

Investigating Ferromagnetic Band Structure with Magnetic Circular Dichroism in Valence Band Photoemission

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The knowledge of the electronic structure of magnetic thin films is of great importance for the interpretation of a variety of effects such as magnetic anisotropy, magnetic interlayer coupling, magneto-optical Kerr effect, etc. These effects are founded on the presence of both the magnetic exchange interaction, which splits electronic states into majority and minority bands, and the spin-orbit coupling, which links the

electron spin to its orbital momentum. For studies of the band structure of solids, angle-resolved photoemission has been widely employed in the last decades. In ferromagnets, the extension of spin-analysis can yield more detailed information. Its use is, however, hindered by low count-rates, and consequently long acquisition times. This is particularly annoying when studying surfaces and thin films. We will show in the following how magnetic circular dichroism in angle-resolved UV photoemission without spin analysis can be employed for band structure investigations.

MCDAD, magnetic circular dichroism in angular distribution (1), is the difference in photoelectron intensity between photoelectron spectra taken with circularly polarized light of opposite helicity. It is thus a differential technique, allowing the comfortable identification of magnetic contributions in a spectrum which may consist also of non-magnetic signal from, e.g., overlayers. Since the effect of MCDAD itself is a result of the simultaneous presence of exchange and spin-orbit interaction, it is highly appropriate to study exchange and spin-orbit split band structures. We will in the following restrict ourselves to highly symmetric experimental geometries. For samples which are magnetized perpendicularly to the surface such a high symmetry can be realized by normal light incidence and detection of the normally emitted photoelectrons. For this geometry, Henk et al. obtained analytically a set of direct relations between the relativistic symmetry character of the valence bands and the observed dichroism (2). Using the expressions of Ref. (2), the dichroism spectra can be correlated to direct transitions in the relativistic band structure.

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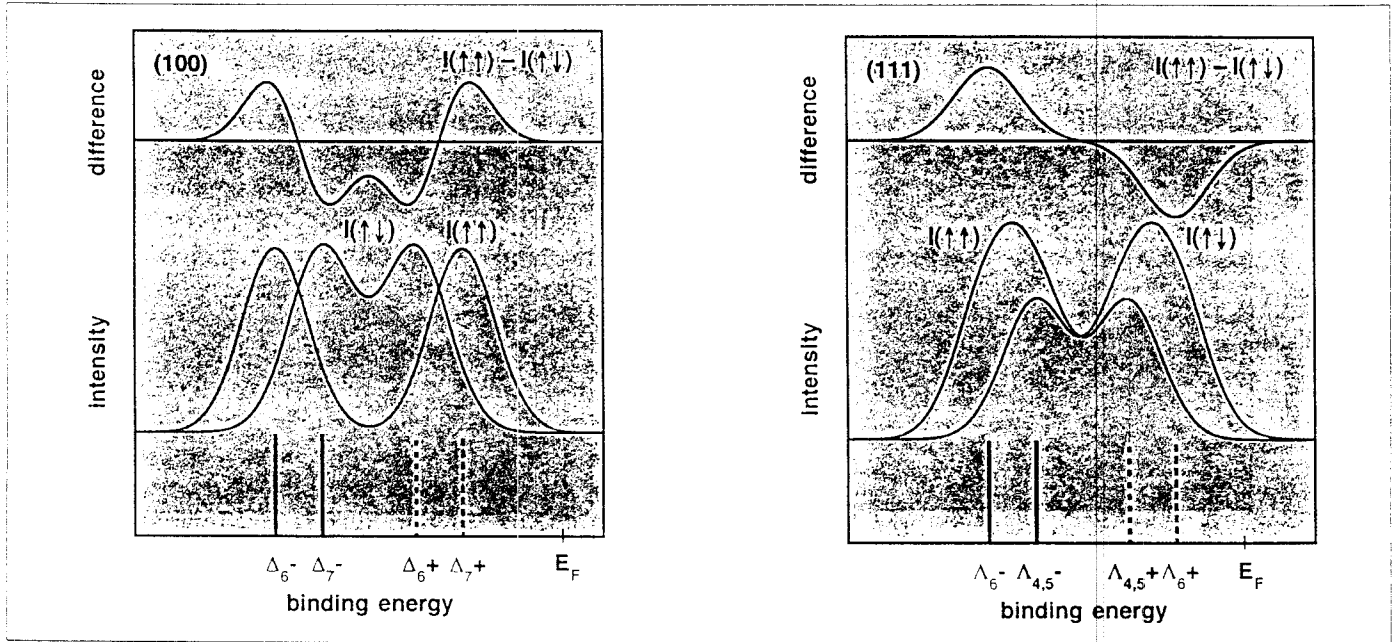


Figure 1. Schematic explanation of the observed dichroism for fcc (100) (left) and (111) surfaces (right). Depending on the alignment of light helicity and magnetization ($I(\uparrow\uparrow)$ or $I(\uparrow\downarrow)$) different initial state bands (bottom) contribute to the photoemission spectra (center). The difference spectra show characteristic plus and minus peaks (top).

Photoelectron spectroscopy in normal emission probes the electronic states along the symmetry axis in momentum space which is parallel to the surface normal. This is the Δ axis for fcc (100) surfaces, and the Λ axis for fcc (111) surfaces. The momentum along this axis can in a first approximation be calculated from the kinetic energy of the photoelectrons, assuming free electron-like final state bands. Varying the photon energy of the exciting radiation, different points in momentum space along this symmetry axis are probed, and the initial state bands mapped.

For the interpretation of the spectra, one has to recall that different electronic bands can exhibit different behavior under symmetry operations. This symmetry character of the bands permits the discrimination of the bands using MCDAD. In a ferromagnet the symmetry is reduced by the presence of the magnetization axis, and bands with different spin character will also exhibit a different symmetry character. Following the nomenclature of Ref. (2), we will label bands on the Δ axis with Δ_{6+} , Δ_{6-} , Δ_{7+} , and Δ_{7-} , and bands on the Λ axis with $\Lambda_{4,5+}$, $\Lambda_{4,5-}$, Λ_{6+} , and Λ_{6-} . This nomenclature follows the irreducible representations of the non-magnetic case.

Note that listed above are only those bands which, according to dipole selection rules, can be excited in the given experimental geometry. The + (-) sign thereby denotes the time reversal symmetry, and not the spin of the electrons, because the latter is not a good quantum number in the presence of spin-orbit coupling. In regions without interband hybridization, that is where the spin character of the bands is preserved, negative time reversal symmetry can be regarded as majority spin, and positive as minority spin of these bands.

Depending on the polarization of the incoming light, only transitions from specific bands are possible. Table 1 summarizes the results of Ref.

Table 1. Initial state bands which contribute to the photoemission spectra for parallel ($\sigma \uparrow \uparrow \mathbf{M}$) and antiparallel ($\sigma \uparrow \downarrow \mathbf{M}$) alignment of light helicity and magnetization. Listed are bands for normal emission from a (100) and a (111) surface according to their symmetry character.

	$\sigma \uparrow \uparrow \mathbf{M}$	$\sigma \uparrow \downarrow \mathbf{M}$
(100)	Δ_{6-}, Δ_{7-}	Δ_{6+}, Δ_{7+}
(111)	$\Lambda_{4,5+}, \Lambda_{4,5-}, \Lambda_{6-}$	$\Lambda_{4,5+}, \Lambda_{4,5-}, \Lambda_{6+}$

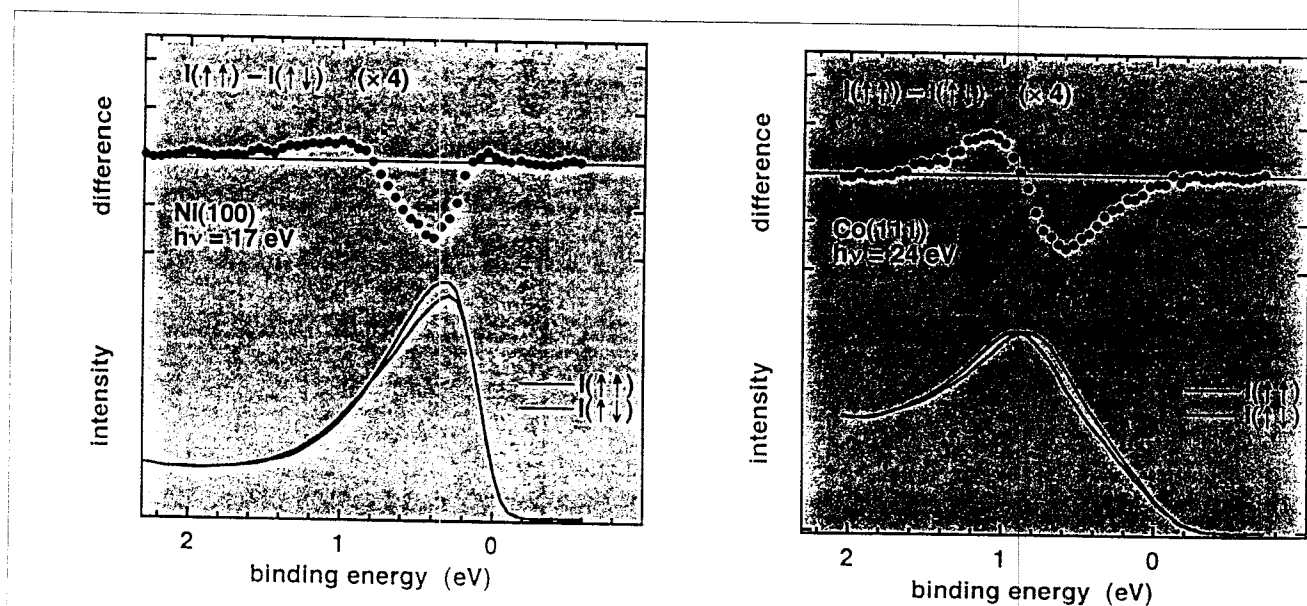


Figure 2. Experimental magnetic circular dichroism of Ni(100) (left) and Co(111) (right) thin films. The bottom panels show spectra for parallel (red) and antiparallel (green) alignment of light helicity and sample magnetization, the top panels the difference between both.

(2) for the geometries considered here. The dichroism thereby only depends on the relative orientation of the vectors of light helicity σ and magnetization M . For σ and M parallel, only electrons from Δ_6^- and Δ_7^+ bands are excited in the case of (100) surfaces, and only electrons from $\Lambda_{4,5}^+$, $\Lambda_{4,5}^-$, and Λ_6^- bands in the case of (111) surfaces.

This excitation of different initial state bands when switching the light helicity is the source of the main dichroism effect. This is schematically illustrated in Figure 1. On the left hand side the situation for a (100) surface is outlined, and on the right hand side for a (111) surface. Energetic positions of the different bands are marked in the bottom panels. The center panels show schematic photoemission spectra for parallel (red) and antiparallel alignment (green) of photon spin and magnetization. The dichroism, i.e., the difference between the two spectra, is depicted in the top panels. For the (100) case it shows a plus-minus-plus shape, with the minus feature located at the energetic positions of the Δ_6^- and Δ_7^+ bands. In the case of the (111) surface, the difference spectrum shows a plus peak at the position of the Λ_6^- band, and a minus peak at the position of the Λ_6^+ band. Spectral features in an MCDAD spectrum are thus directly related to the energetic positions of individual bands. This

allows the experimenter to trace these bands in order to obtain the experimental band dispersion by simply varying the photon energy.

Experimental spectra corresponding to the schematic explanation of Figure 1 are presented in Figure 2. All experimental spectra presented here were taken at the 6.5 m normal incidence monochromator beamline of the Berlin synchrotron radiation source (BESSY). By obscuring the light emitted in the ring plane a circular polarization of about 90% is obtained (3). The overall energetic resolution of the spectra presented here was about 200 meV.

A magnetization perpendicular to the surface can be found in ultrathin Ni films on Cu(100) (4). The left hand side of Figure 2 shows experimental spectra of 15 monolayers (ML) of Ni on Cu(100), taken with a photon energy of 17 eV (6). In the bottom panel the photoemission spectra for parallel (red) and antiparallel alignment (green) of photon spin and magnetization are depicted. The top panel shows the difference between both spectra. It is immediately clear that by circular dichroism a significant plus of information is obtained. Taking the average of the red and the green curve (what would be observed for linearly polarized light) results in a single broad peak, from which it would be very

hard to extract any further information.

The right hand side shows spectra for a 3 ML film of Co on Cu(111) (7). This film exhibits a perpendicular magnetization when it is grown using 1.5 ML Pb as surfactant, and capped by several monolayers of Cu, in our example 3 ML (5). Here the photon energy was 24 eV. Again the circular dichroism clearly yields more information than standard photoemission would.

In both cases a pronounced dichroism is observed, which is qualitatively the same as shown in Figure 1, although the plus and minus features in the experimental difference spectra are not as pronounced as in the explanatory scheme. The exact shape of the spectra depends strongly on the energetic separation between the participating bands and also on the details of the hybridization, and can of course differ from the one assumed in Figure 1. In the (111) case the difference spectrum shows a pronounced plus/minus shape, which clearly is close to the one given in Figure 1. The plus and minus peaks, which are linked to the energetic positions of the respective bands, allow the distinction between the closely lying valence bands of ferromagnets. Having identified the peaks in the dichroism it is now possible to look for the dispersion of the dichroism peaks. This was successfully done for Ni/Cu(100) (6). Comparing the experimental results with fully relativistic photoemission calculations yielded not only the dispersion of the magnetic band structure, but also details of inter-band hybridization. In the case of Co/Cu(111) it was demonstrated that even in a film of only 3 ML a bulk-like band dispersion is observed (7). Because the $\Lambda_{4,5+}$ and Δ_6+ bands, and also the $\Lambda_{4,5-}$ and Δ_6- bands, are little separated in energy (by the spin-orbit splitting, typically 50 meV (6)), the information obtained by MCDAD is comparable to that obtained by spin-resolved photoemission. A plus peak is located at the position where without hybridization the majority bands are found, and a minus peak at positions of the minority bands.

The present examples show how magnetic circular dichroism in a highly symmetric experimental set-up can be used to study the relativistic electronic structure of ferromagnetic materials without the rather time-consuming spin analysis. In highly symmetric configurations the dichroism is linked to the relativistic band symme-

try by simple analytic expressions. Spin-integrated intensity spectra, taken for both directions of either the light helicity or the sample magnetization, are capable of delivering information comparable to spin-resolving techniques. ■

Acknowledgement

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Errata

In the article "Photoelectron Spectroscopy and the Dipole Approximation" by O. Hemmers et al. which appeared in *SRN* Vol. 9 No.6, 1996, Figures 2 and 3 should have appeared in color. The publishers regret this error. The correct versions of these figures are reproduced below.

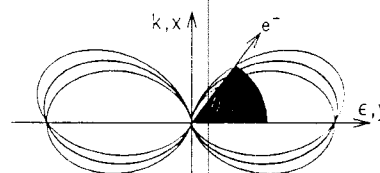


Figure 2

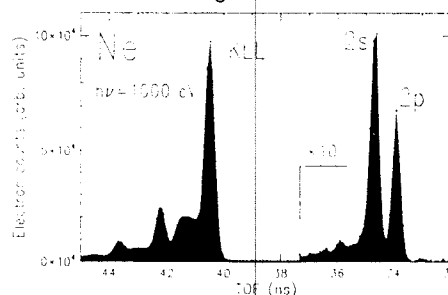


Figure 3