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ORIGINAL PAPER

Magnetic Properties of the Intermetallic Compound HoCuBi

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Abstract We present an investigation on the intermetallic compound formed by HoCuBi which has a monoclinic crystalline $P2$ structure with lattice parameters; $a = 9.8012(26)\,\AA$, $b = 6.0647(6)\,\AA$, $c = 6.1663(13)\,\AA$. In this report, we performed an extensive analysis of the magnetic characteristics, specific heat at low temperature mainly close to the region of the observed antiferromagnetic transition with Nèel temperature about 7 K, and to the field induced spin-crossover; the metamagnetic transition typically observed in antiferromagnetic systems by measurements of M-H, (Magnetization-Magnetic Field) at low temperatures.

Keywords Magnetism · Metamagnetism · Specific heat

1 Introduction

Many intermetallic compound of the type RT(Bi, Sb) have been widely studied in the last 20 years. The importance of these interesting compounds has been related to the many relevant and diverse electronic properties and many different characteristics that they present [1]. The different atomic species that can be introduced may modify the crystalline structure and give place to a number of characteristics [2]. As mentioned, those changes in electronic characteristics are depending on the elements forming the compound [3–5]. If we consider for instances compounds with elements type as RT(Bi, Sb, Se), where R may be a lanthanide atom, T a transition element have been studied in the past. The many different phenomena that can be present are Kondo effect, and/or heavy Fermion behavior at low temperature, antiferromagnetic, ferromagnetic characteristics, and spin glass, and also superconductivity.

The intermetallic alloys with rare earth atoms present physical properties mainly related to its magnetic properties. Those alloys with f-electron shells can form different crystallographic structures and consequently different physical properties. In this study, our investigations were concentrated into the magnetic and thermal behavior. The particular compound studied was HoCuBi. It presents characteristic of spin crossover or as also named metamagnetism at low temperature, antiferromagnetism, and the influence of the magnetic field intensity in the specific heat transition.

As mentioned above, this work is focused on HoCuBi intermetallic alloy. In the literature already published, we found no published study on this compound. In the similar EuCuBi [6, 7] and YbCuBi [8], both show antiferromagnetic ordering with a magnetic phase transition temperature at 18 K, and effective magnetic moment $\mu_{eff} = 7.65$ BM. Also, $Ho5Cu_{0.7}Bi_{2.3}$ is reported [9] with an orthorhombic $Pnma$ structure and no magnetic behavior was reported [10]. This is the first time a complete study was performed on this compound.

2 Experimental Details

The intermetallic compound was prepared by using an arc melting furnace, For the preparation stoichiometry amounts of materials were powdered and pastilled. Elements used were of high purity Ho (99.99%), Cu (99.99%), and Bi

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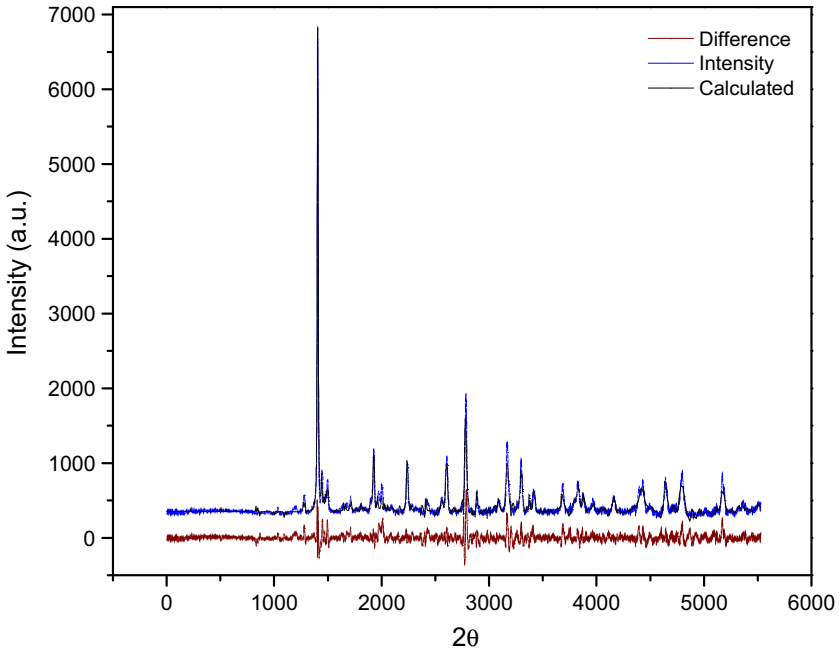

Fig. 1 X-ray diffraction pattern and Rietveld refinement, the *red data line* shows the difference between the calculated and observed pattern. The space group was orthorhombic $P2$ with lattice parameters; $a = 9.8012(26)$ Å, $b = 6.0647(6)$ Å, $c = 6.1663(13)$ Å

(99.99%). The preparation was performed in the arc system with an oxygen free atmosphere in order to prevent oxygen contamination we used a Zirconium getter and ultra-high purity argon atmosphere. Additionally, in order to compensate bismuth losses an excess of bismuth, about 10% was used during the arc melting process. The melting was carried out using low current values for the arc discharge, about 50 Å to minimize any extra loss of bismuth. Samples were remelted several times followed by annealing for 10 days at 900 °C.

The X-ray data of the resulting powders of polycrystalline sample was obtained with a Bruker D8 diffractometer. The unit cell data were derived using DicVol software. The magnetic data reported here were measured with a Quantum Design instrument, MPMS equipped with a SQUID (San Diego, CA) heat capacity more measurements were performed with using a Physical Property Measurement System PPMS, from Quantum Design.

Table 1 Atomic positions parameters of HoCuBi compound. Space group $P2$ (No. 3), $a = 9.8012(26)$ Å, $b = 6.0647(6)$ Å, $c = 6.1663(13)$ Å, $R_F = 8.7\,\%$

Atom	Type of position	x/a	y/b	z/c	Occupation
Cu	4e	0.5244(4)	0.5314(5)	0.8286(0)	1.0
Cu	4e	0.6584(4)	0.1081(8)	0.2697(5)	1.0
Bi	4e	0.9433(9)	0.1374(1)	0.2646(7)	1.0
Bi	4e	0.8390(1)	0.5545(1)	0.4818(0)	1.0
Ho	4e	0.8443(5)	0.6191(6)	0.0314(1)	1.0
Ho	4e	0.7081(7)	0.1662(2)	0.7511(3)	1.0

3 Results

At first X-ray powder diffraction analysis, Fig. 1 was used to solve the crystalline structure and with the help of Rietveld refinement, we carried on and fit the data yielding the lattice parameters; $a = 9.8012(26)$ Å, $b = 6.0647(6)$ Å, $c = 6.1663(13)$ Å in the monoclinic crystalline structure space group type $P2$. Results related to the atomic coordinates are shown in Table 1. It is important to mention that before trying to solve the crystalline structure, we tested various different data bases and found no structure matching it.

The magnetic susceptibility $\chi(T)$ of a specimen of HoCuBi shows a sharp peak at low temperature, the antiferromagnetism at about 7 K. This is the characteristic of a long-range antiferromagnetic order in the sample, with Nèel

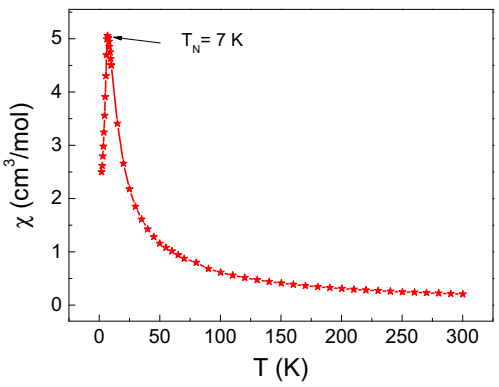

Fig. 2 Magnetic susceptibility $\chi(T)$ from room temperature to 2 K. At low temperatures, the peak corresponds to the maximum of antiferromagnetic ordering ocurring at 7 K, but it is important to remark that the antiferromagnetic transition start at 5.5 K, according to our specific heat measurements

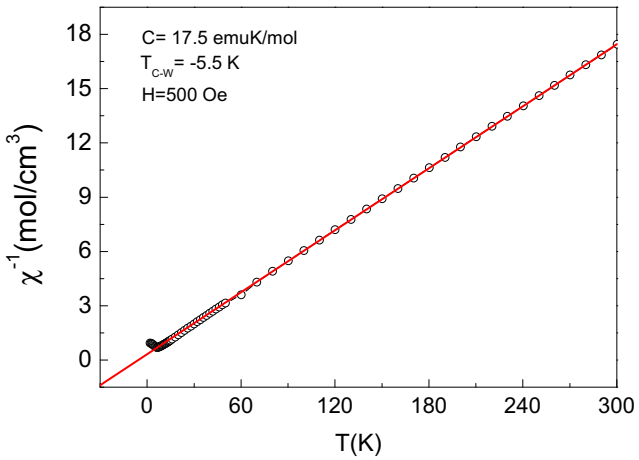

Fig. 3 Inverse magnetic susceptibility $\chi^{-1}(T)$.The *straight line* corresponds to the Curie Weiss law. At low temperature the *data line* presents a change due to the antiferromagnetic transition. The fitting gives a Curie-Weiss temperature of -5.5 K. The Nèel temperature is $T_N = 7$ K, and the Curie constant determined is $C = 17.415(emuK/mol)$

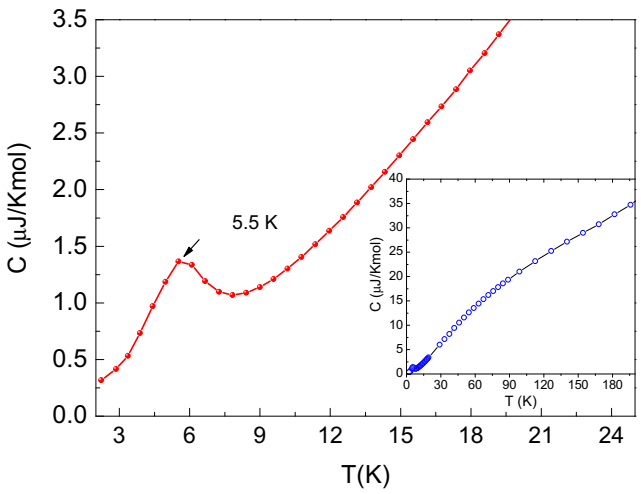

Fig. 5 Specific heat vs temperature determined at zero applied field. the main panel displays the maximum of the transition occurring at 5.5, the onset is at about 7 K. The *inset* displays the overall behavior of the specific heat as function of temperature, at low temperature is observed the transition

temperature $T_N = 7$ K. The temperature dependence of the inverse of the magnetic susceptibility and the fit of the Curie-Weiss law to the data are plotted in Fig. 3 and confirm the antiferromagnetic transition.

X-ray diffraction at room temperature shows that this compound crystallizes in a monoclinic $P2$ structure. The temperature dependence of the magnetic susceptibility χ is shown in Fig. 2. The magnetic susceptibility clearly indicates the antiferromagnetic ordering at about $T_N = 7$ K, showing a steep decrease at $H = 1\,T$. The inverse magnetic susceptibility χ^{-1} is shown in Fig. 3 which has been adjusted by the Curie-Weiss equation. The effective magnetic moment is $\mu_{eff} = 11.80$ is close to the theoretical value for holmium $\mu_{eff} = 10.61$ and $\theta_p = 88$ K.

As our experimental measurements show at low temperature, it was seen an antiferromagnetic transition. In M-H measurements, the applied magnetic field can induce a series of cascade changes from low to high spin flips. Strzyjewski and Giordano, [11] mentioned that the spin flips may be associated to a first order phase transition, in some cases.

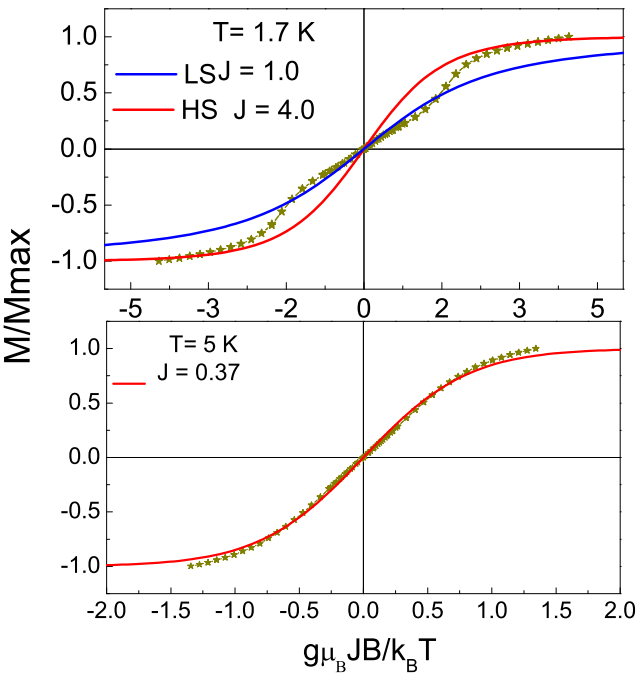

Fig. 4 Magnetization normalized versus magnetic field, M/M_{max} vs H. Brillouin function was used with two distinct J values. The fit indicates a change at low applied magnetic field of a spin crossover from J 1 to 4

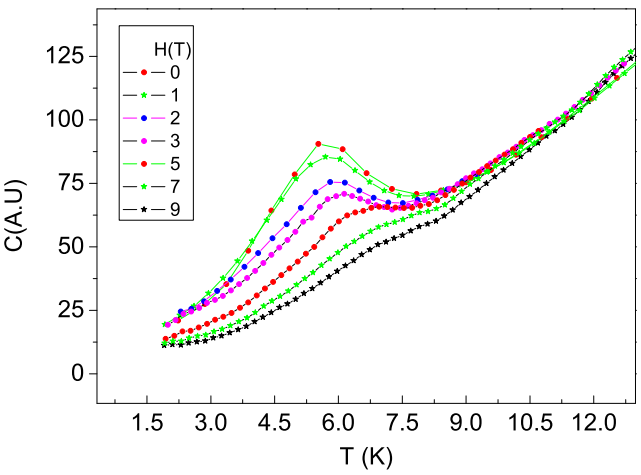

Fig. 6 Changes observed in the specific heat vs temperature, as function of magnetic field, from 0 to 9 T, note that the transition decreases as the magnetic field is increased due to the reduced strength of the exchange force. Measurements were vertically displaced by a constant amount in order to have a better resolution

At low temperature below the Nèel temperature, we see in M-H measurements an appreciable change of the magnetization with the applied field; this behavior is named in the literature, as a spin crossover transition. This feature is seen only at low temperatures indicating a change from low to high spin. This characteristic is observed in measurements of isothermal M-H at 2 K and a little above. The corresponding Brillouin fit indicates variations of J from 1 to 4, and consequently a change of the spins from s = 1/2 to 3/2 (Fig. 4).

Specific heat measurement were carried out and the plot C/T versus T is shown in Fig. 5, applied magnetic field measurements were studied and the plot varying the field from 0 to 9 T is shown in Fig. 6. The specific heat shows the magnetic transition, the sharp peak at 5.5 K indicating the antiferromagnetic ordering of this compound. As the magnetic field is increased, the transition decreases, which is the clear indication that the antiparallel exchange interaction of the spins has been weakened by the strength of the magnetic field.

4 Conclusions

This investigation shows our recent crystallographic, magnetic, and thermal studies performed on the polycrystalline HoCuBi compound which crystallizes in a monoclinic $P2$ structure with lattice parameters; $a = 9.8012(26)\ \AA$, $b = 6.0647(6)\ \AA$, $c = 6.1663(13)\ \AA$. We found several interesting physical features: an antiferromagnetic behavior, with Nèel temperature of $T_N = 7\,K$ and effective magnetic moment $\mu_{eff} = 11.80\ \mu_B$ which is close to the theoretical value for holmium, a metamagnetic characteristic at low temperature (spin crossover), and influence of the magnetic field in the specific heat transition.

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