ESRF

Experiment title: Spin dependent momentum density in nickel		**Experiment number:** HE-056
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Report:

In this experiment, we measured high resolution (~0.4a.u.) magnetic Compton profiles (MCPs) from a single crystal sample of pure nickel. Four projections were taken, the resolved directions being <100>, <110>, <111> and <112>. At this resolution, the existence of discrepancies between experiment and band theoretical calculations is clear, the detailed structure of the experimental profiles at these momenta is smeared out. The aims were (i) to provide a better test of FLAPW theoretical band calculations' for the spin dependent momentum densities than available from previous lower resolution experiments performed elsewhere and (ii) to look for the fine structure expected at high momenta. Also, by taking all four projections in the [110] plane, it was hoped that the 2D [110] projection could be reconstructed from the 1D experimental data.

Figure 1 shows data for the <100> projection. The solid line represents the experimental data obtained during this beamtime; the dotted line represents the theory', convoluted with the experimental resolution function (0.4a.u.). The area under these curves is proportional to the total spin moment of the nickel sample. The large dip near $p_z=0$ is due to the negative polarisation (with respect to the d moment) of the s electrons.

Here, the theory overestimates the experimental momentum density. The <110> projection does clearly indicate the existence of so-called Umklapp features, predicted by theory, but not visible in previous, lower resolution, experiments. However, even at this improved resolution, the existence of these high momentum features cannot be determined in the other directions. Kubo[1] calculated the individual contributions from each majority and minority band and hence we hope to be able to identify the source of the errors in the theory.

At present, data analysis is still in progress. We are investigating the enhancement obtained through partial deconvolution of the resolution function from the experimental profiles, using the MaxEnt algorithm. We are reconstructing the 2D projection in the [110] plane from our 1D MCPs as presented in figure 2.

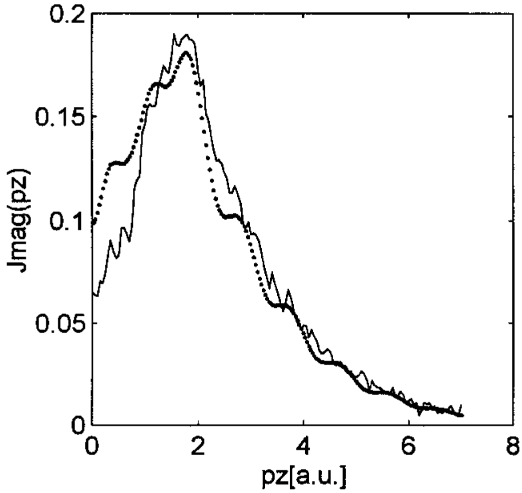

Figure 1. <100> theoretical and experimental MCPs of nickel. See text for details.

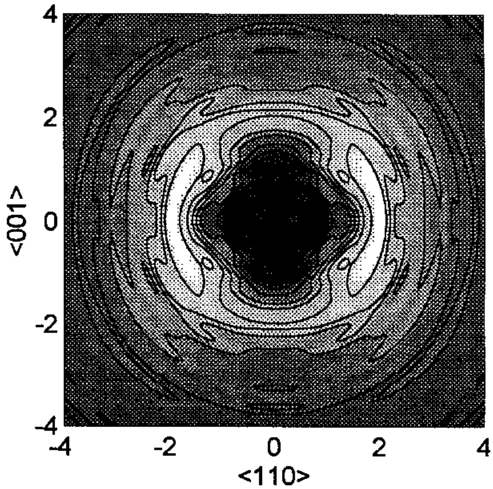

Figure 2. Reconstructed 2D magnetic momentum density for nickel [110].

Comparison of this with (unpublished) spin-polarised 2D-ACAR data' reveals some of the difference between the two techniques, especially the positrons' enhanced sampling of the s electrons, at the expense of the d electrons; the Compton technique being cleaner. Hence the dip near $p_z=0$ is exaggerated in the positron technique, and as a result the data are not related simply to the total spin moment. We have just received Kubo's full 3D theoretical calculations as used in [l], from which we can calculate the 2D projection to compare with our reconstructed experimental data. This will enable us to analyse both the theory and the quality of the reconstruction algorithm when applied to low numbers of projections.

[l] Y. Kubo & S. Asano, (199O)Phys. *Rev. B 42 No.7,4431-46.*

[2] Private communication, A. Manuel, Universite de Geneve; see also P. Genoud et al, J. *Phys.: Condens. Matter* (1991) 3 4201-12.