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ELECTRONIC, MAGNETIC AND TRANSPORT PROPERTIES OF YCo_3B_2 COMPOUND

A. KOWALCZYK, A. JEZIERSKI, L. SMARDZ AND J. BASZYŃSKI

Institute of Molecular Physics, Polish Academy of Sciences
Smoluchowskiego 17, 60-179 Poznań, Poland

We studied the electronic, magnetic and transport properties of the hexagonal YCo_3B_2 compound. The electronic structure was studied by X-ray photoemission spectroscopy and *ab initio* self-consistent tight binding linear muffin tin orbital method. We found a good agreement between the experimental X-ray photoemission spectroscopy valence band spectra and theoretical calculations. Theoretical calculations showed that the YCo_3B_2 is a paramagnet in agreement with experimental results. Electrical resistivity at low temperatures shows a T^2 dependence, implying that the scattering by the spin fluctuactions is dominant in this temperature range.

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1. Introduction

Rare earth (R) and cobalt (Co) can form together a unique group of intermetallic compounds with hexagonal $CaCu_5$ type structure. The RCo_3B_2 compounds crystallize in the $CeCo_3B_2$ type of structure which is derived from the $CaCu_5$ type by replacing Cu atoms at the 2c and 3g sites by B and Co atoms, respectively [1]. The magnetic studies [2] and NMR measurements [3] indicate that the YCo_3B_2 compound is a Pauli paramagnet. On the other hand, Ballou et al. [4] suggest that YCo_3B_2 exhibits paramagnetic behaviour with the maximum of susceptibility at about 150 K. The above disagreement is not yet clear.

In this paper we present the electronic, magnetic and transport properties of the YCo_3B_2 compound.

2. Experimental details

The sample preparation was described in detail in Ref. [5]. The room temperature X-ray diffraction patterns revealed that the YCo_3B_2 compound is prepared as a single-phase material with the lattice constants $a = 5.04$ Å and $c = 3.03$ Å.

The X-ray photoemission spectra (XPS) were measured with Al K_α radiation of 1486.6 eV at room temperature using a SPECS EA 10 PLUS spectrometer. The procedure of the preparation of the sample surface was described elsewhere [5]. All emission spectra were measured immediately after the sample cleaning in vacuum of 8×10^{-11} mbar.

Electrical resistivity measurements were carried out by a standard four-probe technique.

3. Results and discussion

The electronic structure and magnetic moment was calculated by the spin-polarised tight binding linear muffin tin orbital (TB LMTO) method [6]. The self-consistent spin-polarised band calculation were performed for the experimental lattice parameters ($a = 5.04$ Å and $c = 3.03$ Å) and for 270-k points in irreducible wedge of the Brillouin zone. In the band calculations we included the full hybridisation between s, p, and d electrons of yttrium, cobalt, and boron atoms. The calculations of the electronic structure showed that the density of states (DOS) at the Fermi level is dominated by the Co-band (Fig. 1) and is 3.39 states/(eV f.u.). The contribution from Y and B to the DOS at the Fermi level is very small.

The partial replacement of the Co atoms by boron in $Y(Co_{1-x}B_x)_5$ causes the decrease in the Curie temperature T_C, Co magnetic moment, and intersublattice exchange interaction [7]. Basing on *ab initio* LMTO band structure calculations Szajek [8] showed the dependence of the magnetic moments of Co atoms on the local environment in Y–Co–B compounds. The atomic moment was decreased strongly by neighbouring B atoms. In YCo_5 there are two non-equivalent cobalt sites with the different magnetic moments [8]. The different values of magnetic moment on the Co atoms are associated with their various local environments.

In Fig. 1 we present the experimental valence band XPS spectrum (solid line), and the theoretical DOS convoluted by Lorentzians of the half-width 0.4 eV and multiplied by cross-sections (broken line) for the YCo_3B_2 compound. The Fermi level is located at $E = 0$ eV. The main peak in the XPS valence band spectrum located at $E = -1.2$ eV represents the contribution of the Co-d states. The agreement between the experimental XPS spectrum and calculations valence is good.

The temperature dependence of electrical resistivity for YCo_3B_2 is shown in Fig. 2. The resistivity follows a quadratic behaviour in the temperature range 4.2–60 K. The NMR measurements [3] and magnetic studies [2] indicate that YCo_3B_2 is a Pauli paramagnet. The electrical resistivity of the Pauli paramagnet YCo_2 compound [9] shows a fairly large variation proportional to T^2 below 20 K. Ikeda [9] interpreted the T^2 law in terms of the spin fluctuations in agreement with Ueda and Moriya [10]. He concluded that YCo_2 is an enhanced paramagnet and the resistivity is dominated by electron–paramagnon scattering. The magnetic

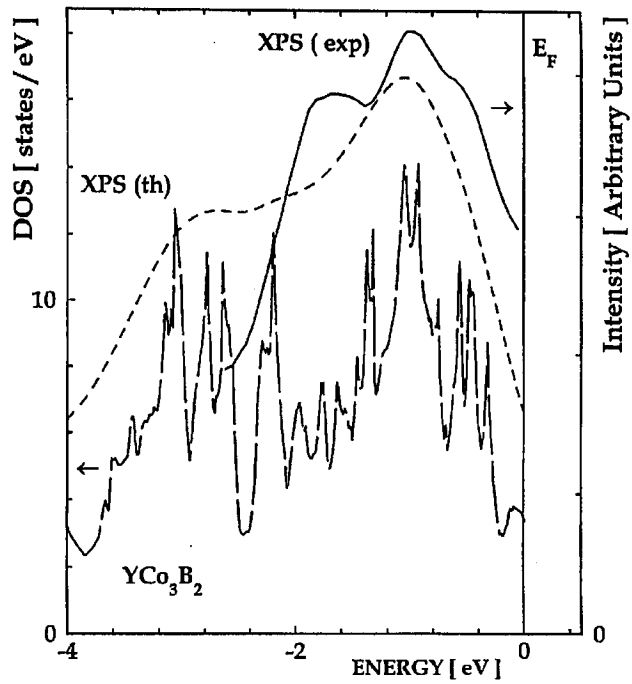

Fig. 1. The measured XPS valence band spectra for YCo_3B_2 compound (solid line), the theoretical density of state (broken curve), and the theoretical density of states convoluted by Lorentzians of the half-width 0.4 eV and multiplied by cross-sections. The Fermi level is located at $E = 0$ eV.

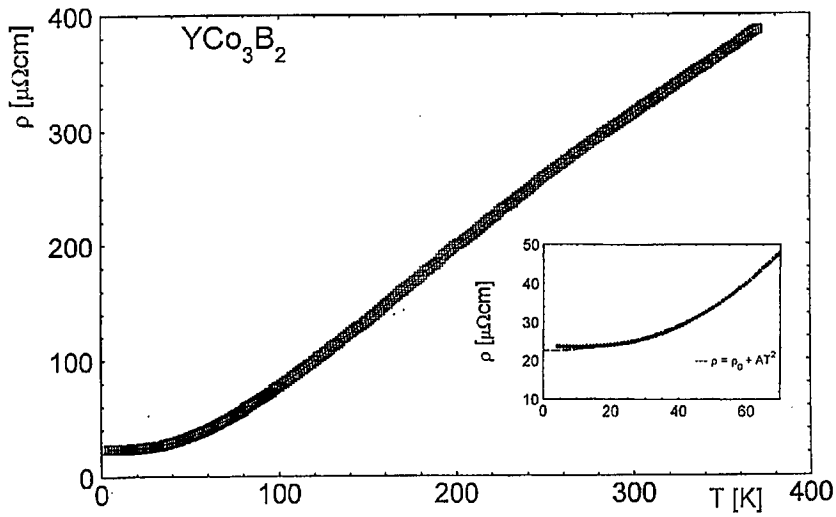

Fig. 2. Temperature dependence of the electrical resistivity for YCo_3B_2 compound. The inset shows the low temperature part in the temperature range 4.2–60 K fitted to the relation $\rho(T) = \rho_0 + AT^2$.

behaviour of cobalt in R–Co–B and R–Co systems shows a typical spin fluctuaction mechanism also predicted by self-consistent renormalization theory [11].

4. Conclusions

The main results are summarized as follows:

1) Electronic structure calculations show that YCo_3B_2 is non-magnetic and near the Fermi level, the density of states is dominated by the Co-band.

2) The experimental XPS valence band spectra agree very well with calculated DOS near the Fermi level.

3) Electrical resistivity at low temperatures shows a T^2 dependence, implying that the scattering by the spin fluctuactions is dominant in this temperature range.

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