behaviour, or the lack of it, of Cu films epitaxially grown on low-index Co substrates. Upon varying the photon energy, films grown on Co(111) exhibited a bulklike continuous dispersion for the sp state, while films grown on Co(100) and Co(110) exhibited nondispersive quantum-well peaks with intensities modulated by the bulk band dispersion. These different behaviours, namely, bulklike versus quantum-well-like, are explained in terms of the band structure. The results are correlated with the magnetic coupling effects in multilayer systems.

Metal films deposited on metal substrates can exhibit quantum size effects. Metals do not have an absolute band gap, yet electrons in the film can be confined by a k -dependent gap, resulting in discrete quantum-well states that can be probed directly by angle-resolved photoemission [1–4]. An important consequence of the quantization is that fine tuning of the microscopic sample structure can result in macroscopic consequences. An example is the thickness-dependent oscillatory magnetic coupling between two ferromagnetic layers separated by a nonmagnetic spacer layer [5]. In this regard, Cu–Co is perhaps the most thoroughly studied bimetallic system. While Cu–Co(100) and Cu–Co(110) both show strong oscillations in magnetic coupling [6, 7], Cu–Co(111) shows no oscillations (or a very weak effect according to some reports) [8]. The reason for this difference has been unclear. It is probably related to the quantum-well properties of the Cu film [4, 9], but there are no comprehensive observations of the electronic structure to directly demonstrate and clarify this relationship.

The present work is to investigate the quantum-well behaviour of Cu films deposited on Co. An emphasis is to look for any significant differences among the three crystallographic directions, for example, the presence or absence of discrete quantum-well peaks in angle-resolved photoemission spectra. As the cross sections of quantum-well transitions are generally unknown, a random search could easily miss these transitions. Our approach is to systematically scan the photon energy in the range where the direct band-to-band transitions of the Cu sp electrons in the bulk are observed. If the Cu electrons are confined in the film, the dispersive direct transition in the bulk will be replaced by a set of nondispersive quantum-well peaks whose intensities as a function of photon energy are modulated by the bulk band dispersion. On the other hand, if the Cu electrons are unconfined due to coupling to the Co states, a dispersive peak similar to the bulk case will be observed. Thus, two kinds of qualitatively different behaviour may exist: quantum-well-like or bulklike. Our results below will show that the Cu–Co(111) system is bulklike, while the Cu–Co(100) and Cu–Co(110) systems are quantum-well-like. These results will be analysed in terms of the

Cu and Co band structures, and the connection to magnetic coupling in multilayer systems will be explained.

Our photoemission data were taken at the Synchrotron Radiation Center, University of Wisconsin–Madison, Stoughton, WI. Co films up to 40 monolayers (ML) thick were deposited on freshly cleaned Cu(100), Cu(110), and Cu(111) surfaces to form the correspondingly oriented Co substrates [10]. Cu layers of various thicknesses were then deposited on these Co surfaces at room temperature followed by a brief anneal to about 200 °C. This procedure resulted in films of high quality as verified by a variety of techniques including electron diffraction (to confirm long range order), Auger electron spectroscopy (to check cleanliness), and angle-resolved photoemission (to observe spectral features indicative of layer quality, e.g., film and surface states).

Figure 1 shows normal-emission spectra from clean Cu single crystals and Cu films on Co for the three different orientations. Figure 1(a) is the results for clean Cu(100). The doublet near a binding energy of 2 eV is derived from the Cu 3d bands. The dispersive peak between 0 and 2 eV binding energy is derived from direct transitions of the Cu sp electrons. These sp electrons play the dominant role in determining the magnetic properties of the Cu–Co composite system because of their proximity to the Fermi level. The same sp transition is seen in figure 1(b) for Cu (110) and in figure 1(c) for Cu(111). The intensity rise near 2 eV binding energy in each case is again caused by d-band emission. Figure 1(c) shows additionally a well known Shockley surface state just below the Fermi level [11].

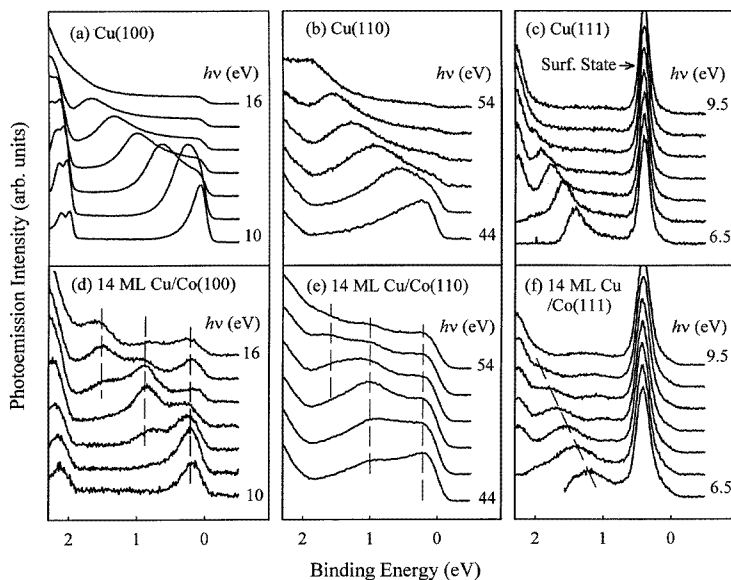


Figure 1. Normal-emission photoelectron spectra for single-crystal Cu substrates and for 14 ML Cu films on Co substrates along three crystallographic directions. Photon energies are evenly spaced between the lower and upper bounds indicated on the graph. The vertical dashed lines for Cu–Co(100) and Cu–Co(110) indicate the positions of quantum-well peaks, while the dashed line for Cu–Co(111) indicates the dispersion of the bulklike peak. The surface state peak in (f) is somewhat broader than that in (c) because of a larger resolution function used in the experiment.

The corresponding spectra for 14 ML Cu films on Co are shown in figures 1(d)–(f). A comparison of figure 1(d) with figure 1(a) shows that the dispersive sp peak for single-crystal Cu(100) is replaced by a set of three nondispersive peaks for the film. The intensities

of these three peaks vary significantly as the photon energy is varied. Each peak at binding energy E_i ($i = 1-3$) attains its maximum intensity at the same photon energy at which the direct transition peak for the single-crystal case is at E_i . This is exactly what is expected for a quantum well. The valence states are quantized, giving rise to discrete peaks, while the matrix-element integral governing the intensities for optical transitions is nevertheless similar to the bulk case (the main difference being that the integral is truncated by the film thickness leading to some momentum broadening).

The results for the (110) orientation are similar. Thus, both the Cu–Co(100) and Cu–Co(110) systems exhibit a quantum-well-like behaviour. The behaviour of the Cu–Co(111) system is different. In figures 1(c) and (f), one sees a dispersive peak for both the single-crystal substrate and the film, indicating that the Cu–Co(111) system has a bulklike electronic structure, and that the interface between Cu and Co does not provide a confinement potential to cause the formation of discrete states. Note that the Shockley surface state for the (111) film is as intense as the single-crystal case. This is strong evidence that the film is smooth, and suggests that the lack of discrete states cannot be caused by roughness in the film. A significant alloying of Cu and Co can be ruled out, as such alloying would affect the (100) and (110) cases as well. Furthermore, a significant roughness or alloying would be easily detected by the appearance of intense Co d-band emission features, but none was detected beyond the usual mean-free-path dependence for different film thicknesses. The Cu surface state is clearly visible for films as thin as 3 ML, again suggesting that the film is smooth and bounded by an abrupt interface. Finally, Cu(111) films were also prepared using a bulk single-crystal Co(0001) as the substrate, and the results were the same [12].

Clues to understanding the differences mentioned above can be found by comparing the band structures of Co and Cu; this comparison along the [100] direction is shown in figure 2. The band structure of Cu [13] consists of several d bands with energies below -2 eV and an sp band, which disperses from 2 eV above the Fermi level down to the d-band region, where it hybridizes with the d bands. The majority and minority spin bands of Co shown in figure 2 have basically the same band topologies, and the main changes from Cu to Co are upward shifts of the bands [13]. There are no obvious gaps in the Co band structure near the Fermi level. It is important, however, to examine the coupling between the Cu sp states and the Co states. Energy regions where none of the Co states couple to the Cu sp states are gaplike, and will provide a confinement potential for the Cu electrons. Such an analysis is carried out using an empirical OPW method [14]. The sp band in Cu or Co is dominated by a few plane waves. The component relevant to quantum-well features is the one that is propagating perpendicular to the film. The vertical bars shown in figure 2 indicate the mixing probability of this plane-wave component for each band (i.e., the absolute square of the projection of the Bloch state onto this plane-wave component). Many of the bands have either zero or such low probabilities that the bars are invisible. As a result, there is effectively a gap as indicated by the shaded regions for the Co bands. This gap depends on the spin direction. The union of the two spin-dependent gaps yields an effective gap in Co where quantum confinement for the Cu sp electrons is expected (for at least one spin component). Because the Cu d-band emission begins to turn on near 1.9 eV binding energy, this imposes a practical limit on the energy range where sp transitions can be clearly observed.

Shown in figure 3 is the Cu band structure along the three crystallographic directions. The shaded region in each case indicates a ‘quantum-well window’ constructed as discussed above, in which one can expect to observe sp quantum-well peaks. Also shown in the figure are horizontal dashed lines indicating the ‘expected’ energy positions of quantum-well states. These positions are first-order approximations, obtained by simply dividing the sp band into

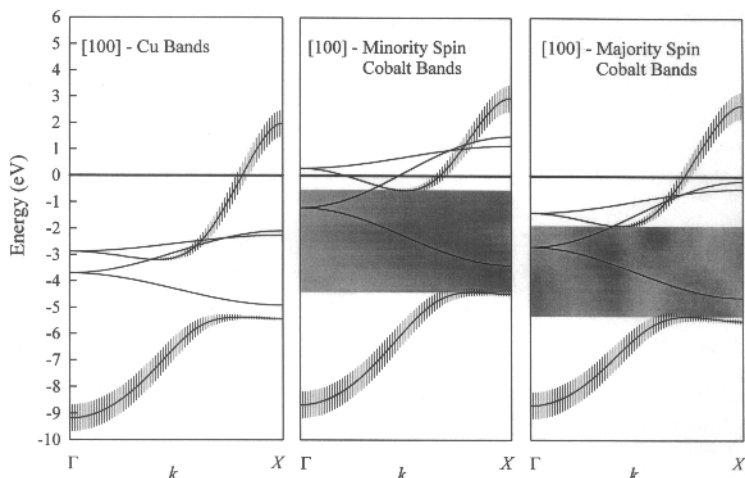


Figure 2. Copper and cobalt bands along the [100] direction. The vertical bars indicate the mixing probability of a free electron wave propagating along [100]. The shaded regions define the effective sp gaps in Co.

14 equal intervals along the Brillouin zone axis (14 is the thickness of the Cu film in ML) [15]. In other words, phase-shift corrections at the film boundaries are ignored. The circles in figure 3 indicate the energy positions of the quantum-well peaks actually observed in our experiment. The agreement is good, considering the phase-shift uncertainties.

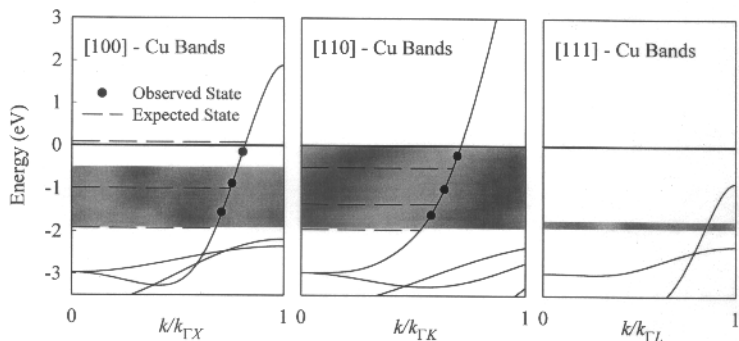


Figure 3. Bulk band dispersions of Cu along three major crystallographic directions. The shaded regions indicate the 'quantum-well windows' described in the text. The horizontal dashed lines indicate the 'expected' energy positions of quantum-well states. The circles are observed energy positions of the discrete peaks in the photoemission spectra.

The above discussion shows that Cu-Co(111) is indeed different from Cu-Co(100) and Cu-Co(110) in that the quantum-well window is too small to support discrete peaks near the Fermi level. Electrons in the Cu film can travel easily across the Cu-Co(111) interface. The basis for the oscillatory magnetic coupling is translayer electronic coupling via quantum-well states, and the oscillation is simply a manifestation of interference effects associated with the layer thickness. The nondispersive quantum-well peaks seen in the (100) and (110) photoemission spectra are likewise a manifestation of the same interference effects. These interference effects are unimportant in the (111) system, and thus no significant oscillations

in the magnetic coupling are expected. There is a simple analogue in optics, the Fabry–Pérot interferometer. A Fabry–Pérot interferometer supports a set of longitudinal optical modes (quantum-well states). As the path length of the interferometer is varied, its optical transmission function oscillates (oscillatory coupling). In this analogy, the Cu–Co(100) and Cu–Co(110) systems correspond to an interferometer with a high finesse.

Our discussion above is limited to the normal-emission geometry. Theoretical calculations have shown that quantum-well states with non-zero parallel momentum (k_{\parallel}) can be important, particularly for the (111) case where Fermi surface nesting occurs near the zone boundary [16]. However, it is known that quantum-well effects are rapidly suppressed for increasing k_{\parallel} due to a finite lateral coherence length [15]. Thus, the nesting near the zone boundary appears to have no practical effect on the issue being discussed here, and the normal-emission geometry provides the most sensitive test for any quantum-well behaviour.

In summary, we have investigated the electronic properties of copper films on Co(100), Co(110), and Co(111). Two different kinds of spectral behaviour are observed when the photon energy is scanned through the range where direct transitions are observed for Cu single crystals. Both Cu–Co(100) and Cu–Co(110) show discrete nondispersive quantum-well peaks with intensities modulated by the bulk band dispersion. Cu–Co(111), in contrast, shows a dispersive bulklike peak. This difference is explained in terms of the Cu and Co band structures and the compositions of the Cu and Co wave functions, which govern the coupling of electronic states across the interface. Our analysis shows that the Cu–Co(111) system, unlike the other two systems, does not have a significant gap near the Fermi level for electronic confinement. The interface is essentially transparent, and the resultant lack of interference effect explains the absence (or extreme weakness) of oscillations in magnetic coupling in this orientation.

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