ESRF	**Experiment title:** Magnetic Compton scattering from Gd and $Gd_{62.4}Y_{37.6}$	**Experiment number:** HE-269
Beamline: ID15a	**Date of experiment:** from: 4.12.97 to: 11.12.97	**Date of report:** 2.98
shifts: 21	**Local contact(s):** J.E McCarthy	*Received at ESRF:* 04 MAR. 1998

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Report:

The objective of this experiment was to investigate the spin moment in one of the ferromagnetic phases in the gadolinium yttrium alloy, $Gd_{62.4}Y_{37.6}$, chosen instead of the original proposed sample, $Gd_{68.9}Y_{31.1}$, for technical reasons: the same phenomena were studied. The magnetic Compton scattering technique used measures a projection of the spin-dependent electron momentum density, revealing the origin of contributing spin moments in a magnetic system, and providing a rigorous test of electronic structure calculations. The measured magnetic Compton profile (MCP) has an area proportional to the total spin of the measured sample.

In the experiment, an induced spin moment of -0.4 μ_B was observed for the first time on the Y conduction electrons in the alloy. Additionally, a pure Gd sample was measured to provide a comparison, revealing the effect of the Y on the momentum space spin density. A detailed comparison of the alloy results with LMTO calculations is in progress, and the pure Gd result is being prepared for publication in its own right, since previous measurements were limited to a much lower resolution, and were made in the phase where the moments are canted rather than collinear.

Pure Gd is the only ferromagnetic 4f metal, whilst Y is non magnetic. Alloys form for all compositions, with a substitutionally disordered hcp structure. It is known that the alloy contains two ferromagnetic and one basal plane antiferromagnetic phase; Y does not simply

behave as a diluent. The main objective in our study was to look for the presence of any induced moment on the Y electrons in the ferromagnetic phase. As well as measurements on ferromagnetic Gd and Gd-Y, the alloy was measured in its antiferromagnetic phase, both with and without afield present; the addition of the field forces the moments to align out of the basal plane, resulting in a non-zero induced moment.

In figure 1, the MCP of pure Gd is presented, together with a band structure calculation performed using the FLAPW method [2]. The sample temperature was maintained at 235K, at which temperature the sample is ferromagnetic, with a moment aligned along the c-axis. The MCP contains two main contributions, as indicated in the figure. The wide component is the 4f contribution to the magnetic moment, of value s = 7 μ_B. The narrower peak is a measure of the spin moment induced on the s,p,d conduction electrons, and its value was determined to be -0.6 μ_B by fitting the 4f part to the high momentum tails. This agrees well with theoretical predictions using the LMTO prescription, within both the local spin density and generalised gradient approximations. The LMTO results are now being used to predict the shape of the MCPs, in order to assess the quality of these approximations in the 4f magnetic system.

In figure 2 the MCP of $Gd_{62.4}Y_{37.6}$ is presented. Also shown, on an enlarged scale, is the difference between the spin densities for the alloy and pure Gd, the curves being normalised to the 4f moment before subtraction. The MCP is very similar to that for pure Gd, showing the large contribution of the 4f electrons. The main differences occur at low momentum, as revealed by the difference plot. This shows changes in the spin-dependent electron momentum density attributed to the presence of an induced moment on those electrons originating from the Y sites. Analysis of the results for the antiferromagnetic phase indicate that the momentum distribution is not observably different from that in the ferromagnetic phase.

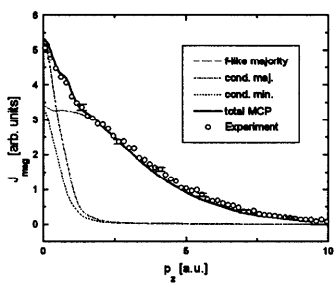

Figure 1. MCP for pure Gd at 233K

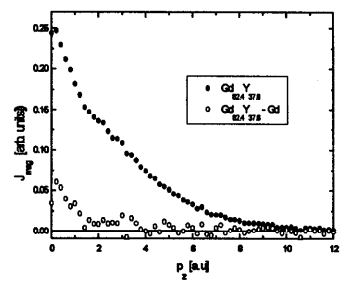

Figure 2. MCP for $Gd_{62.4}Y_{37.6}$, and difference from pure Gd.

A paper on the pure Gd data is in preparation and will be submitted for publication as soon as our LMTO calculations are complete. The Gd-Y results, which unambiguously indicate the presence of an induced moment on the Y conduction electrons will be submitted as a Phys. Rev. Lett. In view of this result, we are extremely eager to study the distribution in the other ferromagnetic phase, in another composition of the alloy.

[1] Y. Kubo and S. Asano (1992) *J. Mag Mag Matt.* **115** 177.

ESRF	**Experiment title:** Spin-Dependent Electron Momentum Distributions in Fe3Al and Fe3Si Single Crystals	**Experiment number:** HE-269
Beamline: ID15	**Date of Experiment:** from: 11/12/97 to: 17/12/97	**Date of Report:** 23.2.98
Shifts: 21	**Local contact(s):** Veijo Honkimaki	*Received at ESRF :* 02 MAR. 1998

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Report:

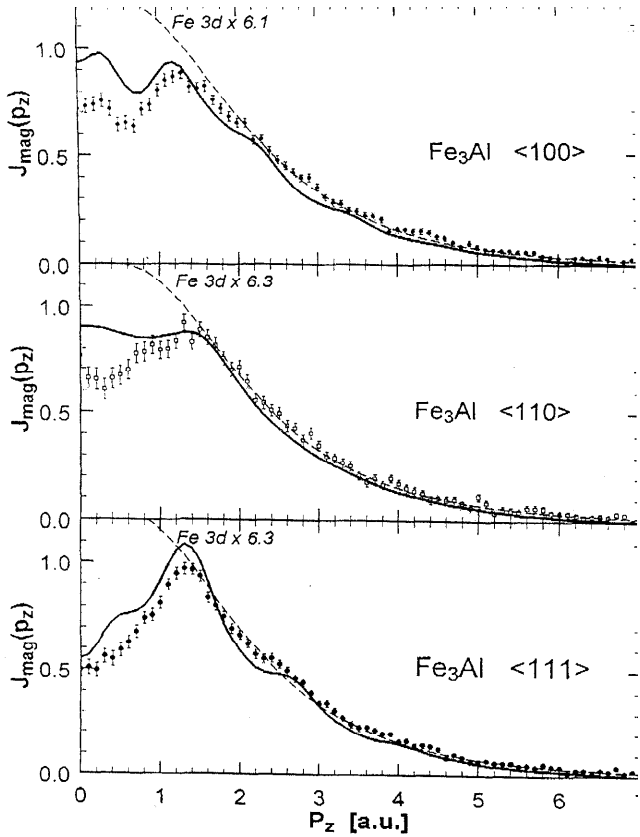
Circularly polarised synchrotron radiation at the ID1 5 has been used to study spin-dependent electron momentum distributions in Fe_3Al and Fe_3Si through studies of their magnetic Compton profiles single crystals. This is a continuation of our ESRF studies of spin density in ferromagnetic Heusler Alloys, the first of which on Cu_2MnAl was published in Dec 1997 [l]. The alloys have the DO3 crystallographic structure (four interpenetrating face-centred cubic sub-lattices) and there are two non-equivalent Fe sites in the compounds: C site with 8 iron atoms as nearest neighbours and B/D site with 4 Fe and 4 Al or Si atoms. Consequently the Fe atoms carry two distinctly different values of the magnetic moments. From polarised neutron data, treated assuming two different states of order, it is known that in Fe_3Si the structure is stable, the degree of order is very high, whereas Fe_3Al is easily subjected to disorder dependent on the sample history. Comparison the two alloys indicates that the Si substantially reduces the magnetic moment of Fe on the B/D site [2,3]. The experiments were carried out for 3 crystallographic directions: [100], [110] and [111] at a momentum resolution of 0.4 a.u.; the incident beam energy was 198keV. .Preliminary data analysis revealed the following features of spin-dependent electron momentum distributions in Heusler alloys under study:

1. The magnetic profiles are very similar for both crystals although one might expect differences due to higher disorder in Fe_3Al sample

2. The agreement of the experiment with KKR-CPA calculation [4] is good for Fe_3Si but a relatively big disagreement for Fe_3Al alloy is observed at low momenta. This is highlighted in the accompanying figure: it is particularly evident in the [100] and [110] directions.

3. Large anisotropies are observed in directional magnetic Compton profiles (up to 30% of their values at pz=0 a.u.) at momenta below 3 a.u. The biggest differences were observed between [111] and [100] directions. The overall characteristics of the anisotropies are similar for both alloys, however the amplitudes of oscillations are about 50% smaller in the case of Fe,Al sample.

4. Conduction electrons appear to contribute a negative polarisation of about 1 μ_B compared with the moment of 2 μ_B per iron atom.



The directional magnetic Compton profiles of Fe_3Al. At high momenta the results approach free-atom Fe 3d electron behaviour (dashed line) whereas the KKR-CPA theory (solid line) is too low: this is a common fault of band theory when too few reciprocal lattice vectors have been included in the momentum expansion. There are other significant discrepancies at low momenta, which are still being analysed. Fe_3Si, which is better ordered, shows much closer agreement with theory.

[1] E Zukowski, A Andrejczuk, L Dobrzynski, MJ Cooper, M AG Dixon, S Gardelis, PK Lawson,T Buslaps, S Kaprzyk, K-U Neumann and KRA Ziebeck J Phys Cond Matter 9 (1997) 10993 -*ESRF work*

[2] J.Moss, P.J.Brown, J.Phys. F2 (1972) 358.

[3] L.Dobrzynski, C.Petrillo and F.Sachetti, Phys.Rev. B42 (1990) 1142.

[4] S.Kaprzyk, Acta Physica Polonica, A9 1 (1997) 135.