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Synthesis and magnetic structure of the $YbMn_2Sb_2$ compound

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Abstract

A neutron diffraction investigation has been carried out on the trigonal La_2O_3-type (*hP*5, space group $P\bar{3}ml$, No. 164; also $CaAl_2Si_2$-type) $YbMn_2Sb_2$ intermetallic. A two-step synthesis route has been tried in this work, and successfully utilised to prepare single phase samples of this compound. This study shows that $YbMn_2Sb_2$ presents antiferromagnetic ordering below 120 K. The magnetic structure of this intermetallic consists of antiferromagnetically coupled magnetic moments of the manganese atoms, in the Mn1 (1/3, 2/3, Z_{Mn}) and Mn2 (2/3, 1/3, $1 - Z_{Mn}$) sites; the direction of magnetic moments of manganese atoms forming a φ and a θ angle, respectively with the *X*- and the *Z*-axis. At 4 K the magnetic moment of the Mn1 atom is $\mu_{Mn} = 3.6(1)\ \mu_B$, with $\varphi = 0^\circ$ and $\theta = 62(4)^\circ$, whilst the Mn2 atom has a magnetic moment $\mu_{Mn} = 3.6(1)\ \mu_B$, with $\varphi = 0^\circ$ and $\theta = 242(4)^\circ$. On the other hand, in this compound no local moment was detected on the Yb site.

Keywords: Rare earth intermetallics; Ytterbium manganese antimonide; Synthesis; Magnetic structure

1. Introduction

The existence of the intermetallic phase $YbMn_2Sb_2$, adopting the La_2O_3-type structure (also called $CaAl_2Si_2$-type; *hP*5, space group $P\bar{3}ml$, No. 164) was earlier reported by Ruhl and Jeitschko [1]: in this structure prototype the Yb atoms occupy the 1a (0, 0, 0) special position, manganese atoms occupy the 2d site (1/3, 2/3, Z_{Mn}) and antimony atoms occupy the 2d site (1/3, 2/3, Z_{Sb}). More recently, moreover, magnetic ordering (with a magnetic transition at about 115(5) K) has been already found for this compound [2].

To determine the type of magnetic ordering and the magnetic structure of $YbMn_2Sb_2$ a neutron diffraction study was carried out; the results are here presented.

2. Synthesis and experimental details

Commercial ytterbium (pieces cut from ingot, with purity 99.9 wt.%), manganese (small grains from a platelet previously surface-cleaned by conc. HNO_3, with purity 99.99 wt.%) and antimony (grains, with 99.999 wt.% purity), were used as the starting components. After few preparations were firstly attempted in an arc-furnace, and due to the fact that preparation of such a kind of samples by arc melting leads to a not negligible weight loss (i.e., as it generally happens for melting and annealing high-melting compounds containing one or more volatile metals), a new synthesis method has been attempted, also. Even being more laborious (since a two-steps procedure), and requiring sealed containers, it has been successfully tried and then utilised to prepare a large and single-phase sample (total weight of about 9 g) utilised in the present work. As a first step, the equiatomic binary alloy MnSb has been prepared by induction melting of the elements in outgassed Ta crucibles, closed by welding under pure Ar, by heating up to 1250–1300 °C; manganese antimonide forms by nearly congruent melting, besides, its formation temperature (840 °C) is relatively low: much lower than that of the melting point of Mn metal (1246 °C) [3]. In the second step, Yb and MnSb have been mixed in the stoichiometric amounts, sealed again under Ar into an outgassed Ta crucible, and reacted by induction heating up to about 1300 °C. The crucibles were then sealed under vacuum in quartz tubes and annealed in a resistance furnace at 800 °C for 7 days; after annealing, they were air cooled. Preparation of MnSb inside a Ta crucible has proved not to give rise to pollution due to reaction towards the container material, as well as no Ta pollution in the final $YbMn_2Sb_2$ was noticed.

The quality of the polycrystalline alloys (MnSb and both arc and induction melted $YbMn_2Sb_2$ samples) was determined using X-ray powder diffraction and analysis by electron microscopy (SEM) equipped with EDX microprobe analysis (a "Camebax" microanalyser was employed to perform microprobe X-ray spectral analyses of the specimens).

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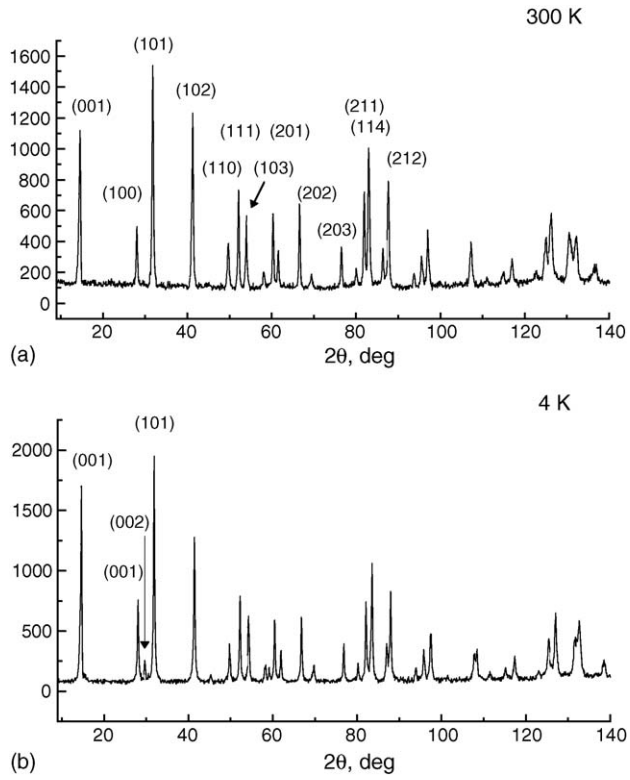

Fig. 1. Neutron diffraction patterns of the $YbMn_2Sb_2$ compound at 300 K (paramagnetic state) (Fig. 1a) and at 4 K (antiferromagnetic collinear type ordering) (Fig. 1b). Neutron wavelength $\lambda = 0.19103$ nm.

X-ray powder patterns were obtained either by a Guinier-Stoe camera (Cu Kα radiation, pure Si as an internal standard: $a = 0.54308$ nm), or on a diffractometer DRON-3 (Cu Kα radiation, $2\Theta = 20$–70°, 0.05° step, 6 s/step). The Guinier patterns were indexed with the help of the Lazy-Pulverix program [4], whilst the diffractograms obtained were identified by means of calculated patterns using the Rietan program [5] in the isotropic approximation; the lattice parameters were calculated by least squares methods.

The neutron diffraction investigation was carried out from 300 to 4 K at the Institute Laue-Langevin, Grenoble, France (on the powder D1A diffractometer, wavelength $\lambda = 0.19103$ nm). The diffraction patterns were indexed, and the calculations performed, by using the Fullprof 98-program [6].

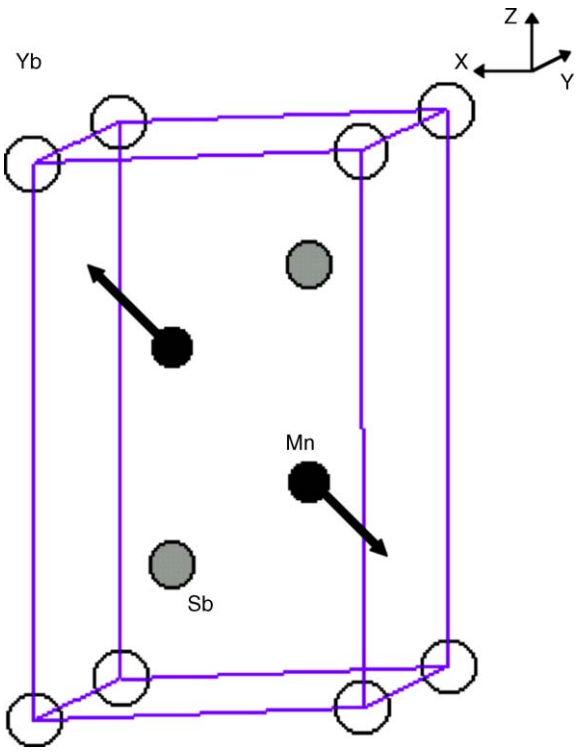

Fig. 2. A sketch of the magnetic structure of $YbMn_2Sb_2$ compound.

3. Results

The above-described synthesis procedure provided us to prepare single phase samples of the compound $YbMn_2Sb_2$; it can be utilised as a preparation method for similar intermetallic systems in future investigations, as well.

Lattice constants of the sample subsequently used for neutron diffraction, as obtained by Guinier pattern, are $a = 0.4532(1)$ nm, $c = 0.7450(1)$ nm; these values are slightly larger than those given in Ref. [1].

Fig. 1 shows the neutron diffraction patterns recorded at the temperatures of 300 and 4 K (Fig. 1a and b, respectively). In the 4 K pattern the reflections pertaining to a commensu-

Table 1
Crystallographic and magnetic parameters of La_2O_2S-type $YbMn_2Sb_2$ compound

T_N	Magnetic type	T	a	c	c/a	V	Z_{Mn}	Z_{Sb}	R_F	μ_{Mn}	θ	R_F^m
	Paramagnetic	300[a]	0.4528(1)	0.7448(2)	1.64488	0.13225	0.629(2)	0.251(2)	4.3	–	–	–
		300	0.45289(4)	0.74503(8)	1.64506	0.13234	0.628(2)	0.256(2)	5.9	–	–	–
		120	0.45181(7)	0.74196(9)	1.64220	0.13117	0.627(4)	0.250(3)	12.0	–	–	–
120	Antiferromagnetic	60	0.45193(3)	0.74026(7)	1.63800	0.13094	0.621(2)	0.252(2)	7.5	Mn1 3.4(1)[b]	Mn1 62(4)	10.6
										Mn2 3.4(1)	Mn2 242(4)	
		4	0.45192(3)	0.73998(6)	1.63741	0.13088	0.621(2)	0.252(2)	6.2	Mn1 3.6(1)	Mn1 62(4)	10.1
										Mn2 3.6(1)	Mn2 242(4)	

Cell parameters a (nm), c (nm), c/a and V (nm^3), atomic position parameters Z_{Mn} and Z_{Sb}, magnetic moment of the Mn atom (μ_B) and θ angle ($^\circ$) at different temperatures T (K). The θ is angle of the Mn magnetic moment with the Z-axis of unit cell, the φ is angle of the Mn magnetic moment with the X-axis of the unit cell ($\varphi = 0$ for all magnetic moments). The temperature T_N refers to a antiferromagnetic transition (K). Reliability factors R_F (crystal structure) and R_F^m (magnetic structure) are given in percent (%).

[a] X-ray data.

[b] Mn1 occupy (1/3, 2/3, X_{Mn}) site and Mn2 occupy (2/3, 1/3, $1 - X_{Mn}$) site in the La_2O_2S-type $YbMn_2Sb_2$ unit cell.

rate magnetic structure well evidently appear. Analysis of the diffraction data shows that below 120 K the magnetic structure of $YbMn_2Sb_2$ consists of antiferromagnetically coupled magnetic moments of the manganese atoms; the crystallographic data and magnetic parameters are given in Table 1.

A sketch of the magnetic structure is shown in Fig. 2.

No local moment was instead detected on the ytterbium site.

Of course, magnetic fields may destroy the antiferromagnetic ordering with the change of the magnetic transition temperature. Likely, and similarly to what happens in the $YbMn_2Sb_2$ compound, in the known homologous compound $EuMn_2Sb_2$ [7] the magnetic moments of the Mn-atoms sublattice might order antiferromagnetically; the overall magnetic structure of this latter could however be much more complicated, due to the possible ordering of the Eu-ions sublattice also. We have so planned to study the magnetic structure of the Eu homologous too.

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