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NON COLLINEAR MOMENT IN SINGLE DOMAIN ANTIFERROMAGNETIC MANGANESE-COPPER

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Abstract. — Diffuse neutron scattering measurements incorporating polarisation analysis have been made on a single domain single crystal of MnCu 90 at. % Mn at 5 K. The atoms are strongly clustered and the long range part of the magnetic defect is transverse to the antiferromagnetic direction.

The face centred tetragonal form of manganese which can be stabilised at room temperature by the addition of small amounts of other elements, is the simplest of the antiferromagnetic structures occurring in the first transition metal series. The structure is one in which the atoms in (001) planes are ferromagnetically coupled and the moment of successive planes alternates along the tetragonal direction.

The first alloy series to be studied with neutron diffraction was MnCu [1, 2]. As well as establishing the magnetic structure, Bacon et al. [2] observed a diffuse peak near the {001} position in their powder diffraction patterns which they inferred was associated with the (001) reciprocal lattice point. More recently Cywinski et al. [3] showed using textured samples and polarisation analysis that the diffuse feature is indeed associated with the (001), magnetic, and most probably due to static magnetisation transverse to the direction of long range magnetic order. No energy analysis was made, and the static nature of the effect was inferred because the experiment was done at low temperatures and with neutrons with an energy less than the magnon band gap.

The data reported here on a single crystal, largely single domain sample of MnCu containing 10 at. % Cu, were taken on the D7 diffuse scattering diffractometer at ILL. No energy analysis was done in the main experiment, but an initial check for a known magnon using time of flight analysis showed that at 5 K, with \( \lambda = 4.85 \AA \), magnon scattering should be very small. Data were collected over a wide area in the (110) scattering plane geometry in a band 0.13 reciprocal lattice units wide running out in the direction of the (001) reciprocal lattice position. This was fitted with Cowley [5] short range order parameters out to sixth neighbour. The parameters are shown in table I. The above is not a satisfactory fit because the atomic clustering is much longer ranged than to the sixth neighbour shell. This can be seen because of the large magnitudes of the outer Cowley parameters. Long range clustering was also seen in the nuclear data of [3]. The data was scaled according to the fitted value of the \( \kappa \) independent part of the scattering to equal \( c(1 - c)(b_{\text{Cu}} - b_{\text{Mn}})^2 \) with \( c \) the concentration. Figure 1 shows the data plotted as a function of the \( z \) component of \( \kappa \) along with the fitted function. The same factor was also used to scale the magnetic data to obtain cross-sections.

Table I. — The fitted Cowley short range atomic order parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha_1 )</td>
<td>0.23 ± 0.07</td>
</tr>
<tr>
<td>( \alpha_2 )</td>
<td>0.04 ± 0.04</td>
</tr>
<tr>
<td>( \alpha_3 )</td>
<td>0.09 ± 0.02</td>
</tr>
<tr>
<td>( \alpha_4 )</td>
<td>0.07 ± 0.01</td>
</tr>
<tr>
<td>( \alpha_5 )</td>
<td>0.12 ± 0.04</td>
</tr>
<tr>
<td>( \alpha_6 )</td>
<td>0.18 ± 0.04</td>
</tr>
</tbody>
</table>

1Now at MASPEC, Parma, Italy.
The high values near the (001) reciprocal lattice point are due to a “leak through” from the magnetic scattering because of the imperfect separation of the two cross-sections. The highest three points were not included in the fit.

The magnetic diffuse scattering at (001) is extremely sharp. From the data shown in figure 2 it would be easy to mistake it for a Bragg peak. However powder diffraction patterns, for example [3], show it to be diffuse. The cross-sections shown in figure 2 are from the transverse part of the magnetic scattering plus one third of the nuclear spin incoherent cross-section. The sharp feature at the (001) position is absent from the longitudinal magnetic cross-section except for a small effect which can be attributed to “leak through” as with the nuclear defect cross-section. The absolute cross-sections are obtained with reference to the nuclear defect cross-section as described before. The data selected are in a narrow band within 0.03 Å⁻¹ of the [001] and [110] directions.

The widths of the peak in the two directions are partly determined by instrument resolution and crystal quality. The crystal had a mosaic spread of about 2° FWHM and the slightly greater width in the [110] direction is probably due to this. Similar data but without polarisation analysis has been obtained by Tsunoda and Nakai [6].

The simplest model which would explain this remarkable magnetic scattering feature is one in which each magnetic defect has a long range component which is canted away from the antiferromagnetic direction. At the same time the canting direction for each defect must be different so that there is no nett staggered magnetisation. This is necessary because no Bragg peak is observed at the (001) position. The cross-section for this simple model is given by

\[
\frac{d\sigma}{d\Omega} = c(1-c) \left[ \frac{e^2 \gamma}{2mc^2} \right]^2 S(\kappa - r) f^2(\kappa) M_t^2(\kappa)
\]

where \( S \) is the short range order function with \( r \) the antiferromagnetic periodicity, \( f \) is the atomic magnetic form factor for Mn, and \( M_t \) is the transverse part of the staggered magnetisation around each defect. At \( \kappa = r \) which is the (001) reciprocal lattice point, \( S \) is sharply peaked with a FWHM of much less than 0.8 Å⁻¹. However the FWHM of the magnetic diffuse peak is about 0.1 Å⁻¹ indicating that the range of the magnetic defect is much longer than that of the atomic clustering, roughly 30-40 Å. The magnitude of \( M_t(r) \) can also be estimated. \( S(0) \) from the fitted nuclear defect scattering is at least 12, which gives a value for \( M_t(r) \) of 12 \( \mu_B \). The best name for such an entity is a “giant staggered moment”.

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