STAGGERED FIELD EFFECT ON THE ONE-DIMENSIONAL S=1/2 ANTIFERROMAGNET Yb_4As_3

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Polarized neutron diffraction and inelastic neutron scattering experiments on Yb_4As_3 revealed that it exhibits typical behaviors of a one-dimensional S=1/2 Heisenberg-type antiferromagnet at low temperatures due to the formation of one-dimensional arrays of Yb^{3+} ions by the charge ordering transition. Staggered field effects on the Yb^{3+} chains induced by applying a magnetic field were also detected by the neutron scattering experiments.

Yb_4As_3 has an anti-Th_3P_4 type cubic crystal structure at temperatures above 290 K, below which it shrinks slightly along a [111] direction giving a trigonal structure. From several experimental observations, the phase transition was suggested to be accompanied by a charge ordering as shown in Fig. 1. The existence of charge ordering in the low temperature phase of Yb_4As_3 was directly proved by experiments performed at the polarized neutron diffractometer 5C1 at LLB [1], where flipping ratios of about 20 Bragg peaks were measured by applying a magnetic field H perpendicular to the [111] direction, using an incident neutron beam with wavelength of 0.84 Å.

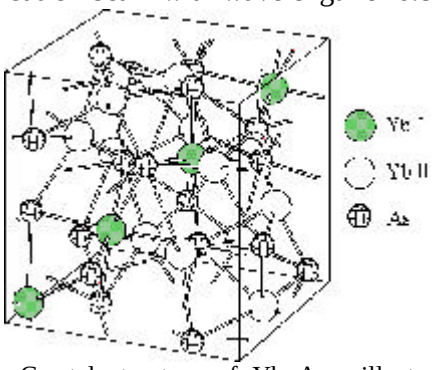

Figure 1. Crystal structure of Yb_4As_3, illustrating the expected charge ordering in the trigonal phase (T < 290 K). In the cubic phase, Yb_I and Yb_{II} are equivalent.

From the least squares fit analysis of the data, it was found that the induced moment of the four Yb ions aligned along the [111] direction (Yb_I) is much larger than that of the rest of 12 Yb ions (Yb_{II}); for example, the induced moments of Yb_I and Yb_{II} are m_I = (0.33 ± 0.01) m_B and m_{II} = (0.009 ± 0.006) m_B, respectively, at 1.5 K and H = 7 T. This clearly indicates that Yb_I is mainly trivalent whereas Yb_{II} is almost divalent.
The charge ordering gives rise to the formation of one-dimensional arrays of Yb^{3+} ions as seen in Fig. 1. In order to investigate the spin dynamics of the system, inelastic neutron scattering experiments on a single crystal (single domain) sample of Yb_4As_3 were performed at the triple axis spectrometers 4F2 at LLB, 6G and C11 at JAERI and IN14 at ILL [2].

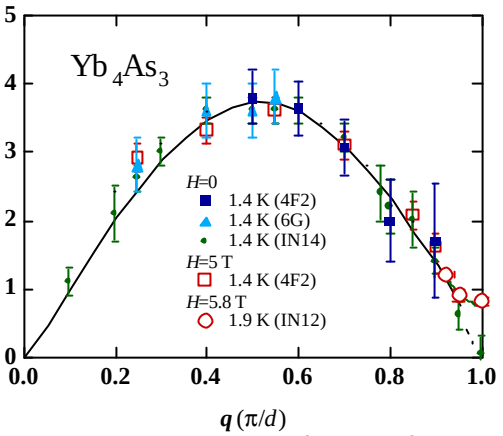

Figure 2. Dispersion relation of peaks of spin excitation spectra of Yb_4As_3 in the one-dimensional representation.

The observed spectra are well explained by the calculation based on the Müller ansatz for a one-dimensional spin 1/2 Heisenberg system with a nearest-neighbor antiferromagnetic coupling (1D-HAF) [3]. Fig. 2 depicts the dispersion relations of the peak positions of the observed spectra at 1.4 K against the 1D wave vector q in the unit of π/d for the Yb_I chains along the [111] direction, where d (=3.8 Å) is the atomic distance in the chain. The dashed curve in Fig. 2 shows the peak position of the resolution convoluted spectra of a 1D-HAF system which corresponds to the so-called des Cloizeaux-Pearson spin-wave mode $E_1(q) = \pi J/2|\sin(dq)|$ with the exchange interaction value of J = 2.23 meV. Since the observed crystal field excited levels (14, 21, 29 meV) are well above the J value [2], can be the 1D-HAF properties ascribed to the ground state doublet of the Yb^{3+} ions,
Thus, it becomes clear that the low-energy properties of the 1D chains of Yb^{3+} ions caused by the charge ordering are explained well by the 1D-HAF model when there is no magnetic field. However, experimental results of specific heat under magnetic field exhibit unusual properties which indicate the opening of a gap in the low energy excitations of Yb_4As_3 by applying a magnetic field [4]. This is not

consistent with the simple Zeeman effect on the 1D-HAF model which does not cause any energy gap [3]. The gap opening phenomenon was directly observed by the inelastic neutron scattering experiments under magnetic field performed on the spectrometers 4F2 at LLB and IN12 at ILL [5]. We found that, by applying a magnetic field perpendicular to the [111] direction, the spectrum at the 1D wave vector around q = 1 [π/d] changes drastically from the gap-less one with the spinon excitation continuum of the 1D-HAF system to the spin-wave-like sharp one at a finite excitation energy. The peak positions of the spectra at H = 5.8 T (IN12) and 5 T (4F2) are shown in Fig. 2 by open circles and squares, respectively. The magnetic field dependence of the peak position at q = 1 was found to be well proportional to $H^{2/3}$. This is in good agreement with the theory presented by Oshikawa et al. [6] which argues that the gap is opened by the staggered field on Yb^{3+} ions induced by the uniform magnetic field perpendicular to the chains due to existence of Dzyaloshinsky-Moriya interaction in the Yb^{3+} chains.

In order to check the staggered field model, we have also performed a polarized neutron diffraction experiment at 5C1 diffractometer under a magnetic field parallel to the [111] direction. Flipping ratios were measured at several temperatures under the same conditions as in the case of the perpendicular field as described above. Fig. 3 shows the obtained temperature dependence of the induced moment of Yb_I under the magnetic field of 7 T for both parallel and perpendicular field cases. As seen in Fig. 3(a), m_I under magnetic field parallel to the chain direction exhibits a broad maximum around 20 K as is expected for the 1D-HAF model, whereas that for perpendicular field, see Fig.3(b), does not show such a pronounced peak and instead shows an unusual enhancement below about 10 K. The difference of the magnetic field dependence of m_I is actually explained well by the staggered field model[7]. The solid lines in the figures are the sum of the calculated magnetization due to the crystal field ground state doublet

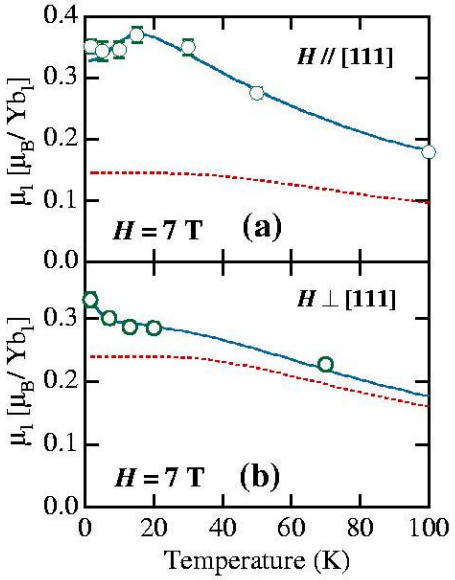

Figure 3. Temperature dependence of induced moment μ_I for *(a) H // [111] and (b) H ^ [111]*. See text .

and Van Vleck-type one due to the excited states (dashed lines in Fig. 3), where the former is calculated by the density matrix renormalization group method (DMRG) for the 1D-HAF system with and without the staggered field and only the first excited state contribution was taken into account in the calculation of the Van Vleck term. The effective g-value of the ground state doublet and the scaling factor of the Van Vleck term were determined by using least squares fit procedures, where the anisotropy of the g-factor determined from the scattering vector dependence of the spin excitation spectra was taken into account. The nice fit between the observation and calculation strongly supports the staggered field model.

The experimental results described above revealed that Yb_4As_3 is an ideal quantum spin system providing the new interesting problem of the staggered field. However, it is metallic, and its electrical resistivity shows a heavy-electron-like anomaly though the carrier density is extremely low (~10^{-3}/formula) at low temperatures [8]. Further study on this material is necessary.

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