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Letter

Magnetic structure of the $TbCu_2In$ compound

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Abstract

We have performed neutron diffraction experiments on a polycrystalline $TbCu_2In$ compound. This compound crystallizes in the cubic $L2_1$-type crystal structure and orders antiferromagnetically at T_N = 7.5 K. Below T_N, the Tb magnetic moments equals 8.81(19) μ_B, and forms a sine-wave modulated structure which is stable down to 1.5 K.

Keywords: Rare earth compounds; Magnetic structure; Neutron diffraction

1. Introduction

The Heusler alloys (cubic $L2_1$ structure) with the general chemical formula RT_2X, where R is a rare earth element, T is d-electron element and X is p-electron element are the subject of intensive investigations because of interesting magnetic and superconducting properties including co-existence of superconductivity and antiferromagnetism [1].

The types of magnetic ordering in these compounds are determined only for some compounds and are manifold [1]. In our laboratory systematic investigation of these compounds are planned with the purpose to determine their magnetic ordering.

In this work, the low-temperature neutron diffraction measurements of the $TbCu_2In$ compound are presented. From these data the magnetic structure of this compound is determined.

According to the data in Ref. [2], $TbCu_2In$ crystallizes in the cubic structure of the $L2_1$-type and is antiferromagnet with the Néel temperature equal to 6 K.

2. Experimental details and results

The polycrystalline sample was synthesized by arc melting of stoichiometric amounts of high-purity Tb, Cu and In elements in the argon inert atmosphere. The ingot was homogenized in an evacuated sealed quartz tube at 800 °C for one week. In order to check the purity of the obtained sample, X-ray powder diffraction measurements were performed. The results reveal that sample have the cubic $L2_1$-type structure. The determined lattice parameter *a* equals 6.623(1) Å and is in good agreement with the data published, previously

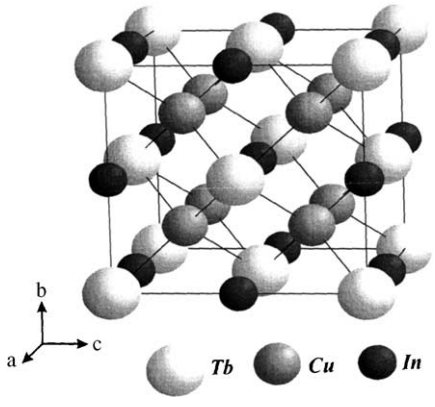

Fig. 1. Crystal structure of $TbCu_2In$ (the $L2_1$-type).

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[2]. Additional peaks of small intensity corresponding to the $TbCu_4In$ phase are observed.

The E6 diffractometer at the Berlin Neutron Scattering Center was used to perform neutron diffraction measurements in the temperature range 1.5–15 K with the incident neutron wavelength 2.4415 Å. The neutron diffraction data were analyzed using the Rietveld-type program Fullprof [3].

Previous X-ray diffraction study [2] revealed that $TbCu_2In$ exhibits the cubic $L2_1$-type crystal structure (space group F*m3m*) with atoms at the following sites:

- 4 Tb atoms in 4(a) site: 0, 0, 0;
- 8 Cu atoms in 8(c) site: 1/4, 1/4, 1/4;
- 4 In atoms in 4(b) site: 1/2, 1/2, 1/2.

The crystal structure of $TbCu_2In$ is displayed in Fig. 1. The refined neutron diffraction pattern collected in the paramagnetic state at 15 K is presented in Fig. 2. The crystal structure of $TbCu_4In$ was also determined. This compound exhibits the cubic crystal structure (space group $F\bar{4}3m$). The atoms

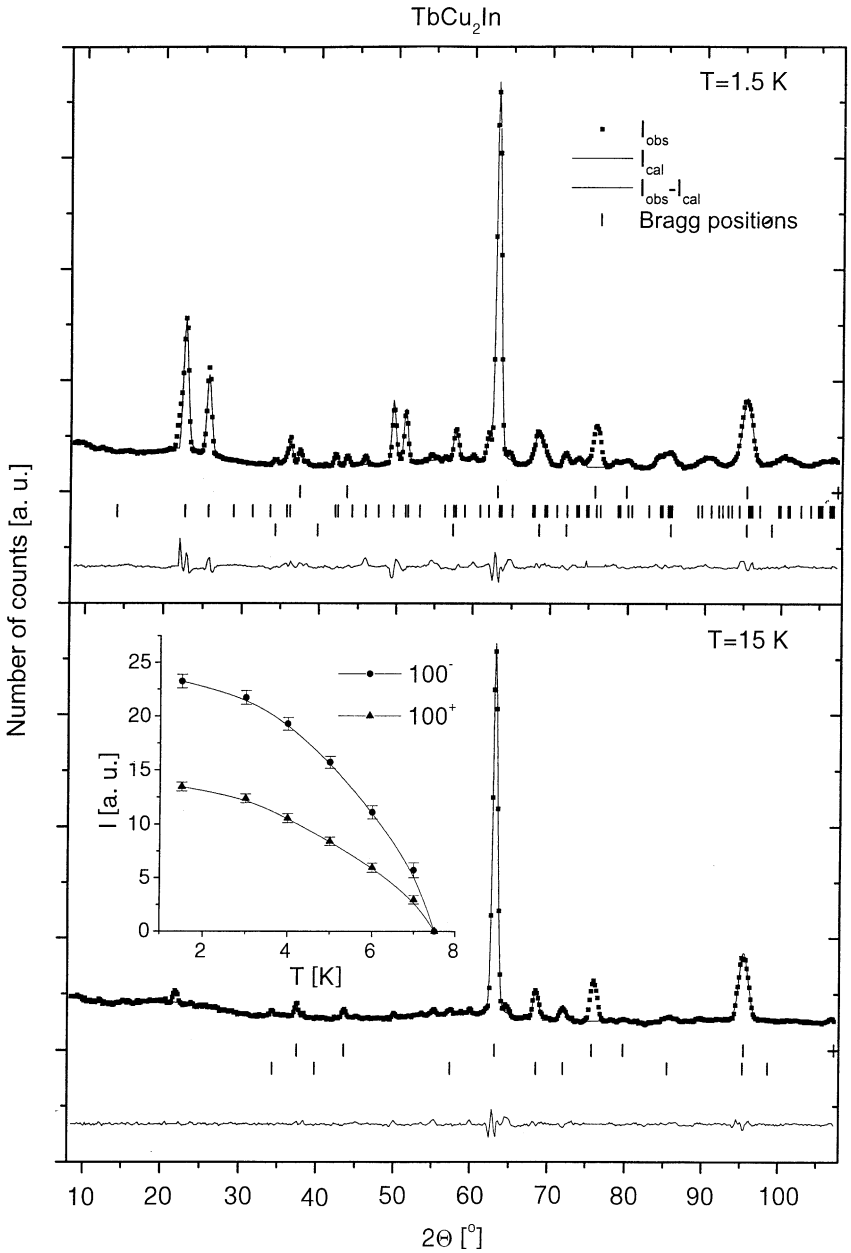

Fig. 2. Neutron diffraction patterns of $TbCu_2In$ compound at 1.5 and 15 K. The squares represent experimental points, the solid lines are the calculated profiles for the crystal and magnetic structure described in the text and the difference between the observed and calculated intensities is plotted at the bottom of each diagram. The vertical bars indicate the positions of the Bragg peaks of nuclear and magnetic origin. One interval of 2θ is excluded owing to cryostat reflections. The inset shows the temperature dependence of the 100^- and 100^+ magnetic peaks intensities.

Table 1
Crystal structure parameters of $TbCu_2In$ and $TbCu_4In$

T(K)	1.5	15	293	Reference
$TbCu_2In$				
a(Å)	6.6054(9)	6.6134(14)	6.623(1), 6.616	This work, [2]
R_{Bragg}(%)	1.15	0.74	9.8	
R_{prof}(%)	1.73	1.02	13.1	
$TbCu_4In$				
a(Å)	7.2020(21)	7.213(2)	7.221(3)	*Thiswork*
x	0.628(7)	0.631(4)	0.644(8)	
R_{Bragg}(%)	10.9	7.21	12.6	
R_{prof}(%)	10.3	10.3	12.9	

occupy the following positions:

- 4 Tb atoms in 4(a) site: 0, 0, 0;
- 16 Cu atoms in 16 (e) site: x, x, x;
- 4 In atoms in 4 (c) site: 1/4, 1/4, 1/4.

The crystal structure parameters for both compounds are summarized in Table 1.

The neutron diffractogram of $TbCu_2In$ recorded at 1.5 K is shown in Fig. 2. All additional reflections of the magnetic origin could be indexed assuming an antiferromagnetic order described by the propagation vector $\boldsymbol{k}$ = (0, 0, 0.3438(5)). The best fit was obtained for the following model of the magnetic structure:

- In the crystal unit cell, four Tb^{3+} ions are located at 0, 0, 0 ($\mathbf{S}_1$); 1/2, 1/2, 0 ($\mathbf{S}_2$); 1/2, 0, 1/2 ($\mathbf{S}_3$) and 0, 1/2, 1/2 ($\mathbf{S}_4$). The analysis of the intensity of peaks indicates the following sequence of the antiferromagnetic structure $\mathbf{S}_1-\mathbf{S}_2-\mathbf{S}_3+\mathbf{S}_4$, which corresponds to the magnetic structure of the first type [4].
- The Tb moment equal to 8.81(19) μ_B and parallel to the c-axis forms a sine-wave modulated structure (see Fig. 3) (R_{mag} = 9.1 %). The observed value of the magnetic moment of Tb^{3+} ion in $TbCu_2In$ at 1.5 K is close to the free ion value (9.0 μ_B).

Temperature dependence of the 100^- and 100^+ intensities leads to the Néel temperature of 7.5 K (see the inset in Fig. 2).

3. Discussion

Our neutron diffraction analyses show that $TbCu_2In$ crystallizes in the cubic $L2_1$-type structure and orders antiferromagnetically below T_N = 7.5 K. Previous magnetic measurements give a lower T_N value equal to 6 K [2].

The determined magnetic structure of $TbCu_2In$ is similar to the one observed in the isostructural $TbAg_2In$. In this compound magnetic ordering is also non-collinear described by the propagation vector $\boldsymbol{k}$ = (0, 0, k_z) (k_z = 0.344) [5].

The magnetic ordering in both compounds is different from those observed in other Heusler compounds based on rare earth atoms [6–8], as well as in isostructural RTSb compounds [9–12]. In all these compounds the magnetic structure is similar to that observed in MnO [13], where the magnetic lattice consists of parallel (1 1 1) planes within which all rare earth moments are coupled ferromagnetically, while adjacent (1 1 1) planes are coupled antiferromagnetically.

The interatomic distance between terbium atoms in the isostructural TbT_2X compounds (being $a/\sqrt{2}$) is large enough to exclude any direct magnetic interaction. Therefore, the magnetic order observed at low-temperatures is stabilized by long-range interaction, probably of the RKKY-type. According to the RKKY theory T_N is an oscillatory function of the interatomic distance. Fig. 4 shows the dependence of the Néel temperature on the lattice parameter for isostructural TbT_2X compounds which shows the oscillatory character.

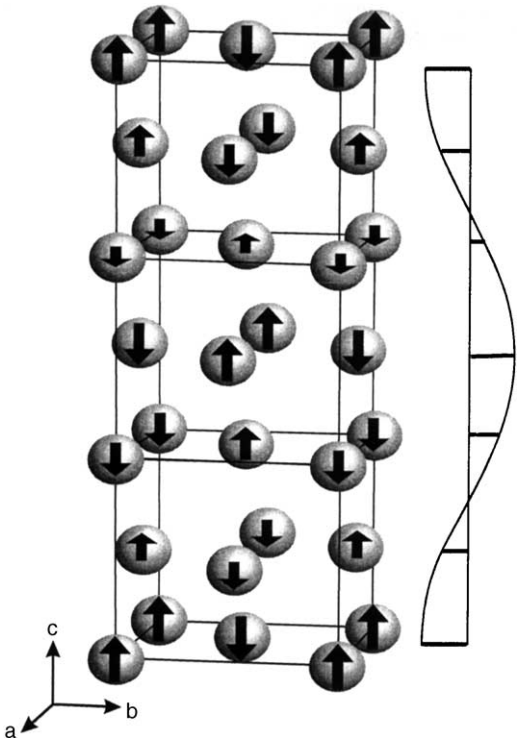

Fig. 3. Magnetic structure of $TbCu_2In$.

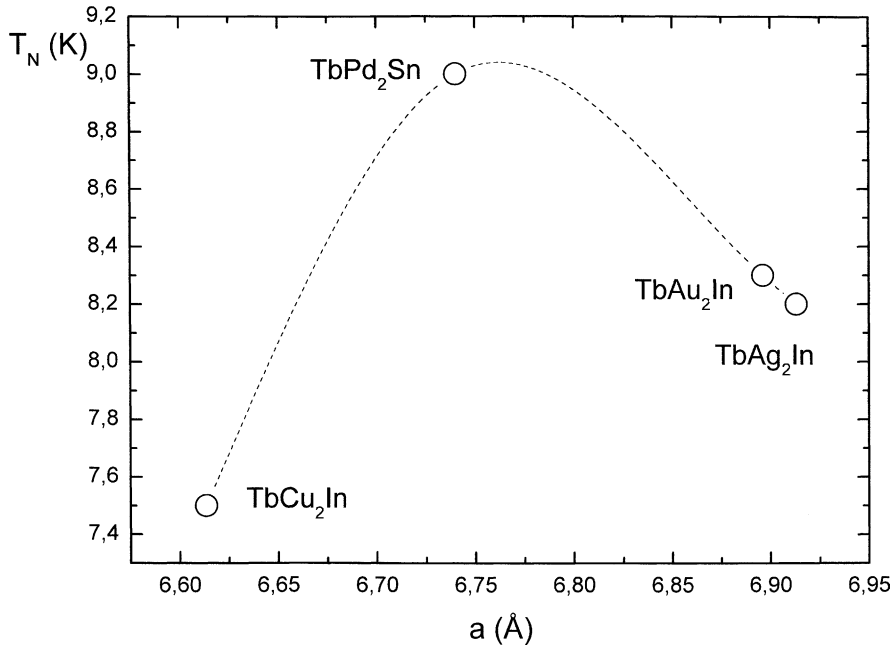

Fig. 4. Néel temperature vs. lattice constant *a* for some terbium Heusler alloys. Data are from Refs. [5,14,15].

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