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LETTER TO THE EDITOR

Spin dependent anisotropy in the momentum density of ferromagnetic nickel metal

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Abstract. Directional spin dependent Compton profiles of ferromagnetic nickel metal have been measured with 55 keV circularly polarised synchrotron radiation and the results have been compared with an APW calculation of the electron momentum density. At low momenta where the negatively polarised 4s–p band reduces the spin dependent momentum density, the model predicts accurately the contribution to the [100] lineshape but significantly underestimates the [111] profile.

The existence of spin dependent terms in the x-ray scattering cross section provides the means to study the properties of the spin oriented electrons in magnetic materials [1, 2]. The development of bright synchrotron sources, at which it is possible to select both a particular photon energy and a polarisation state has made magnetic x-ray scattering experiments possible, albeit with difficulty.

Measurements of the spin dependent Compton profiles of all the soft polycrystalline ferromagnetic elements have been undertaken with circularly polarised synchrotron radiation (CPSR), [3–6]. Recently a measurement of the magnetic anisotropy in the electron momentum density of single-crystal iron was reported by some of us [7]. Data of improved statistical quality enabled the majority and minority directional difference profiles to be separated to provide a more specific test of band theory [8]. This letter reports a further directional measurement on ferromagnetic nickel.

Compton scattering experiments with unpolarised radiation measure a one-dimensional projection of the total electron momentum density distribution, $n(\boldsymbol{p})$, summed over all spin states [9]. This projection is commonly referred to as the Compton profile, $J(p_z)$ and defined as

$$J(p_z) = \int_{p_x} \int_{p_y} (n_\uparrow(\boldsymbol{p}) + n_\downarrow(\boldsymbol{p}))\, \mathrm{d}p_x\, \mathrm{d}p_y \qquad (1)$$

where p_x, p_y and p_z are the Cartesian momentum coordinates, the direction z being parallel to the scattering vector. The use of circularly polarised radiation leads to a magnetic scattering contribution of order $\hbar\omega/mc^2$, where $\hbar\omega$ is the photon's energy. For transition metals where the orbital moment is quenched, the magnitude of the magnetic contribution when compared to the leading charge scattering term is

$$\Delta = [P_c(1 - \cos\phi)/mc]\, \boldsymbol{S} \cdot (\boldsymbol{k}_i \cos\phi + \boldsymbol{k}_f) J_{\mathrm{mag}}(p_z) \qquad (2)$$

where P_c is the degree of circular polarisation of the beam, $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ are the incident and

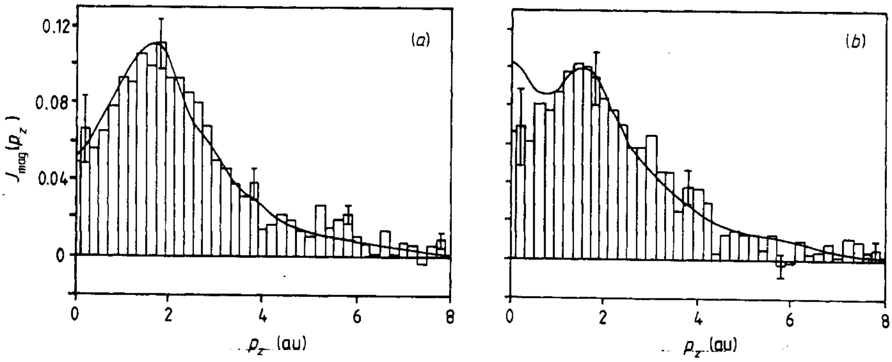

Figure 1. The measured (*a*) [100] and (*b*) [111] directional magnetic Compton profiles of nickel, as defined by equation (3), shown at intervals of 0.2 au, after left–right averaging the data obtained with 55 keV CPSR. The APW theoretical profiles (full curve) have been convoluted with a gaussian of FWHM = 0.7 au to mimic the experimental resolution function.

scattered wavevectors and ϕ is the scattering angle. The z axis is parallel to $\boldsymbol{k}_i - \boldsymbol{k}_f$. In addition, only a small proportion of electrons give rise to a magnetic scattering contribution; hence for photon energies of $\sim\frac{1}{10}mc^2$, the magnetic scattering amplitude is usually little more than a few per cent of the total scattering amplitude. The quantity $J_{mag}(p_z)$ is a magnetic Compton profile and is obtained by forming the difference between Compton profiles recorded with the electron spin direction parallel ($\uparrow$) and antiparallel ($\downarrow$) to the photon polarisation, i.e.

$$J_{mag}(p_z) = \int_{p_z}\int_{p_y} (n_\uparrow(\boldsymbol{p}) - n_\downarrow(\boldsymbol{p}))\, dp_x\, dp_y. \tag{3}$$

In soft ferromagnets $J_{mag}(p_z)$ can be obtained by reversing the spins in the sample. The alternative of switching the handedness of polarisation is not yet a practical proposition. This operation enables the core contribution from the paired electron spins to be removed leaving the unpaired electron spin momentum density.

The present study was carried out under the same conditions as reported in an earlier single-crystal study on iron using a new spectrometer designed for magnetic Compton experiments in which the scattering is observed in transmission through the sample, thereby facilitating the observation of directional effects [8]. The CPSR was obtained from the three-pole wiggler port at the Daresbury storage ring by viewing the elliptically polarised radiation that is emitted at a small inclination to the synchrotron's orbital plane (see [10] and [11] for an explanation of this technique). The radiation was scattered through an angle of 145 ± 2° in transmission through a magnetised 200 μm thick {110} single crystal of nickel after monochromating the incident white beam with a flat Ge 220 crystal to select a photon energy of 55 keV. Great care was taken to ensure parallelism between the magnetisation direction, the scattering vector and the required crystallographic axes. The magnetisation direction was reversed in an asynchronous cycle with a minimum dwell time of 5 s and the data for the two spin directions were stored in separate memories.

A total of 25 h of data collection resulted in 7×10^7 counts under each directional Compton profile and the resulting difference profiles contained 3×10^5 counts. The spin-up and spin-down data sets were first corrected for the low energy tail of the detector response and then for the energy dependence of the magnetic inelastic scattering cross section and absorption within the sample. The effects of multiple scattering on the spin dependent profiles were neglected in line with the prediction of Sakai [12] that they should be negligible. Finally the data were averaged in momentum intervals of 0.2 au (1 au of electron momentum $\equiv 1.99 \times 10^{-24}$ kg m s^{-1}) and then folded about $p_z =$ 0 au. There was insufficient machine time available to record the 110 or other profiles.

The [100] and [111] directional magnetic Compton profiles of nickel and APW theoretical profiles [13] are shown in figures 1(*a*) and 1(*b*) plotted as a function of the electron momentum. The latter have been convoluted with a Gaussian of FWHM 0.7 au to mimic the experimental resolution and all profiles are normalised to an area of 0.7 (the number of unpaired electrons in atomic nickel) in the momentum range −8 to +8 au.

For the [100] profile, good agreement with the APW calculation is observed at all values of momentum. On the other hand, the theory predicts that there is no central dip in the [111] profile whereas a significant dip is observed experimentally. This observation of a central dip in the [111] profile is consistent with a measurement of poorer rsolution, but improved statistical accuracy performed at the Photon Factory, Japan, using CPSR obtained from the elliptical wiggler magnet on the Accumulation Ring [14].

This measurement highlights a deficiency in the APW model which is echoed in the analogous directional measurements on iron where the central dip in the [100] profile is also poorly reproduced. Further band calculations of the momentum density would help to identify the cause of this discrepancy

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