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Spin Correlations in Mn_3Pt

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The ordered alloy Mn_3Pt is an antiferromagnet and shows a first order AF-AF transition at T_t=400 K below Néel temperature (T_N=475 K) .The magnetic structure is triangular (D-phase) below T_t and collinear (F-phase) above T_t. In the F-phase, one third of Mn spins has no magnetic moment. The neutron scattering measurements were performed to investigate the dynamical behavior of these special spins in the F-phase. Inelastic diffuse scattering extending along the [010] axis was obtained at low excitation energy (3 meV) on the 001 scattering plane in the F-phase. The special Mn spins feel strong frustrations with nearest neighbor spins, although they have rather strong parallel coupling with second neighbor spins.

KEYWORDS: frustration, inelastic magnetic diffuse scattering, spin correlations

§1. Introduction

The ordered alloy Mn_3Pt has a Cu_3Au-type atomic structure at room temperature and is an antiferromagnet with Néel temperature T_N=475 K. Below the Néel temperature, a first order AF-AF transition takes place. This transition temperature sensitively depends on the atomic concentration of the sample. The transition temperature increases with increasing of Mn concentration. Krén *et al.* reported to be T_t=365 K from their susceptibility, neutron powder diffraction and X-ray diffraction measurements.[1] H.Yasui *et al.* studied the transition temperature T_t more accurately, using the samples with less than 1 % deviations from the nominal stoichiometry and determined T_t as 400 K.[2] The magnetic structure is triangular below T_t (D-phase) and collinear above T_t (F-phase), as illustrated in Fig.1. At this phase transition, the magnetic moments of Mn atoms change from 2.2 (D-phase) to 3.3 (F-phase) μ_B per Mn atom accompanied with the unit cell volume expansion of 2.25 %.[3] In the D-phase, the magnetic moments lie on the (111) plane and point to the [211] direction. In the F-phase, the magnetic unit cell is double atomic cells and the spin coupling of second neighbor Mn atoms are inconsistent for the directions in this spin structure. One third of Mn atoms have no moment in the F-phase, although it has a moment in the D-phase. Under the hydrostatic pressure, the F-phase disappears with increasing the pressure.[3] The similar alloys, Mn_3Ir and Mn_3Rh, do not have the F-phase with the collinear structure below T_N. Thus, the F-phase is a characteristic of the Mn_3Pt alloy. We have interested in this special character of Mn_3Pt alloy and preformed neutron scattering measurements to investigate the dynamical behavior of the special spins in the F-phase.

§2. Sample Preparation and Experiments

Both the powder and single crystal specimens of Mn_3Pt were prepared for the present experiments. Mn and Pt with purities of 99.99 % were used as raw materials for those samples. The single crystal was grown by the Bridgman method in a furnace with a carbon heater system under an Ar gas atmosphere and then cooled down in the furnace. The ordering anneal was done at 1050 K for 80 hours for both specimens in a quartz tube. Single crystal has a volume of about 2 cc. The neutron scattering measurements were performed at the T1-1 (HQR) triple axis spectrometer installed at a thermal guide of JRR-3M, JAERI, Tokai. Measurements for both powder and single crystal specimens were performed at room temperature (300 K) and at 422 K which correspond to the temperature of D-phase and that of F-phase, respectively.

§3. Experimental Data

From a consideration of the symmetry of the F-phase, the molecular field at the position where one third of Mn atoms with zero moment is located, would be zero. Therefore, at first, we assumed that the relevant Mn spins are paramagnetic in the F-phase. To examine this point, the experiments were performed using powder specimen. If this is true, paramagnetic scattering, the

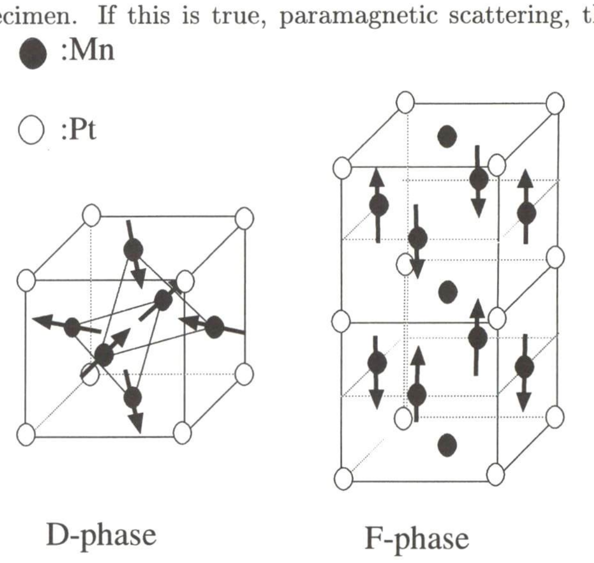


Fig. 1. Magnetic structures for Mn_3Pt in the D- and F-phases.

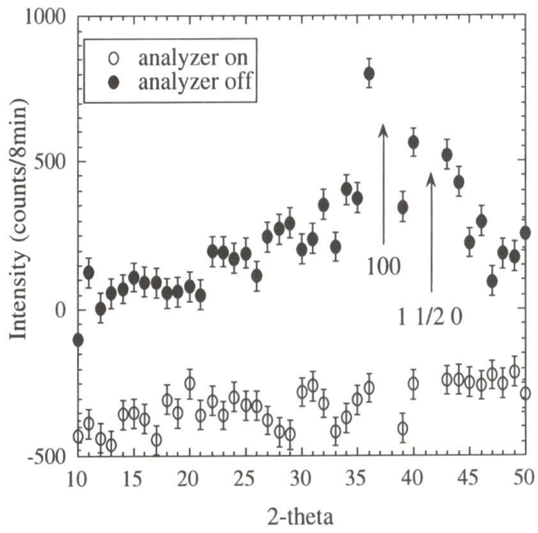


Fig. 2. The data for powder sample with analyzer on and off. The data at D-phase were subtracted form those at F-phase.

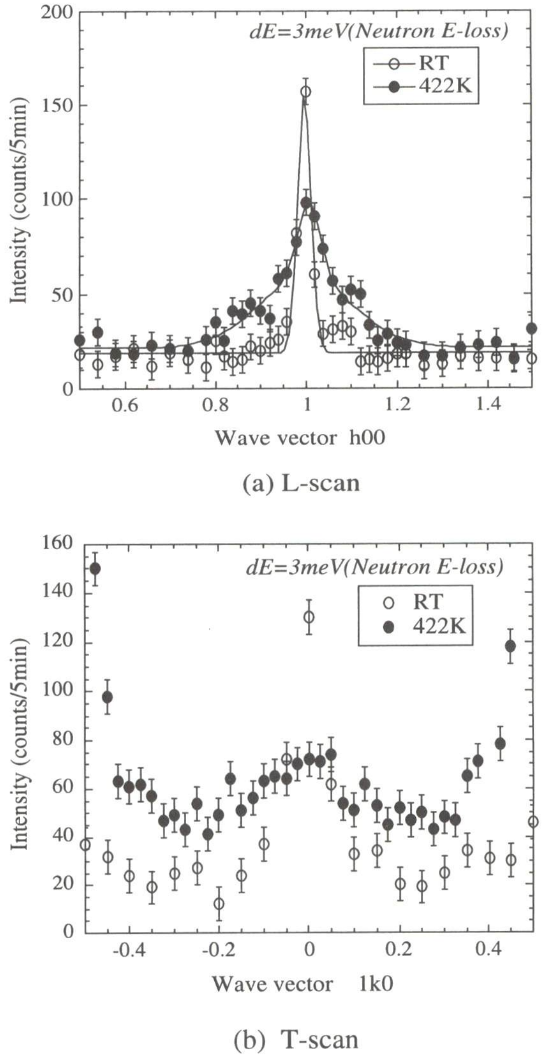
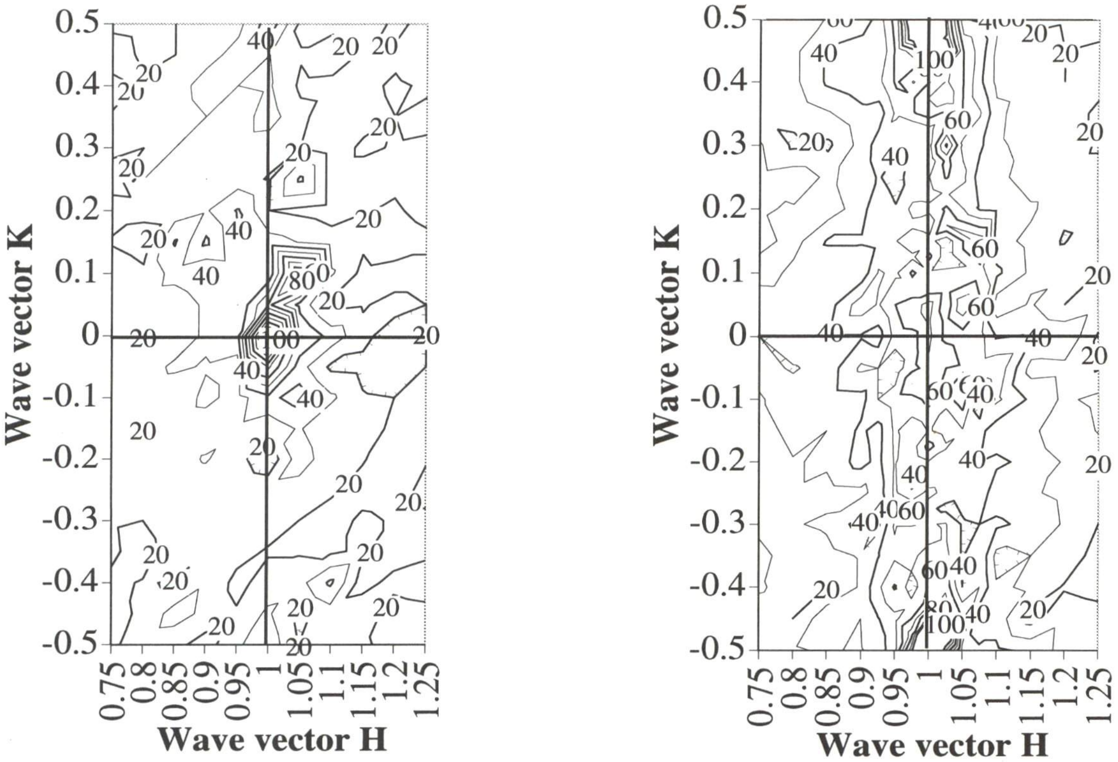


Fig. 3. Neutron inelastic scattering data obtained around 100 for single crystal specimen.

intensity of which depends on the scattering angle and varies as the magnetic form factor, would be observed only in the F-phase. Since paramagnetic scattering is basically inelastic scattering, elastic (analyzer-on) and inelastic (analyzer-off) measurements were performed, both in the D-phase and the F-phase, then the data at D-phase were subtracted from those at F-phase. The subtracted data for both analyzer -on and -off are given in Fig.2. On the contrary to the expectation, the inelastic scattering data show broad peak around the 100 reciprocal lattice point (RLP) and elastic scattering data do not have any diffuse peaks. The data indicate that the spins in the F-phase are not paramagnetic but are dynamically fluctuating with some spin correlation. To determine the exact location of the inelastic diffuse peak, we made inelastic neutron scattering measurements using a single crystal specimen. Diffraction patterns obtained at low excitation energies (3 meV) by scanning along the [100] (L-scan) and the [010] (T-scan) directions on the (001) scattering plane are given in Fig.3-(a) and Fig.3-(b), respectively. In both F- and D-phase, rather sharp peaks located at the 100 RLP in the L-scan are identified to be magnon scattering.[4] Comparing the data of both phases, inelastic diffuse scattering is observed only in the F-phase as a tail of magnon peak. Intensity contour maps of inelastic diffuse scattering studied at low excitation energy (3 meV) on the 001 scattering plane in the D-phase and the F-phase are given in Fig.4-(a) and Fig.4-(b),respectively. The inelastic diffuse scattering intensities extend along the [010] direction in the F-phase, but no diffuse peaks are observed in the D-phase except for the sharp magnon peak at 100.

§4. Discussion

Since the inelastic diffuse scattering along the [010] direction is observed only in the F-phase, we can consider that the inelastic diffuse scattering comes from the one third of Mn atoms, which was described as zero moment in Fig.1. These Mn spins have a strong correlation. From the present experimental data, we can draw the following picture for the one third of Mn spins in the F-phase. Although our measurements were performed only in the (001) plane, inelastic diffuse scattering is considered to extend on the plane perpendicular to the [100] axis in the reciprocal lattice space from the symmetry of the spin structure of Fig. 4. Thus, the Mn spins, which are located at the zero molecular field, couple ferromagnetically along the [100] direction on the (001) plane. This spin configuration would be consistent with the nearest neighbor (n-n) AF coupling along the [100] direction but inconsistent with the n-n AF coupling along the [010] direction. Then, the Mn spins would turn up side down immediately. However, although the n-n AF coupling is consistent for the [010] direction, it is inconsistent for the [100] direction in this time. Thus, the Mn spins turn up and down from time to time at the frequency of the order of 10^{11}-10^{12} Hz with strong ferromagnetic correlations along the each cubic axis. From the diffuse peak line width, the correlation length along the cubic axis is estimated to be 5 times the lattice parameter. These Mn spins feel always strong frustrations with nearest neighbor spins, although they have rather strong parallel coupling with second neighbor spins. Thus, the F-phase



(a) D-phase **(b) F-phase**

Fig. 4. Intensity contour maps of inelastic diffuse scattering studied at δE=3 meV.

of Mn_3Pt is considered to be a partially frustrated spin system. Further measurements around the Néel temperature are now in progress.

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