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NEUTRON SCATTERING STUDY OF SPIN WAVES IN AN ANTIFERROMAGNET $FePt_3$

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Spin wave dispersion relations in an antiferromagnetic ordered alloy of $FePt_3$ were determined along three crystallographical axes by neutron scattering. Well defined magnon groups could be observed up to the magnetic zone boundary. The dispersion relation could be interpreted in terms of the Heisenberg model using more than four exchange parameters.

$FePt_3$ IS A METALLIC antiferromagnet with the $CuAu_3$ type ordered structure where iron atoms occupy a s.c. lattice. Below the Néel temperature of about 170 K, the antiferromagnetic structure with the antiferromagnetic wave vector $Q_0 = [110]\pi/a$ is established [1]. The iron atoms carry a magnetic moment of $3.3\,\mu_B$, while no appreciable moment has been detected on the Pt atoms [1]. The static susceptibility above T_N decreases with increasing temperature, suggesting the existence of a localized moment in the paramagnetic region. Therefore Pt_3Fe is one of the best system to explore the spin dynamics in the antiferromagnetic metals as an example of the quasi-localized spin system [2]. The study of the magnetic coupling of this system would also give us an answer to the question why $FePt_3$ becomes antiferromagnetic, while other similar ordered alloys $FePd_3$ [3] and $MnPt_3$ [4] are ferromagnetic. This paper describes the results of neutron spin wave scattering from $FePt_3$.

Neutron scattering experiments at 5 K were first performed on a triple axis spectrometer IN1 at the High Flux Reactor at ILL and the measurements below 20 meV were repeated at 5 and 77 K using a triple axis spectrometer TUNS at JRR-2 of JAERI. The sample used in the experiments is a single crystal of about $3\ cm^{-3}$ in volume grown by Bridgman method. The chemical analysis shows a composition of $Fe_{22.6}Pt_{77.4}$. The antiferromagnetic structure with an antiferromagnetic wave vector $Q_0 = [110]\pi/a$ was confirmed by the temperature dependence of the intensity of the (1/2, 1/2, 0) reflection. We also found the (0, 0, 1/2) reflection below about 80 K whose intensity is about 4% of the (1/2, 1/2, 0) reflection at 5 K. Therefore two kinds of antiferromagnetic structures coexist below 80 K as reported previously [1]. We expect, however, that the (0, 0, 1/2) antiferromagnetic phase is too small to disturb the main phase, and we disregarded it in our analysis.

The spin wave measurements were made around the (1/2, 1/2, 0) and (1/2, 1/2, 1) reciprocal lattice points in the (1, $\bar{1}$, 0) plane. The spin wave dispersions determined along three principal crystal axes are shown in Fig. 1. The uncertainty of the peak positions of the spectra are shown by error bars. Typical magnon

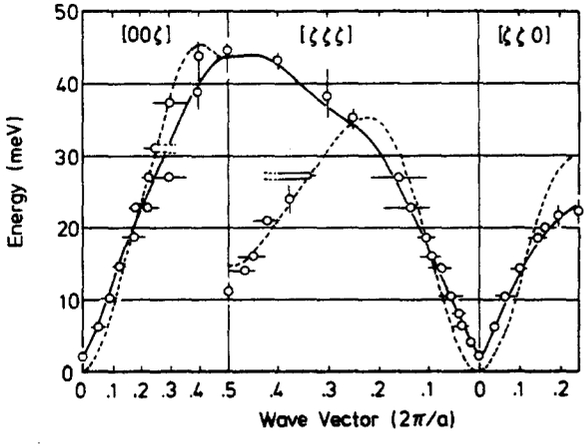

Fig. 1. Spin wave dispersion relations of $FePt_3$ at 5 and 77 K. Solid and broken lines are calculated for 5 K based on the Heisenberg type Hamiltonian using six exchange parameters. The solid lines correspond to the spin waves in the [1/2, 1/2, 0] domain to which the wave vector in the figure is referred. The broken lines correspond to the spin waves in the [1/2, 0, 1/2] and [0, 1/2, 1/2] domains.

* A part of experiment was performed by temporary affiliation to ILL.

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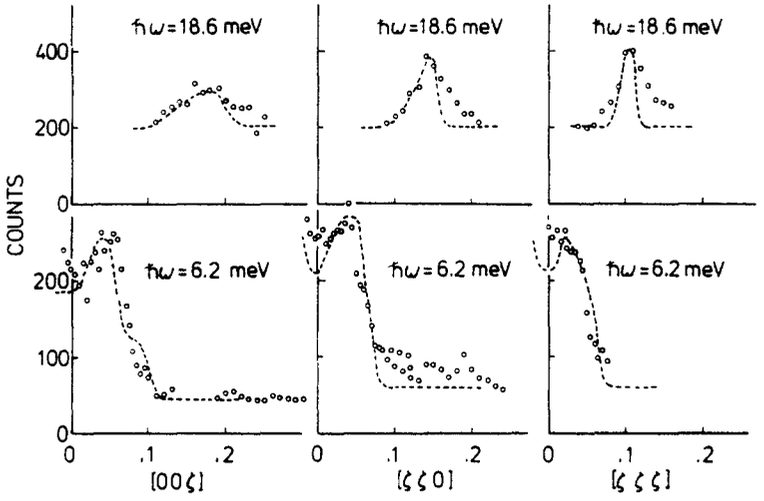

Fig. 2. Typical constant E scans at 5 K. The broken curves represent calculated spin wave profiles obtained by convolution of calculated dispersion relations with the resolution function.

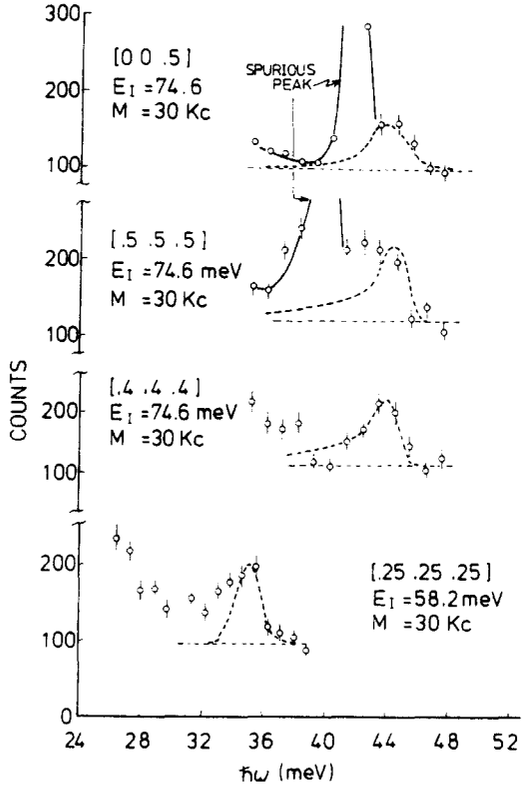

Fig. 3. Typical constant Q scans at 5 K. The broken curves represent the calculated spin wave profiles obtained by convolution of calculated dispersion relations with the resolution function.

groups observed in both low and high energy regions are displayed in Figs. 2 and 3 respectively. The spin wave spectra show simple single peak shapes for the energy transfers of less than 20 meV, but the spectra in the [001] and [110] directions become complicated with two or three peaks for energy transfers of more

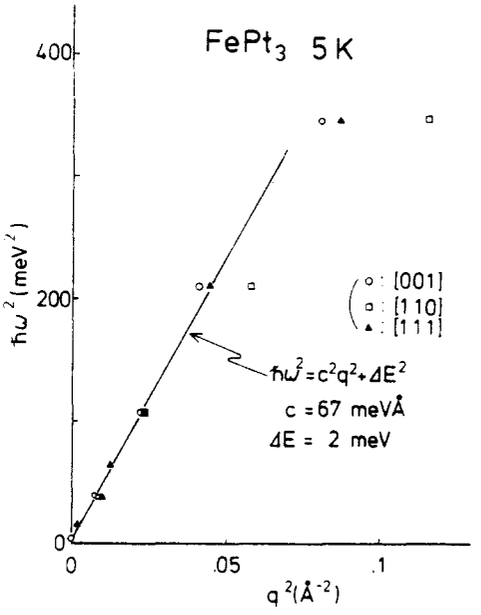

Fig. 4. Spin wave dispersion for small wave vectors.

than 20 meV. This may be due to the multi-domain effect as described below. The spectra near about 24 meV may also suffer from the contamination of optical phonon branch.

An isotropic and linear dispersion relation was found to hold at a small wave vector region as shown in Fig. 4. This gives the spin wave velocity of 67 meV Å for $q \lesssim 0.16$ Å^{-1} and the energy gap of 2 meV at the zone centre.

The spin wave dispersion relations at 5 K are analyzed using the Heisenberg type Hamiltonian

$$H = -\sum_{\langle ij \rangle} 2J_{ij}\mathbf{S}_i\mathbf{S}_j - \sum_i DS_{iz}^2, \quad (1)$$

where J_{ij} is the effective exchange interaction between the ith and jth iron atoms and D is the one ion type anisotropy constant. The spin wave dispersions in an antiferromagnet with $Q_0 = [1/2, 1/2, 0]\,\pi/a$ in the s.c. lattice was calculated based on the Hamiltonian (1), and the exchange parameters J_{ij} as well as D were determined by least squares fit to the data, where the effect of the multi-domain structure was taken into account. Equal distributions of magnetic domains were confirmed by equal intensities of three equivalent magnetic Bragg reflections (1/2, 1/2, 0), (1/2, 0, 1/2) and (0, $\overline{1/2}$, 1/2).

Solid lines in Fig. 1 are calculated for the domain with $Q_0 = [1/2, 1/2, 0]\,2\pi/a$ with six exchange parameters and one anisotropy constant: $J_1 = 1.56$, $J_2 = -0.85, J_3 = 0.73, J_4 = 0.27, J_5 = 0.08, J_6 = 0.20$, and $D = 0.06$, in the unit of meV. Broken lines are the dispersion relations calculated for other antiferromagnetic domains. If we use less than four exchange parameters, the theory can not be made to reproduce the observations. Significant improvement of agreement between the theory and the experimental data could not, however, be achieved even using more than six exchange parameters. The parameters thus obtained suggest that the exchange interactions between iron atoms extend in long range and they show an oscillatory character just as was the case with Heusler alloys [5]. The Fourier transform of the exchange parameters $J(Q)$ was found to have a maximum at the wave vector $Q_0 = [1/2, 1/2, 0]\,2\pi/a$, confirming that they stabilize the [1/2, 1/2, 0]-type antiferromagnetic structure. The spin wave spectra were calculated by folding the resolution function [6] to the dispersion relation without life time and are displayed by broken lines in Figs. 2 and 3. The peak positions of the calculated spectra agree well with the observed ones except near (0.25, 0.25, 0), but the agreement of the spectrum shapes between the calculation and observation is not satisfactory for some of constant E scans (Fig. 2). The observed neutron groups by constant Q scans at high energy transfers are, however, rather well reproduced by the calculation as shown in Fig. 3. Therefore it seems not reasonable to assume a large line width for the spin wave excitations in order to remedy the discrepancy at lower energy transfers.

It is not clear, in the present stage, that the localized model or the Heisenberg-type Hamiltonian (1) is completely applicable to $FePt_3$ system. The experimental fact that the magnetic excitations with long life times exist up to the zone boundary favors the localized model, because in the itinerant antiferromagnet the collective excitations interact with the single particle modes at virtually all energies, resulting in the significant line broadening [7, 8] just as were observed in some typical itinerant antiferromagnets γMn(Ni) [9] and γFeMn alloys [10]. The best justification of the localization of the moment can be checked by investigating the temperature dependence of the excitations as was done for the Heusler alloys [4], which is now in progress.

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