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Antiferromagnetic interactions in the semimetallic Yb_4As_3: field-dependent specific heat and magnetization data

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Abstract

The $S=\frac{1}{2}$ antiferromagnetic Heisenberg model with the Dzyaloshinsky–Moriya interaction is applied to a semimetallic compound Yb_4As_3. The field dependent specific heat and the magnetization of this model are calculated by the numerical quantum transfer-matrix method and compared with experiment. New specific heat experimental results for the polydomain sample in the field applied are presented and compared with the theoretical predictions obtained without adjustable microscopic parameters.

The Yb_4As_3 is a pnictide compound which belongs to the family of R_4X_3 (R = rare earth, X = As, Bi, P, Sb) compounds of the anti-Th_3P_4 structure [1]. Above $T_{co} \approx 295$ K Yb_4As_3 is a homogeneous intermediate metal (IV) with a valence ratio of $Yb^{2+}/Yb^{3+} = 3:1$, where the Yb ions reside statistically on four equivalent families of chains along the space diagonals of a cube [1]. At $T_{co} \approx 295$ K the IV state exhibits such a charge-ordering instability that far below T_{co} one of the four Yb ions becomes trivalent and forms a one-dimensional spin $S=\frac{1}{2}$ chain along the $\langle 1\ 1\ 1 \rangle$ direction. The remaining Yb ions take non-magnetic divalent states. The crystal structure is trigonal with the angle 90.8° [1]. The Yb^{3+} ion has one hole in the 4f closed shell. The $J=\frac{7}{2}$ ground multiplet splits into four doublets under the crystal field. Thus, the low-temperature dynamics is described by an effective $S=\frac{1}{2}$ spin chain. The neutron scattering experiments on Yb_4As_3 confirmed that the excitation spectrum is well described by the one-dimensional $S=\frac{1}{2}$ isotropic Heisenberg model [2] in the absence of magnetic field. The interchain interactions are small and ferromagnetic, leading to a low-T spin-glass freezing [1]. On the other hand, the field-dependent data confirm the existence of a gap related to the Dzyaloshinsky–Moriya (DM) interaction [3] which can be mapped onto the anisotropic Heisenberg model with both uniform field B^x and staggered field B_s^y [4].

To characterize the finite-temperature properties of the Yb_4As_3, we consider the $S=\frac{1}{2}$ Heisenberg model with DM interaction [4,5] in a wide range of magnetic field ($B = 0$–25 T). Following the scheme described in Ref. [5], we have performed transfer-matrix simulations of the specific heat and magnetization using the parameters: $g_{\parallel} = 2.9$, $g_{\perp} = 1.3$ [6], $J/k_B = -26$ K [2] and $\tan(\theta) = 0.19$ [4]. The high-field data are new and interesting due to the gap opening [3].

The specific heat results determined in the magnetic fields are presented in Fig. 1. The open symbols represent our experimental results for a polydomain sample with the magnetic field ($B = 4$–19.5 T) applied along the cubic $\langle 1\ 1\ 1 \rangle$ direction and the filled symbols are numerical results. For the experimental data the phonon contribution $C_{ph} = 2.05 \times 10^{-3} T^3$ J/(K^4 mol) has been subtracted [3]. The measurements were performed for a polydomain sample in which 25% of

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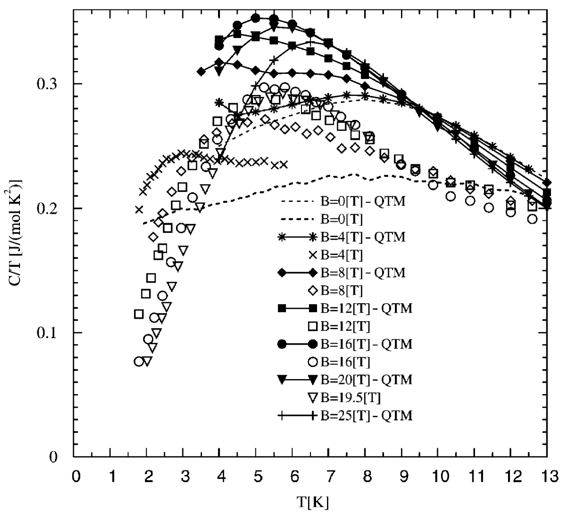

Fig. 1. Comparison of the measured specific heat after phonon subtraction and QTM calculation for Yb_4As_3.

the domains were oriented with the spin chains parallel to the applied field B and about 75% of the domains were aligned so that the effective field component $B\sin(70^{\circ})$ was perpendicular to the spin chains. With increasing magnetic field the molar specific heat C/T maximum increases, shifts to the right and the C/T curves intersect at about 9 K, which is consistent with the new experimental findings. However, our theoretical specific-heat data systematically overestimate the experimental results. This has not been understood so far.

Instead, we have decided to analyze the magnetization data. To achieve the convergence of our extrapolations up to $B = 25$ T, we performed simulations of the field-dependent magnetization at $T = 3$ K. In Fig. 2 we present these results for the polydomain sample by full circles, where vanVleck-type ($\chi_{\perp} = 0.0324$ and $\chi_{\parallel} = 0.0205$) contributions [6] are added. We also plot the corresponding experimental data extracted at 0.6 K [3] and supplement them with the averaged results of

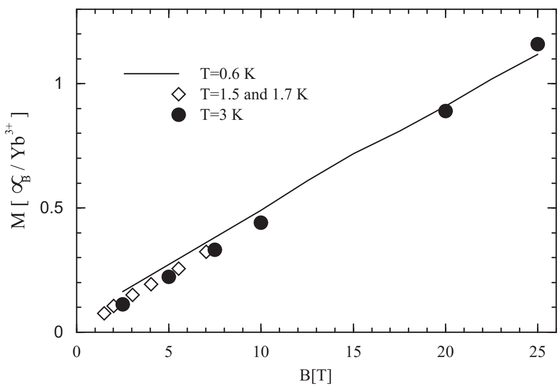

Fig. 2. The field-dependent magnetization for Yb_4As_3: experiment (◇ and continues line) and theory (•).

Iwasa et al. [6] for $T = 1.5$ and 1.7 K, represented by diamonds (consistent with DMRG calculations [6]).

In conclusion, we have presented the experimental field-dependent specific heat and magnetization data and successfully compared them with the quantum transfer-matrix calculations performed for the Heisenberg model with the Dzyaloshinsky–Moriya interactions, revealing at least the qualitative agreement with experiment.

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