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LETTER TO THE EDITOR

The spin-dependent Compton profile of gadolinium

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Abstract. Monochromated circularly polarised synchrotron radiation with an energy of 46.3 keV has been used to measure the spin-dependent Compton profile of polycrystalline gadolinium. The lineshape is in good agreement with the superposition of the profile of an atomic 4f electron distribution ($7\mu_B$), and a small ($0.55\mu_B$) free-electron parabola.

Compton scattering is an established method of studying electron momentum density distribution, $n(\boldsymbol{p})$. With unpolarised radiation it yields the projection, $J(p_z)$, commonly referred to as the Compton profile (see Williams 1977), i.e.

$$J(p_z) = \int_{p_x}\int_{p_y} n(\boldsymbol{p})\, \mathrm{d}p_x\, \mathrm{d}p_y \tag{1}$$

where p_x, p_y and p_z are Cartesian components of the momentum $\boldsymbol{p}$ with the z axis parallel to the x-ray scattering vector: $n(\boldsymbol{p})$ is insensitive to the spin distribution, and is summed over all the electronic contributions.

Platzman and Tzoar (1970) were the first to suggest that in ferromagnets the unpaired-spin distribution can be isolated in a difference experiment in which circularly polarised photons are used and the magnetisation direction is reversed. The magnetic part of the scattering cross section (Lovesey 1987, Blume 1987) has the form

$$\Delta\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}\omega}\right) = P_c\left(\frac{1-\cos\varphi}{mc}\right)\boldsymbol{S}\cdot(\boldsymbol{k}_i\cos\varphi + \boldsymbol{k}_f)J_{\mathrm{mag}}(p_z) \tag{2}$$

where P_c is the degree of polarisation, φ is the scattering angle and $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ are the incident and scattered wavevectors. The magnetic Compton profile, $J_{\mathrm{mag}}(p_z)$, is defined as the difference between the profiles with spin parallel, $n_{\mathrm{up}}(\boldsymbol{p})$, and anti-parallel, $n_{\mathrm{down}}(\boldsymbol{p})$, to the photon polarisation,

$$J_{\mathrm{mag}}(p_z) = \int_{p_x}\int_{p_y} (n_{\mathrm{up}}(\boldsymbol{p}) - n_{\mathrm{down}}(\boldsymbol{p}))\, \mathrm{d}p_x\, \mathrm{d}p_y. \tag{3}$$

The circularly polarised synchrotron radiation (CPSR) was extracted from the three-pole wiggler port at the Daresbury storage ring source by moving the apparatus either above or below the orbital plane (see Holt and Cooper 1983, Cooper *et al* 1986). For

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example at 0.15 mrad above the orbital plane $P_c = 0.7$ and the flux has dropped by less than an order of magnitude in comparison with its value in the orbital plane for photon energy of the order of 50 keV.

Previous work has concentrated on the 3d transition metals (see Cooper *et al* 1986, Mills 1987, Sakai and Sekizawa 1987). The first measurement for a rare earth, gadolinium, was made by Mills (1987) using CPSR produced by an x-ray phase plate at the Cornell High Energy Synchrotron Source.

The present experiment was carried out under the same conditions as reported in an earlier study on iron (see Cooper *et al* 1988). A Ge 220 monochromator was used to select radiation at 46.3 keV, i.e. below the Gd K-absorption threshold at 50.24 keV in order to avoid overlap of the Compton profile with the gadolinium fluorescence lines. The photons were detected by a solid-state detector (SSD) after being scattered through 149° ± 2° in transmission through a 250 μm thick foil. The resolution of the experiment (330 eV at 46 keV) was equivalent to a Gaussian of full width at half maximum 0.7 au of momentum (1 au = 1.99×10^{-24} kg m s^{-1}). The magnetic field was reversed at intervals of 10 and 20 s and data for two spin directions stored in separate memories (see Cooper *et al* 1986, Timms *et al* 1988). The Curie temperature of gadolinium is 293.2 K (Moon *et al* 1972) and it was therefore necessary to cool the magnetised sample to well below room temperature. Nitrogen gas, cooled by passage through liquid nitrogen, was blown onto the sample and the magnet, which were insulated in a polystyrene box. The consequent beam attenuation at 46 keV was negligible and the temperature of the sample stabilised around 200 K.

Approximately 5×10^5 counts were accumulated in the Compton peak for each magnetic field direction in the 15 h measurement period. The resulting difference profile contained 4×10^3 counts. The energy interval for data collection was 70 eV which is equivalent to 0.15 au of momentum. The difference spectrum was converted to an electron momentum scale, then corrected for the energy dependence of both the magnetic inelastic scattering cross section and the sample absorption. A correction for the efficiency of the SSD was not necessary because it is effectively constant and close to 100% across the energy range of interest. The multiple-scattering correction is predicted by Sakai (1987) to be insignificant (i.e. less than 1%) in the magnetic data for this thin sample.

According to the non-relativistic augmented-plane-wave calculation by Dimmock and Freeman (1964), the calculated conduction bands are not free-electron-like—they resemble markedly those of the 3d transition metals. This is mainly due to the fact that the atomic 6s and 5d states are overlapped, and that the bands near the Fermi level are of mixed s–d character and consequently are much flatter than would be expected from the free-electron model. The ground-state properties of gadolinium are also described by Harmon (1979) and Sticht and Kubler (1985) using the local-spin-density functional approximation where the magnetic moment is well determined when the 4f states of gadolinium are not included in the core states but are considered as valence states. The magnetic 4f shell lies well inside the atom, i.e. the 4f band is about 6 eV below the bottom of the conduction electrons band (see Moon *et al* 1972). Hence 4f electrons have a negligible overlap with the 4f shells of the neighbouring ions, and their only significant exchange interaction is with the conduction band.

The spin-dependence of the Compton profile of gadolinium is due largely to the inner unpaired 4f bound electrons which consequently give a broader profile than 3d ferromagnets. This can be seen in figure 1 where the magnetic profile extends well beyond 5 au. There is an extra, small magnetic moment (see Moon *et al* 1972, White *et*

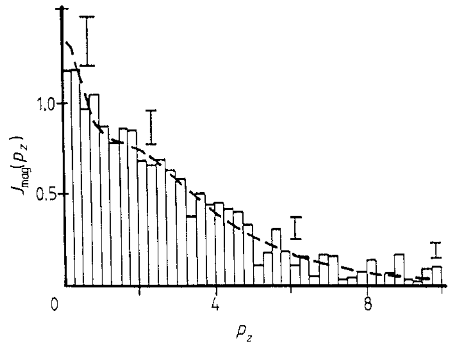

Figure 1. The magnetic Compton profile (see equation (3)) of ferromagnetic gadolinium normalised from -10 to 10 au to an area of 7.55 electrons. The curve represents the superposition of atomic 4f contributions which account for a moment of $7\mu_B$ and a free-electron contribution for the remaining $0.55\mu_B$. The theory has been convoluted with the experimental resolution function.

al 1976, Roeland *et al* 1975) arising from the spin polarisation of the conductions electrons ($6s^25d$) and this contributes significantly to the Compton profile at low momenta. In the absence of any theoretical calculation the experimental profile is compared with the superposition of the Compton profiles of the seven unpaired 4f electrons deduced from the atomic calculation by Biggs *et al* (1975) and a free-electron component equivalent to 0.55 electrons. It is clear that the profile due to the atomic 4f electrons alone does not adequately describe the experimental spin-dependent momentum distribution at low momenta. The small low-momentum peak was not apparent in the earlier measurement by Mills (1987) which was of poorer statistical quality and lower resolution, the latter accounting for the smaller magnetic peak heights reported by Mills for both Gd and Fe. A result similar to that reported by Mills has been obtained recently at the Japanese Photon Factory using an elliptical multipole wiggler (Itoh 1989). Our result is qualitatively in agreement with the simple theory outlined above, but greater statistical accuracy is needed if the central feature is to be investigated quantitatively.

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References

Biggs F, Mendelsohn L B and Mann J B 1975 *Nucl. At. Data Tables* **16** 252
Blume M J 1987 *Appl. Phys.* **57** 3615–8
Cooper M J, Collins S P, Timms D N, Brahmia A, Kane P P, Holt R S and Laundy D 1988 *Nature* **333** 151–2
Cooper M J, Laundy D, Cardwell D A, Timms D N, Holt R S and Clark G 1986 *Phys. Rev.* B **34** 5984–7
Dimmock J O and Freeman A J 1964 *Phys. Rev. Lett.* **13** 750–2
Harmon B N 1979 *J. Physique Coll.* **40** C5 65–70
Holt R S and Cooper M J 1983 *Nucl. Instrum. Methods* **213** 447–52
Itoh F 1989 private communication
Lovesey S W 1987 *J. Phys. C: Solid State Phys.* **20** 5625–39
Mills D M 1987 *Phys. Rev.* B **36** 6178–81
Moon R M, Koehler W C, Cable J W and Child H R 1972 *Phys. Rev.* B **5** 9976–1015
Platzman P and Tzoar N 1970 *Phys. Rev.* B **2** 3556–9
Roeland L W, Cook G J, Muller F A, Molemann A C, Jordon R G and McEwan K A 1975 *J. Phys. F: Met. Phys.* **5** 12 L233–7
Sakai N 1987 *J. Phys. Soc. Japan* **56** 2477
Sakai N and Sekizawa H 1987 *Phys. Rev.* B **36** 2164–9

Sticht J and Kubler J 1985 *Solid State Commun.* **53** 529–32
Timms D N, Brahmia A, Collins S, Collins S P, Cooper M J, Holt R S, Kane P P, Clark G and Laundy D 1988 *J. Phys. F: Met. Phys.* **18** L57–61
White H W, Beaudry B J, Burgardt P, Legvold S and Harmon B N 1976 *AIP Conf. Proc.* **29** 329–30
Williams B G (ed.) 1977 *Compton Scattering* (New York: McGraw-Hill)