



	<b>Experiment title:</b> <b>Magnetic Linear Dichroism in X-ray Emission Spectroscopy</b>	<b>Experiment number:</b> HE-317
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## Report

In this experiment we study the Magnetic Linear Dichroism (MLD) effect in 2p<sub>4d</sub> x-ray emission spectra of Yb. MLD is well known in x-ray absorption, where it is defined as the difference in absorption of p-polarised x-rays ( $q=\pm 1$ ) and s-polarised x-rays ( $q=0$ ). The x-ray absorption MLD effect can be detected by measuring the x-ray absorption parallel and perpendicular to the magnetic ordering direction, in other words it identifies with the angular dependence of the x-ray absorption cross section with respect to the magnetic vector. In analogy, the x-ray emission MLD effect is the angular dependence of the x-ray emission cross section with respect to the magnetic vector.

We have carried out 2p<sub>1/2</sub>4d x-ray emission experiments on Yb-garnet. In case of Yb-garnet, the Yb ground state has one 4f hole present, and the Yb<sup>3+</sup> ions have 4f<sup>13</sup>[2F<sup>7/2</sup>] symmetry. The excitation energy has been chosen some 100 eV above the Yb 2p edge, to avoid the complications of resonance effects. The intermediate state is 2p<sup>5</sup>4f<sup>13</sup> plus an electron of high kinetic energy. In the 2p<sub>4d</sub> x-ray emission step, a 4d electron fills the 2p hole and the final state is 4d<sup>9</sup>4f<sup>13</sup>. A crucial ingredient is the large overlap of the 4d and 4f wave functions, the so called 'multiplet effects' in the final state. This creates the specific 2p<sub>4d</sub> XES spectral shape, and it is the angular variation of this shape that can be studied.

Figure 1 shows the 2p<sub>1/2</sub>4d x-ray emission spectral shape and measured at detection angles  $\theta=20^\circ$  and  $\theta=60^\circ$ . The spectral shapes are similar, but a small difference is visible. It is noted that the integrated intensity is equal at the

two detection angles, which offers an additional normalisation check. If the magnetic field is turned off, the spectral difference between the detection angles of  $\theta=20^\circ$  and  $\theta=60^\circ$  disappears completely. This proves that the origin of the linear dichroism is the magnetic ordering.

Figure 2 shows the comparison between theory and experiment. Indicated are the experimental  $2p_{1/2} 4d$  XES spectral shape together with the difference between the two detection angles, which is proportional to the MLD spectral shape. The theoretical stick spectrum has been convoluted with a Lorentzian broadening of 2.5 eV (HWHM) of and a Gaussian broadening of 0.75 eV (HWHM). The theoretical spectra have been shifted to align the peak position with experiment and the peak intensities of experiment and theory have been made equal. The theoretical MLD curve has been calculated by applying a magnetic field in the  $z$ -direction and determining the difference between the  $q=\pm 1$  and  $q=0$  dipole channels. The shoulder at 9770 eV is related to the  $^1H_5$  state. The peak is related to the combination of the three states  $^3P_2$ ,  $^3D_3$  and  $^3G_4$ . The comparison shows that an overall the experimental shape is reproduced. Some small differences are visible, for example the position of the high-energy shoulder is a bit higher in theory than in experiment. Also there is a small shoulder visible in the negative lobe of the MLD spectrum and the MLD spectrum has a small non-zero offset around 9785 to 9790 eV. We believe these small discrepancies are essentially due to uncertainties in the precise values of the Slater integrals, which have been determined from the 80% reduced Hartree-Fock values. We conclude that the  $2p_{1/2} 4d$  XES and MLD spectral shapes can be described in great detail with the  $2p_{1/2}4f^{13}$  to  $4d^9 4f^{13}$  atomic dipole transitions. We note that this is not obvious, as one could expect screening effects in the intermediate state to affect the spectral shape. For example, in case of  $1s3d$  XES spectral shape of nickel compounds, these screening effects are known to be important

**Figure 1:**

The  $2p_{1/2}4d$  x-ray emission spectral shape at the detection angles  $\theta=20^\circ$  (points) and  $\theta=60^\circ$  (line)

**Figure 2:**

Comparison of the  $2p_{1/2}4d$  XES and MLD spectral shape with the broadened theoretical spectrum

