Vol. 32 (2001) *ACTA PHYSICA POLONICA B* No 10 Special Issue

MAGNETIC STRUCTURES AND MAGNETIC PHASE TRANSITIONS IN RAuIn (R = Tb, Ho) COMPOUNDS*

W. Bażela

Institute of Physics, Cracow University of Technology
Podchorążych 1, 30-084 Kraków, Poland

Ł. Gondek, B. Penc, A. Szytuła

Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Kraków, Poland

N. Stüsser,

BENSC, Hahn-Meitner Institute, 14-109 Berlin, Germany

and A. Zygmunt

W. Trzebiatowski Institute of Low Temperature and Structure Research
Polish Academy of Sciences
P.O. Box 1410, 50-950 Wrocław, Poland

(Received June 21, 2001)

TbAuIn and HoAuIn compounds crystallize in the hexagonal ZrNiAl-type structure and order magnetically below 35 K for R = Tb and 4.8 K for R = Ho. In the case of TbAuIn a noncollinear antiferromagnetic structure described by the propagation vector $\boldsymbol{k} = (0, 0, \frac{1}{2})$ is stable in the temperature range from 1.5 K up to $T_{\rm N}$. The magnetic structure of HoAuIn determined at 1.5 K is noncollinear antiferromagnetic one. This low temperature magnetic structure could be described by two propagation vectors $\boldsymbol{k}_1 = (0, \frac{1}{2}, \frac{1}{2})$ and $\boldsymbol{k}_2 = (0, 0, \frac{1}{2})$. At $T = 2.5$ K an additional phase transition to a modulated structure is observed.

PACS numbers: 75.25.+z, 75.30.Kz, 75.50.Ee

* Presented at the XII School of Modern Physics on Phase Transitions and Critical Phenomena, Lądek Zdrój, Poland, June 21–24, 2001.

1. Introduction

This paper, concerning magnetic properties of RAuIn, reports a part of our systematic study of rare earth intermetallic compounds. RAuIn compound crystallize in the hexagonal ZrNiAl-type of crystal structure [1]. Magnetic properties of these compounds have not been investigated till now.

This paper reports the results of magnetic and neutron diffraction measurements which have been carried out to determine magnetic properties as well as the crystal and magnetic structure of TbAuIn and HoAuIn.

2. Experiment and results

The polycrystalline samples were prepared from high-purity rare earth, gold and indium elements by arc melting in a purified argon atmosphere. The reaction product was annealed at 800° C for several days. X-ray powder diffraction (CuK_α radiation) analysis show that the samples have hexagonal structure with the lattice parameters $a = 7.7018(11)$ Å, $c = 3.9355(7)$ Å for TbAuIn and $a = 7.6755(8)$ Å, $c = 3.8920(5)$ Å for HoAuIn. These parameters are in fair agreement with the data reported in Ref. [1].

Magnetic susceptibility and magnetization data were collected using a SQUID (in low magnetic fields) and a vibrating sample (up to $H = 50$ kOe) magnetometer in the temperature range 1.9–300 K. Neutron diffractograms were obtained using the E6 diffractometer at the BER II reactor, Hahn–Meitner Institute, Berlin (with the incident neutron wavelength 2.441 Å) in the temperature range from 1.5 up to 70 K. The Rietveld-type program FULLPROF [2] was adopted for processing the neutron diffraction data.

X-ray (at room temperature) and neutron diffraction patterns recorded in the paramagnetic state have confirmed that TbAuIn and HoAuIn have the hexagonal crystal structure of the ZrNiAl-type ($P\bar{6}2m$ space group). The unit cell contains three formula units. The atoms occupy the following positions: R atoms in $3(g)$ site: $x_{\mathrm{R}}, 0, \frac{1}{2}$; Au atoms in $1(b)$ site: $0, 0, \frac{1}{2}$ and $2(c)$ site: $\frac{1}{3}, \frac{2}{3}, 0$ and In atoms in $3(f)$ site: $x_{\mathrm{In}}, 0, 0$. The values of the lattice parameters a and c as well as the positional parameters corresponding to the minimum of the reliability factor are listed in Table I.

The temperature dependence of the magnetization at low magnetic fields (50 and 100 Oe) and 10 kOe are shown in Fig. 1. The parameters determined on the basis of magnetometric data are collected in Table II. They indicate that both compounds are antiferromagnets at low temperatures. The magnetization curve $M(H)$ at 1.9 K shows the existence of metamagnetic transition at the critical field H_{cr} equal 20.5 kOe for TbAuIn and 8 kOe for HoAuIn.

Magnetic peaks observed in the neutron diffraction pattern of TbAuIn collected at $T = 1.5$ K are indexed with the propagation vector $\boldsymbol{k} = (0, 0, \frac{1}{2})$

TABLE I

The refined structural parameters of TbAuIn and HoAuIn (space group $P\bar{6}2m$ (No. 189)); standard deviations are given in parentheses.

Compound	TbAuIn			HoAuIn		
T (K)	70	40	1.5	10	2.5	1.5
a (Å)	7.674(5)	7.672(5)	7.642(2)	7.628(4)	7.624(2)	7.619(2)
c (Å)	3.909(3)	3.901(3)	3.883(2)	3.866(3)	3.859(1)	3.857(1)
$\frac{c}{a}$	0.5094(7)	0.5085(7)	0.5081(4)	0.5068(6)	0.5062(3)	0.5062(3)
V(Å^3)	199.35(42)	198.84(42)	196.38(20)	194.81(35)	194.25(15)	193.89(15)
x_R	0.596(2)	0.597(2)	0.588(2)	0.598(2)	0.595(2)	0.599(2)
x_{In}	0.250(5)	0.253(5)	0.272(7)	0.265(5)	0.287(6)	0.290(5)
R_{Bragg}(%)	13.1	10.9	14.8	12.6	12.2	9.5
R_{prof}(%)	11.0	8.3	11.7	11.8	13.9	6.4

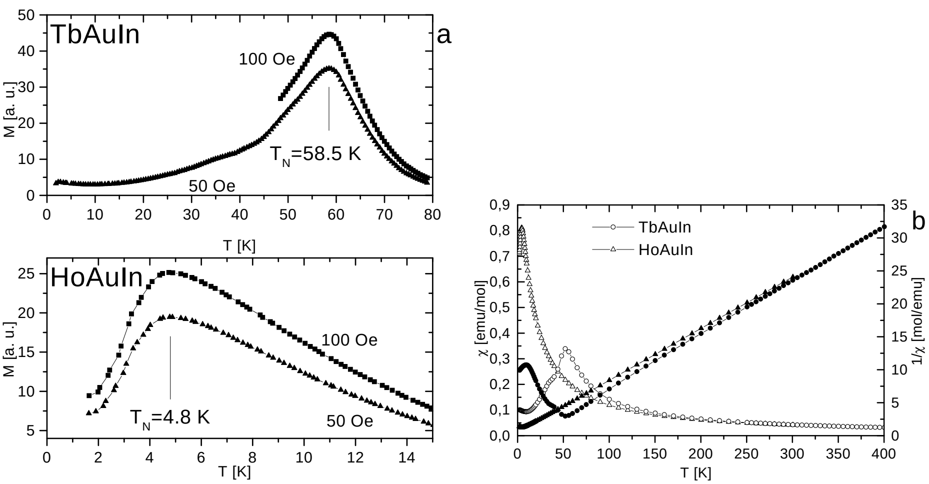

Fig. 1. Temperature dependence of the (a) magnetization of TbAuIn and HoAuIn at low magnetic fields (50 and 100 Oe) and (b) magnetic susceptibility and reciprocal magnetic susceptibility at $H = 10$ kOe.

(Fig. 2). The Tb magnetic moments, which are equal to $8.98(18)\mu_B$, form in the 001 plane a non collinear magnetic structure typical for a triangular lattice (see Fig. 3(a)). The temperature dependence of the peak intensity gives the Néel temperature of 35 K (Fig. 3). In the neutron diffraction pattern at 40 K only peaks connected with the crystal structure are observed.

The peaks of the magnetic origin on the neutron diffraction pattern of HoAuIn collected at 1.5 K are indexed by the propagation vector

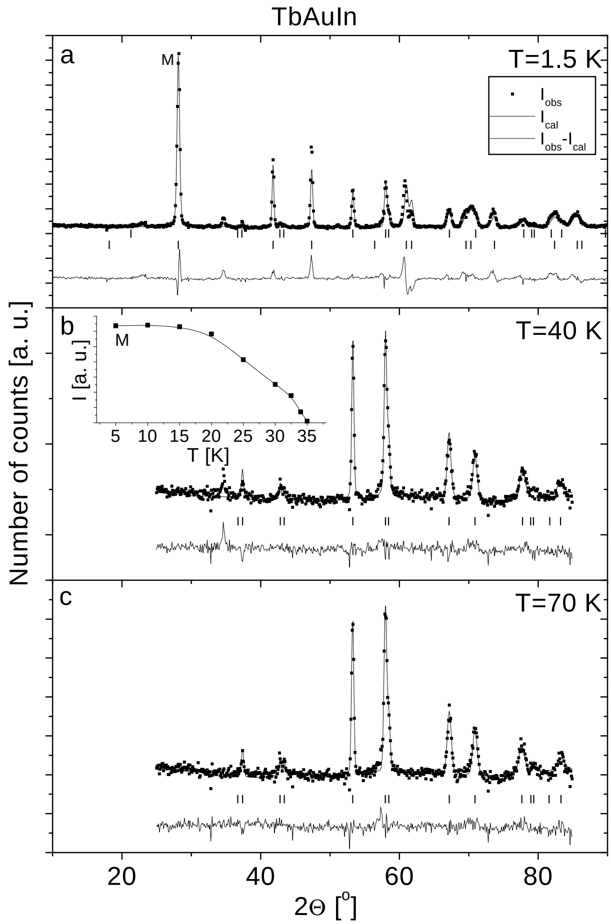

Fig. 2. Neutron diffraction patterns of TbAuIn at 1.5, 40 and 70 K. The squares represent experimental points; the solid lines are the calculated profiles for crystal and magnetic structure model (as described in the text) and the difference between the observed and calculated intensities at the bottom of each diagram. The vertical bars indicate Bragg peaks of nuclear and magnetic sublattices. The insert shows the temperature dependence of $000^{\pm}$ magnetic peak.

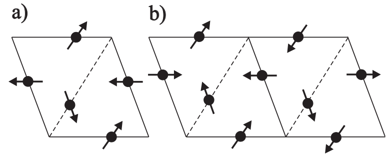

Fig. 3. Projection of the magnetic structures of (a) TbAuIn and (b) HoAuIn on the 001 plane.

TABLE II

Magnetic data of TbAuIn and HoAuIn: T_{N}-Néel temperature, T_t-metamagnetic transition temperature, θ_p-paramagnetic Curie temperature μ_{eff}-effective magnetic moment, μ-magnetic moment, LH — low field, HF — at 10 kOe.

Compound	T_{N} (K)	T_t (K)	θ_p (K)	H_{cr} (kOe)	μ_{eff} (μ_{B})		μ (μ_{B})		
					exp.	theor.	exp.		theor.
							M	ND	R^{3+}
TbAuIn LF	58.5	37						8.98(18)	9.0
HF	53.8	37	17	20.5	9.8	9.72	1.5		
HoAuIn LF	4.8							6.0(1)	10.0
HF	4.5		−9	8	10.1	10.61	4.9		

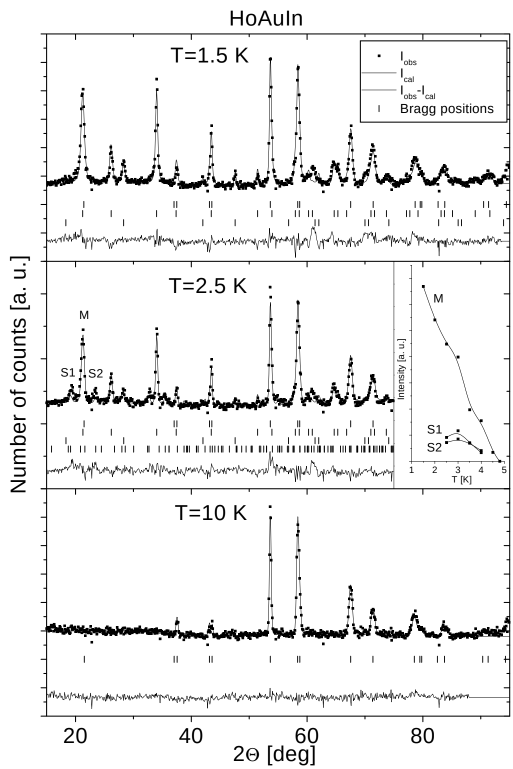

Fig. 4. Neutron diffraction patterns of HoAuIn at 1.5, 2.5 and 10 K. The squares represent experimental points; the solid lines are the calculated profiles for crystal and magnetic structure model (as described in the text) and the difference between the observed and calculated intensities at the bottom of each diagram. The vertical bars indicate Bragg peaks of nuclear and magnetic sublattices. The insert shows the temperature dependences of the magnetic peaks.

$\boldsymbol{k}_1 = (0, \frac{1}{2}, \frac{1}{2})$ (high intensity peaks) and by $\boldsymbol{k}_2 = (0, 0, \frac{1}{2})$ (low intensity peaks) (Fig. 4). In the resulting structure the Ho moments equal to 6.0(1) μ_{B} form a non collinear structure with components in the 001 plane and perpendicular to it (see Fig. 3(b)). While increasing temperature additional peaks of low intensity appear at 2.5 K. They could be indexed, as satellite pairs, with the propagation vector $\boldsymbol{k}_3 = (0, 0, 0.1365)$. The dependence of the intensities of magnetic peaks give the Néel temperature equal to 4.5 K.

3. Discussion

The neutron diffraction data for TbAuIn and HoAuIn compounds confirm the crystal structure of the ZrNiAl-type and lead to complicate magnetic structures for these compounds. For TbAuIn large difference between the values of the Néel temperature determined from magnetic (58.5 K) and neutron diffraction (35 K) data is observed. This could not be explained on the basis of the data collected in this work and new measurements on a single crystal are necessary. In HoAuIn neutron diffraction measurements indicate the additional phase transition at $T = 2.5$ K connected with the long-range modulation of the magnetic structure observed at low temperatures.

Kind hospitality and financial support extended to the three of us (ŁG, BP and AS) by the Berlin Neutron Scattering Center, Hahn-Meitner Institute is gratefully acknowledged. This work was supported by European Commission under the Access to Research. Infrastructures of the Human Potential Program (contact number HPRI-CT-1999-00020) and for the Polish State Committee for Scientific Research (KBN) Grant no 2 P03B 107 15.

REFERENCES

[1] A.E. Dwight, Proc. 12th Rare Earth Research Conf., ed. C.E. Lundin, Denver, CO: Denver Research Institute, 1976, p. 480.

[2] J. Rodriguez-Carvajal, *Physica* **B192**, 55 (1993).