PHOTOEMISSION OF CO/CU(100). NON-RELATIVISTIC SPIN- AND ANGLE-RESOLVED NORMAL EMISSION.

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ABSTRACT

The Co/Cu(100) system is the first system known where the contributions to the spin polarisation of spin-orbit coupling and the ferromagnetic overlayer were clearly distinguished experimentally. In order to get a first understanding of the photoemission data non-relativistic spin-polarized photoemission calculations are performed for one and two overlayers of Co on Cu(100).

INTRODUCTION

As can be seen from Fig. 1 the Co/Cu(100) system shows thickness dependent magnetic behaviour which results into a large reduction of the critical temperature for thin Co coverages [1]. Furthermore Co films exhibit a considerable big magnetic anisotropy, which gives rise to an orientation dependency of spin-polarized photo-emission spectra with respect to the magnetisation in the surface. Band structure calculations reveal that the magnetic moment of the Co monolayer is $1.8\mu_B$ [2], i.e. is 15% bigger than the corresponding bulk value ($1.56\mu_B$ [3], $1.65\mu_B$ [4]). This enhancement, however, is considerably smaller than for instance in Fe/Cu(100) ($2.85\mu_B$ for the Fe monolayer vs. $2.12\mu_B$ in bulk Fe [5]).

COMPUTATIONAL DETAILS

We used a one-step-model for the calculation of the photoemission spectra of a Co monolayer on a Cu substrate. Table I displays all computational details. Since the FLAPW calculations do not provide information concerning the lifetimes for the final and the initial (hole) states we followed the results of McRae [6]. The theoretical spectra are convoluted with a Gaussian spectrometer function of 0.2 eV full width at half maximum and are individually normalized to the highest peak. Taking into account that the local density approximation (LDA) usually leads to a rigid shift of at least 0.3 eV towards higher binding energies, the present photocurrent calculations with the listed values for

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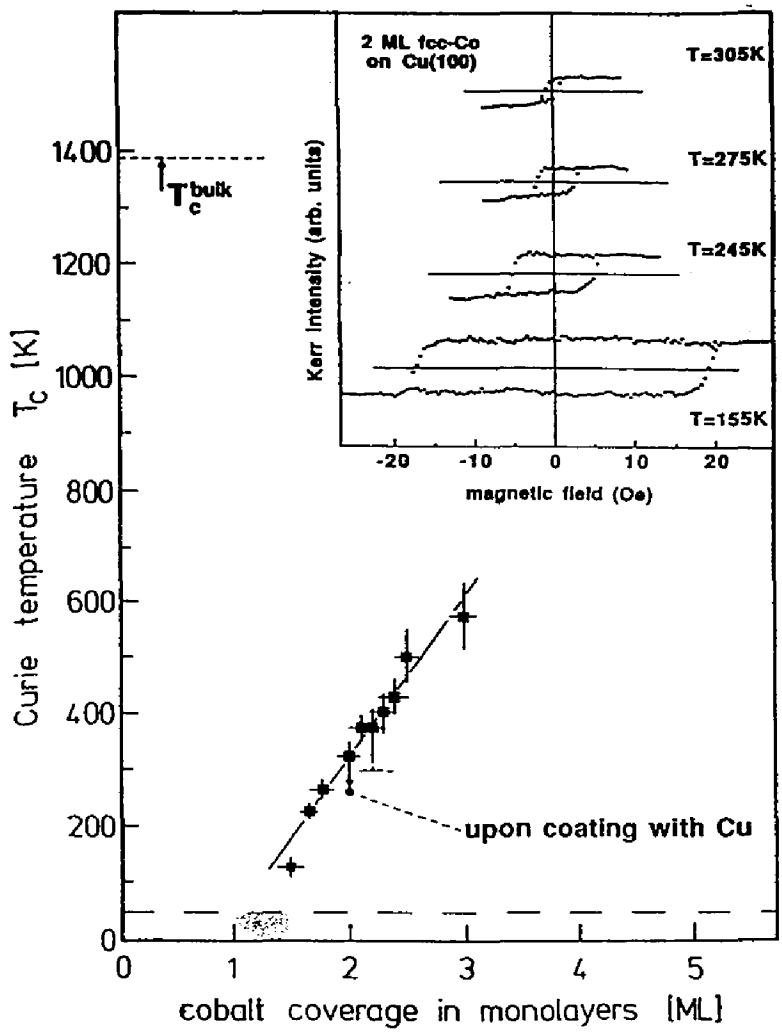

Fig. 1: Thickness dependence of the Curie temperature of fcc-Co films. Inset: Hysteresis loops from a 2ML film as a function of sample temperature.

TABLE I.: Computational parameters

potential: Co/Cu(100)	muffin-tinized FLAPW 7 layer slab [2]
2Co/Cu(100)	muffin-tinized FLAPW 9 layer slab [8]
vacuum region	z-dependent [9]
highest l value	4
beams	21
layer doubling:	
initial state	128 layers
final state	16 layers
photon energy range	11 to 21 eV
absorptive potential:	
initial state	0.135 eV
final state	0.54 to 1.63 eV with increasing photon energy

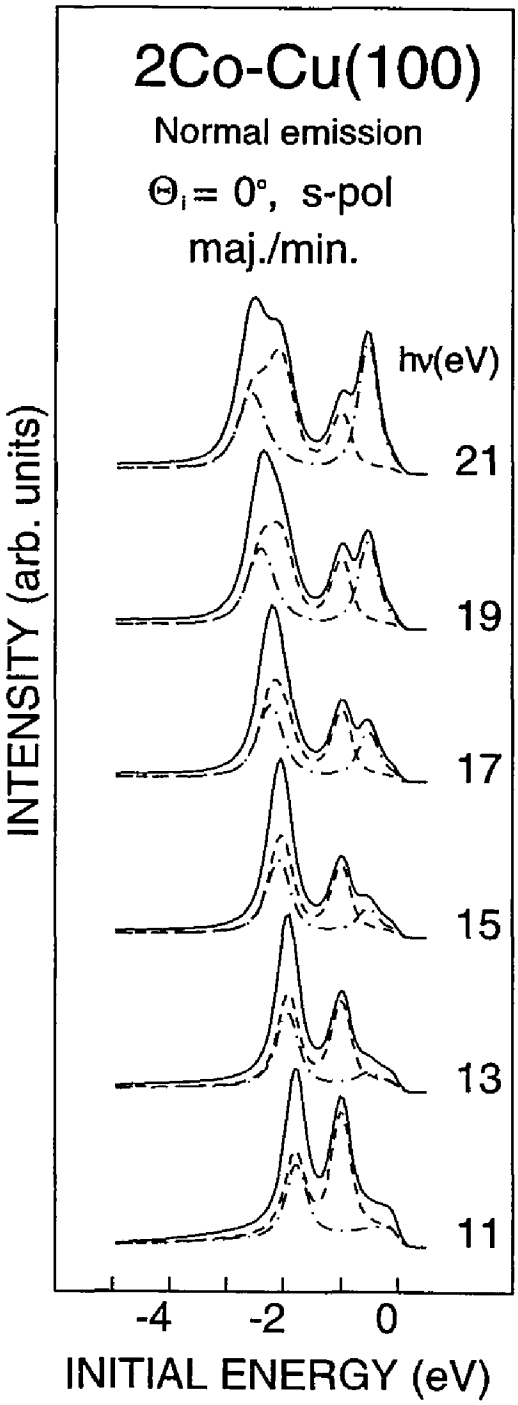

Fig. 2: s-polarized normal photoemission for two overlayers of Co on Cu(100): dashed-dotted line: minority spin contribution, dashed line: majority spin contribution, full line: total contribution.

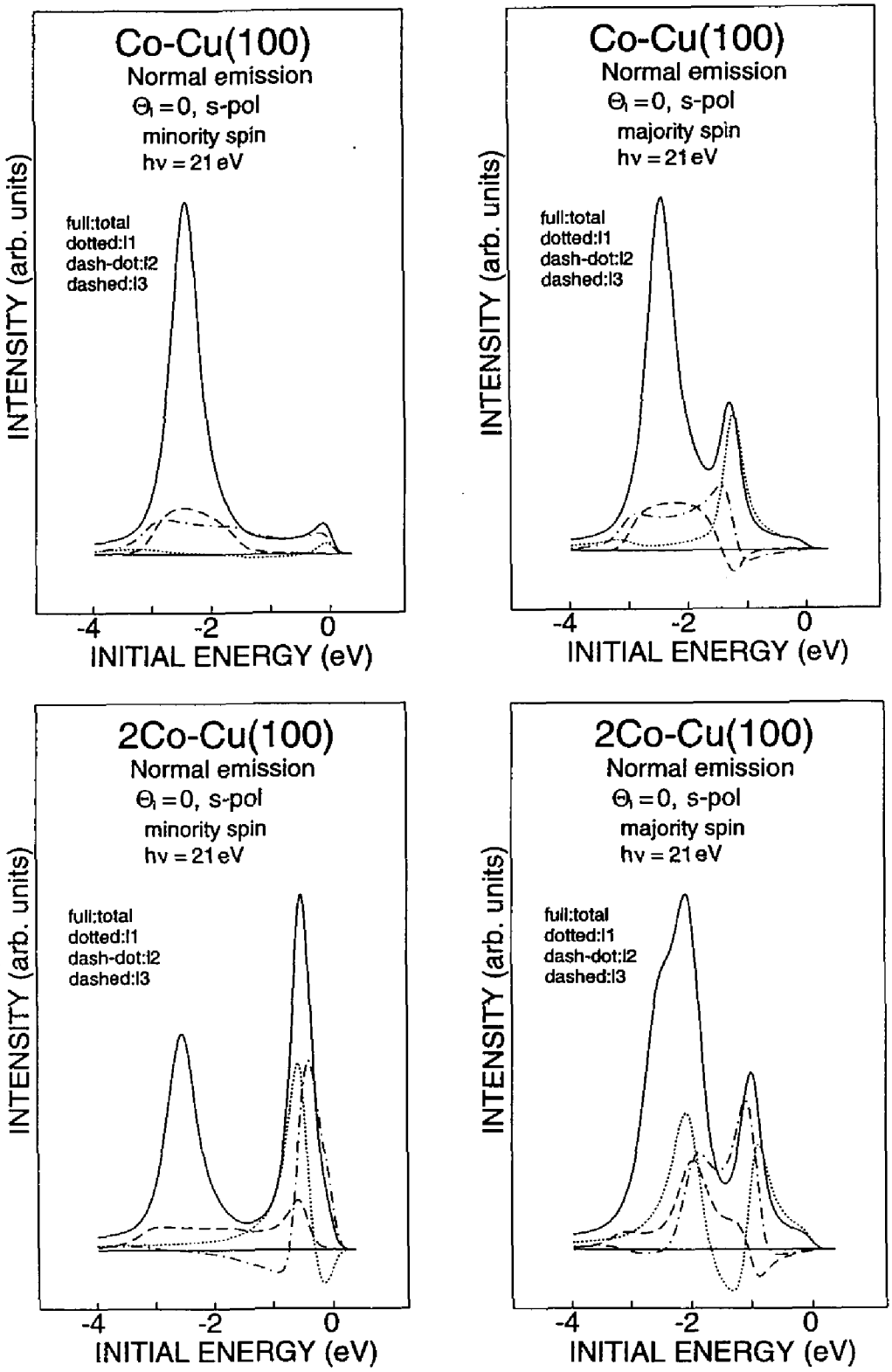

Fig. 3: Layer resolved contributions to the s-polarized normal photoemission at 21 eV. For Co/Cu(100): l1: Co-layer, l2: first Cu-layer, l3: second Cu-layer. For 2Co/Cu(100): l1: first Co-layer, l2: second Co-layer, l3: first Cu-layer.

the imaginary part of the potential yielded an excellent agreement with experimental data for Cu(100) of Schneider *et al.* [7].

RESULTS

We calculated photoemission spectra for normal emission and angles of 0° and 60° for the incident light. According to the experimental data [1] the photon energy varied from 11 to 21 eV. As normal emission requires totally symmetric final states (Δ_1), Cu-bulk transitions are allowed from Δ_5 initial state bands for s-polarized light, and from Δ_1 and Δ_5 initial state bands for p-polarized light.

Fig. 2 presents the normal incidence spectra for the majority and the minority contributions and the total photocurrent. The lowest peak in these spectra in the vicinity of –1.7 eV to –2.5 eV follows the dispersion of the Cu Δ_5 initial state band. In addition we find peaks which do not change their position with varying photon energy. In the majority spectra they appear at –1.0 eV and –2.1 eV whereas in the minority spectra they can be found at –0.5 eV. Clearly these peaks do not arise from Bloch-like initial states. The layer-resolved spectra reveal that indeed the corresponding initial states are highly localized in the first two to three layers. Whereas at least for low photon energies the majority inital states seem to affect the contributions from the first Cu layer (i. e. the 3rd layer), this effect does not occur in the the case of minority spin.

Inital states, which are predominantly confined to the Co overlayers in the 2Co-overlayer system give rise to two quite narrow peaks, mapping a typical bonding/antibonding situation, whereas the single Co overlayer exhibits only one peak situated energetically inbetween the former two peaks (see in particular the comparison in Fig. 3)

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