

## Spin-polarized X-ray emission spectroscopy for disordered semi-infinite systems

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### ABSTRACT

X-ray emission spectra of  $\text{Fe}_x\text{Co}_{1-x}/\text{Cu}(100)$  are presented using a spin-polarized fully relativistic multiple-scattering theory in order to emphasize new features in comparison with a non-spin-polarized description. The variations in the calculated Co and Fe spectra with respect to the layer thickness are explained by means of electronic structure calculations using the screened Korringa–Kohn–Rostoker method. X-ray emission spectra for ferromagnetic and antiferromagnetic aligned films are compared.

### §1. INTRODUCTION

Recently, we developed a theoretical description for spin-polarized X-ray emission spectroscopy using fully relativistic multiple-scattering theory (Pustogowa *et al.* 1998). As opposed to the theoretical investigation by Strange *et al.* (1991) and experiments by Hague *et al.* (1993), and Duda *et al.* (1994, 1995), analysing the total photon emission generated by transitions to core holes created by different polarized radiation, we calculate the intensities of polarization-resolved emission independent of the core hole creation.

We have calculated X-ray emission spectra and their magnetic dichroism for Co and Fe in  $\text{Fe}_x\text{Co}_{1-x}/\text{Cu}(100)$  for alloy film thicknesses up to 7 monolayers (ML). In this paper we compare total emission spectra and the magnetic dichroism for films with ferromagnetic and antiferromagnetic coupled layers corresponding to  $x = 0.8$  by discussing in quite some detail the contribution of the surface and the alloy–substrate interface to the spectrum of the total film.

### §2. THEORETICAL DESCRIPTION

The electronic transition intensity to a well defined core state  $\psi_{Qc}(\mathbf{r})$  at a given site  $n$  (Pustogowa *et al.* 1998) is defined as

$$I_{Qc}^{q\lambda n}(\varepsilon) \propto (\varepsilon - \varepsilon_{Qc}) \sum_{Q_1, Q_2} \mathcal{M}_{Q_1}^{q\lambda n}(\varepsilon) \text{Im} \tau_{Q_1 Q_2}^{nn}(\varepsilon) \mathcal{M}_{Q_2}^{q\lambda n}(\varepsilon), \quad (1)$$

with transition matrix elements

$$\mathcal{M}_{Q}^{q\lambda n}(\varepsilon) = \int d^3 r_n Z_Q^n(\mathbf{r}_n; \varepsilon)^+ (\boldsymbol{\alpha} \cdot \mathbf{a}_\lambda) \psi_{Qc}(\mathbf{r}_n), \quad (2)$$

for a fixed polarization of the emitted photons  $\mathbf{a}_\lambda$  and using regular scattering solutions  $Z_Q^n(\mathbf{r}_n; \varepsilon)$  to describe the initial valence states. The magnetic dichroism is defined as the difference between the intensities for left-handed and right-handed circular polarized emission.

## §3. RESULTS AND DISCUSSION

In the present paper, X-ray emission  $L_3$  spectra of Co and Fe in a (homogeneously) disordered alloy  $\text{Fe}_x\text{Co}_{1-x}$  on Cu(100) are investigated. As follows from total energy calculations (Zabloudil *et al.* 1998a) for  $x = 0.8$ , the films 5 and 7 ML thick are coupled antiferromagnetically with two ferromagnetically aligned surface layers. At this particular concentration, the alloy films 1, 2, 3, 4 and 6 ML thick favour ferromagnetic coupling.

All calculations reported here are based on the fully relativistic spin-polarized screened Korringa–Kohn–Rostoker method (Szunyogh *et al.* 1995) and the coherent potential approximation (Weinberger *et al.* 1996) for generating the corresponding self-consistent potentials and spin-polarized partial local densities of states.

In figure 1 the total  $L_3$  emission spectra of Co and Fe for several  $\text{Fe}_{0.8}\text{Co}_{0.2}$  films are shown. Both, the Co and the Fe spectra for the 3 and 6 ML case differ only marginally from the 4 ML case, while the 5 ML spectrum is very similar to the 7 ML spectrum. In the 1 ML case and for the antiferromagnetically coupled films, a pronounced peak at around 1.3 eV occurs in the Fe spectrum, whereas, in the Co spectrum, only an enhancement is found.

Figure 2 shows the magnetic dichroism spectra of Co and Fe for the same systems as in figure 1. Obviously, the dichroism for the antiferromagnetically coupled film spectra is an order of magnitude smaller than for ferromagnetically coupled films. As is to be expected, the largest dichroism is found for the monolayer film.

In figures 3 and 4, the layer-resolved contributions to the total spectra and the magnetic dichroism for the 7 ML film are shown. The total emission spectra from Co sites in different layers show no distinct variations. Only the Fe spectrum corre-

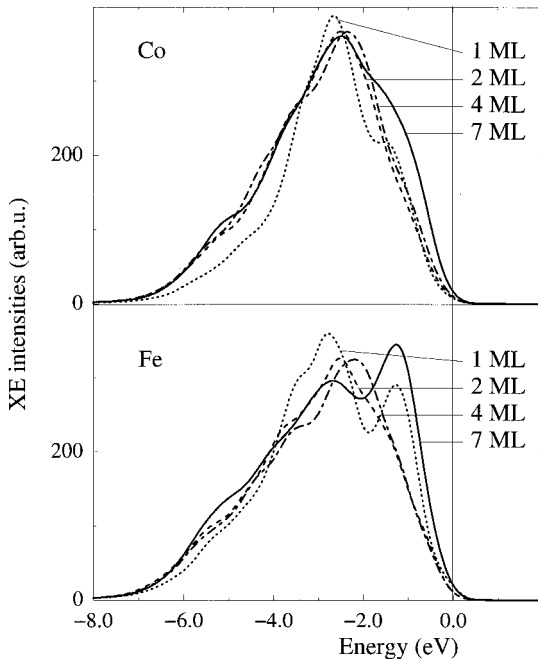


Figure 1. X-ray emission  $L_3$  spectra of Fe and Co in  $\text{Fe}_x\text{Co}_{1-x}$  films on Cu(100).

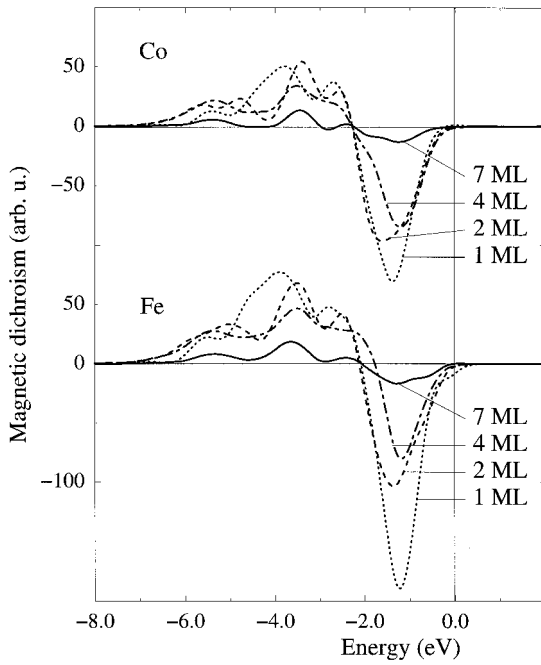


Figure 2. Magnetic dichroism in X-ray emission of Fe and Co in  $\text{Fe}_x\text{Co}_{1-x}$  films on Cu(100).

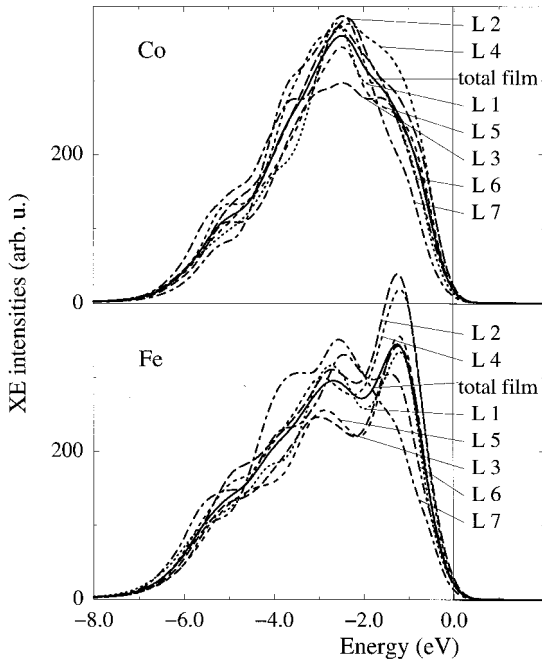


Figure 3. Layer-resolved contributions to the X-ray emission  $L_3$  spectra in a  $\text{Fe}_x\text{Co}_{1-x}$  film 7 ML thick on Cu(100).

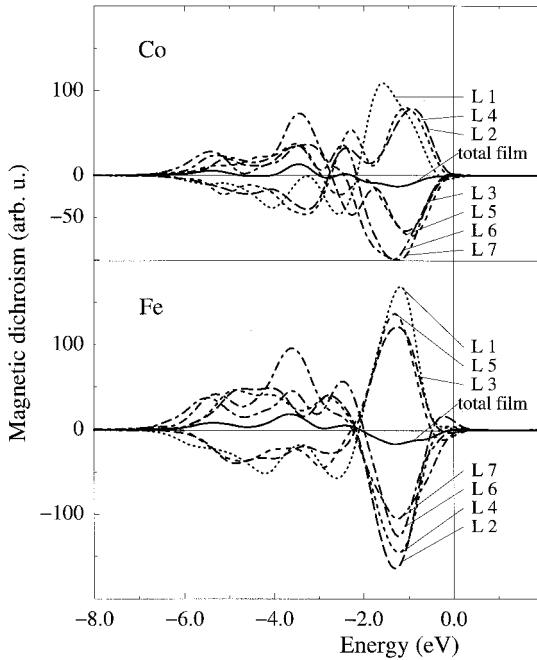


Figure 4. Layer-resolved contributions to the magnetic dichroism in X-ray emission in a  $\text{Fe}_x\text{Co}_{1-x}$  film 7 ML thick on Cu(100).

sponding to the surface layer differs noticeably. The Fe layer-resolved spectra clearly show that the peak around 1.3 eV does not originate from the emission from surface Fe atoms but results from all antiferromagnetically deeper-lying layers. The dichroism spectra in figure 4 show characteristic changes in sign due to antiferromagnetic coupling of neighbouring layers. For Fe sites this behaviour corresponds to a type of layer coupling, whereas, for Co, layers 2–5 (layer counting starting from the Cu–alloy interface) the sign of dichroism is reversed compared with the Fe case. These results fit very well the layer-resolved calculated magnetic moments (Zabloudil *et al.* 1998b). In contrast with the total emission spectra, the shape of the total dichroism spectra is determined by the dichroism of the surface emission. For a ferromagnetically coupled film (6 ML, not shown here) the largest magnetic dichroism occurs at the surface and the interface layers, for Co as well as for Fe sites.

In conclusion, we have shown the origin of characteristic features in Fe and Co X-ray emission spectra using layer-resolved calculations of the total spectra and the corresponding magnetic dichroism. Surprisingly, the structure of the total spectra is determined by the antiferromagnetically-coupled bilayers, with the emission from the surface playing a less important role.

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