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Transport Properties of $CeCo_{12}B_6$ in Vicinity of Phase Transition

Y. Skorokhod[a], Z. Arnold[a], O. Isnard[b], H. Mayot[b], M. Míšek[a] and J. Kamarád[a]

[a]Institute of Physics AS CR v.v.i.
Na Slovance 2, 182 21, Prague 8, Czech Republic
[b]Institut Néel, CNRS/Univ. J. Fourier
BP166x, 38042 Grenoble cedex, France

Study of resistivity and specific heat on $CeCo_{12}B_6$ compound was performed in a temperature range 2.5–300 K. The specific heat exhibits pronounced λ-type anomaly in the vicinity of the Curie temperature T_{C}. Using the Debye–Einstein model the following parameters were obtained: the Debye temperature $\theta_{\mathrm{D}} = 185$ K, coefficient of the electron specific heat $\gamma_{\mathrm{el}} = 115$ mJ/mol K. The parabolic temperature dependence of resistivity $\rho(T) = \rho_0 + A_\rho T^2$ was observed below T_{C} in agreement with ferromagnetic state. Comparison of $\mathrm{d}\rho/\mathrm{d}T(T)$ with $C_{\mathrm{M}}(T)$ allows to confirm their similar character, accordingly to theory of critical behavior.

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1. Introduction

The $CeCo_{12}B_6$ compound crystallize in the rhombohedral $SrNi_{12}B_6$-type structure (space group R-3m) [1] with the Co atoms located at the 18g and 18h sites and the Ce atoms at the 3a ones. The Curie temperatures T_{C} below 200 K and low Co magnetic moments are attributed to hybridization of B(p) and Co(d) electrons bands as a consequence of small distances between Co and B atoms (2.05 Å). X-ray absorption near-edge structure (XANES) studies showed that the Ce atoms are in intermediate mixed valence state [2]. From preliminary magnetic characterization follows that $CeCo_{12}B_6$ goes through the paramagnetic (PM) – ferromagnetic (FM) phase transition at $T_{\mathrm{C}} \approx 140$ K, the saturation magnetization of $4.8\mu_{\mathrm{B}}$/f.u. was obtained [3]. Measurement of transport properties is one of the most relevant ways of studying of changes in spin system near a phase transition. In this work we present results of resistivity and specific heat measurements on $CeCo_{12}B_6$.

2. Experimental

Samples were prepared using the method described in [2]. The crystal structures were determined by X-ray powder diffraction. Within the limits of resolution of the X-ray technique, the samples were found to be single phase.

The molar specific heat (C_p) of the studied compound was measured by relaxation two-τ method in commercial PPMS experimental setup (Quantum Design) in the temperature range 2.5–300 K. The resistivity of $CeCo_{12}B_6$ was measured on bar-shaped samples in temperature range 3.5–290 K in a close-cycle refrigerator. The measurement was made using lock-in amplifier by standard four-point method.

3. Results and discussion

The C_p vs. T curve shows regular solid-state behavior in both PM and FM regimes. A pronounced λ-type anomaly was observed in vicinity of FM–PM phase transition which is typical of second-order transition (Fig. 1a).

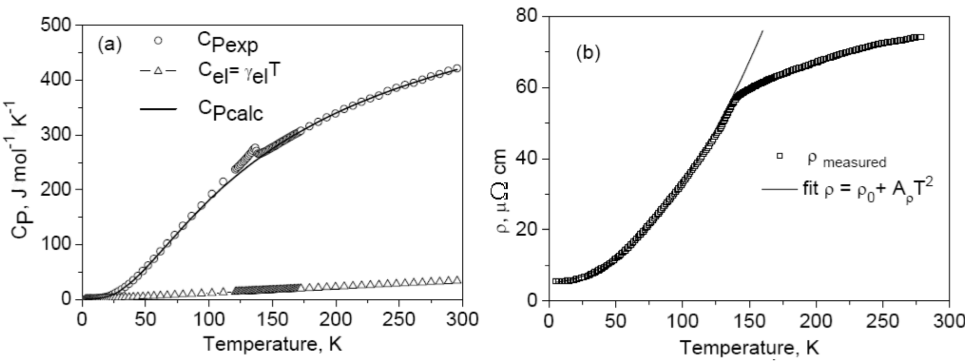

Fig. 1. Temperature dependence of specific heat (a) and resistivity (b) of $CeCo_{12}B_6$. Experimental data are depicted by open circles; the solid line indicates calculated values.

Magnetic part of C_p can be obtained by subtraction of calculated lattice and electron contributions from the experimental data. The electron specific heat is considered as $C_{\mathrm{el}} = \gamma_{\mathrm{el}}T$. The coefficient γ_{el} is obtained as intersection of C_p/T vs. T^2 plot with C_p/T axis: $\gamma_{\mathrm{el}} = 115$ mJ mol^{-1} K^{-2}.

Analysis of lattice specific heat C_{ph} was performed with the use of the Debye–Einstein model for heat capacity [4, 5]. Here, total spectrum of phonon contribution is splitted up to 3 acoustic branches, described by Debye's integral and $3N_{\mathrm{f.u.}} - 3$ optical branches, described by Einstein's exponential formula, where $N_{\mathrm{f.u.}} = 19$ is number of atoms in formula unit (for details see Ref. [5]). It is necessary to denote the importance of appropriate splitting of optical part by several sets of branches described by the same parameters. On the one hand, big number of parameters causes significant complication of fitting procedure. On the other, reducing of their number leads to rough approximation of the experimental data and the magnetic specific heat can be unsatisfactorily overestimated. In our case five sets of optical branches were chosen as optimal configuration. It was found that the anharmonic contribution to the specific heat is not negligible and

TABLE

Part of the phonon spectra.

	Multiplicity of the branch	Characteristic temperature, K	Anharmonic coefficient, K^{-1}
Acoustic (Debye)	3	185	4.2×10^{-4}
Optical (Einstein)	4	162	8×10^{-4}
	9	235	3.5×10^{-4}
	11	342	2.5×10^{-4}
	13	417	1.2×10^{-4}
	17	697	4.2×10^{-4}

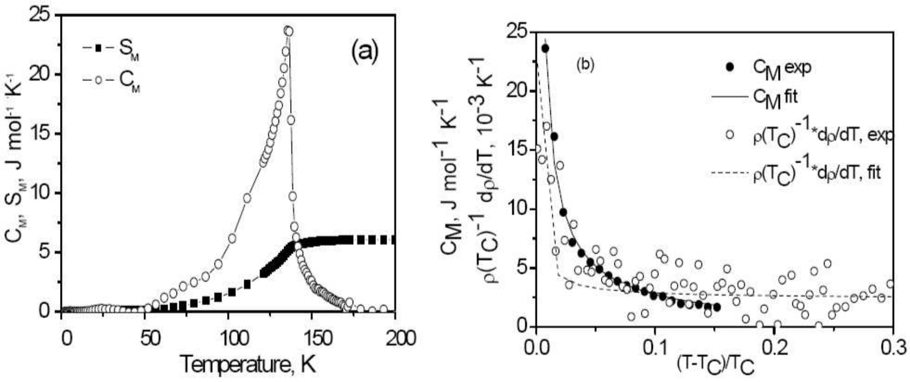

Fig. 2. Temperature dependence of magnon specific heat $C_{\rm M}$ and magnetic entropy $S_{\rm M}$ (a) and temperature derivative of the resistivity with theoretically fitted values together with magnon specific heat $C_{\rm M}$ (b).

should be taken into account [4]. Parameters of the best fit at both low and high temperatures are collected in Table.

Resulting temperature dependence of magnetic specific heat $C_{\rm M}$ is plotted in Fig. 2a. The $C_{\rm M}$ value is close to zero at temperatures 0–50 K and above 175 K that corresponds to FM and PM regimes, respectively. At 50 K it begins to increase and reaches its maximal value $C_{\rm Mmax} \approx 24$ J mol^{-1} K^{-1} at $T = 135.5$ K which is considered as transition temperature. In the framework of phase transition theories the magnetic contribution $C_{\rm M}$ to specific heat above the $T_{\rm C}$ is given by the following power law:

$$C_{\rm M} = (A'/\alpha) * (|t|^{-\alpha} - 1), \tag{1}$$

where reduced temperature $t = (T - T_{\rm C})/T_{\rm C}$ and $\alpha = 0.785$ (Fig. 2b).

The magnetic entropy $S_{\rm M}(T)$ was calculated from the $C_{\rm M}$ by numerical integration (Fig. 2a). It saturates to value ≈ 6 J mol^{-1} K^{-1} above the magnetic phase transition.

Temperature dependence of resistivity is presented in Fig. 1b. Below the transition temperature resistivity can be described as $\rho = \rho_0 + A_\rho T^2$, where ρ_0 is residual resistivity, as is typical of the ferromagnets. Calculated values of ρ_0 and A_ρ are 5.27 $\mu\Omega$ cm and 2.76×10^{-9} $\mu\Omega$ cm K^{-2}, respectively. Above the T_C the resistivity data were fitted to the prediction of the theory of critical phenomena [6, 7]:

$$\frac{1}{\rho(T_\mathrm{C})}\frac{\mathrm{d}\rho}{\mathrm{d}T} = \frac{A''}{\alpha}\left(|t|^{-\alpha} - 1\right) + B'', \tag{2}$$

where A'' and B'' are constants and α is calculated from the specific heat data. Keeping T_C fixed, the values of A'' and B'' are determined: $A'' = 0.7 \times 10^{-4}$ K^{-1}, $B'' = 2.42 \times 10^{-3}$ K^{-1}.

4. Conclusions

The detailed analysis of specific heat of $CeCo_{12}B_6$ compound was performed in the temperature range 2–300 K. Magnetic contribution to the specific heat and magnetic entropy near T_C was obtained using the Debye–Einstein approximation for lattice heat capacity. Temperature dependence of magnetic specific heat $C_\mathrm{M}(T)$ and temperature derivative of resistivity $\mathrm{d}\rho/\mathrm{d}T(T)$ above T_C can be described within the framework of short-range spin fluctuation model [8].

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