15 May 2002

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Satish K. Malik

Zili Chu

Amish G. Joshi

Jinbo Yang

et. al. For a complete list of authors, see https://scholarsmine.mst.edu/phys_facwork/221

Recommended Citation

S. K. Malik et al., "Magnetic and Neutron Diffraction Studies on $PrMnSb_2$," *Journal of Applied Physics*, vol. 91, no. 10, pp. 7842-7844, American Institute of Physics (AIP), May 2002.
The definitive version is available at https://doi.org/10.1063/1.1453938

Magnetic and neutron diffraction studies on $PrMnSb_2$

S. K. Malik
Tata Institute of Fundamental Research, Colaba, Mumbai 400-005, India

Z. Chu[a)]
Department of Physics, University of Missouri-Columbia, Columbia, Missouri 65211

Amish G. Joshi
Tata Institute of Fundamental Research, Colaba, Mumbai 400-005, India

J. B. Yang and W. B. Yelon
Graduate Center of Materials Research and Departments of Chemistry and Physics, University of Missouri-Rolla, Rolla, Missouri 65409

Q. Cai
Department of Physics, University of Missouri-Columbia, Columbia, Missouri 65211

W. J. James
Graduate Center of Materials Research and Departments of Chemistry and Physics, University of Missouri-Rolla, Rolla, Missouri 65409

K. Kamaraju
Department of Physics, University of Missouri-Rolla, Rolla, Missouri 65409

Magnetic and neutron diffraction studies have been carried out on $PrMnSb_2$. Magnetization data in the temperature range of 5–400 K show two magnetic transitions: one at ~175 K attributed to the antiferromagnetic ordering of the Mn moments, and the other at ~35 K possibly due to the antiferromagnetic ordering of the Pr moments. The magnetization-field isotherms at various temperatures are consistent with the above. Neutron diffraction data obtained at various temperatures can be fitted with a nearly antiferromagnetically coupled Mn moment of $\sim 3\mu_B$ at 70 K. At 10 K, moments both on Mn ($\sim 3.5\mu_B$) and Pr ($\sim 0.94\mu_B$) are ordered antiferromagnetically with small canting angles. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1453938]

I. INTRODUCTION

Ternary rare earth intermetallic compounds with the general formula $RMnSb_2$ (R = La, Ce, Pr, Nd, and Sm) crystallize in the tetragonal $ZrCuSi_2$ type structure (space group $P4/mmm$, No. 129). These show magnetic ordering of the Mn moments in the temperature range of 100–520 K.[1] Furthermore, the rare earth sublattice also appears to order magnetically below 50 K in the abovementioned compounds with Ce, Pr, and Nd. The Mn–Mn distance in these compounds is large enough to induce ferromagnetic interaction in them reminiscent of the Mn-based Heusler alloys. We have started a systematic investigation of the magnetic structure of these compounds using magnetization and powder neutron diffraction studies. We present here the results of such studies on $PrMnSb_2$.

II. EXPERIMENTAL DETAILS

The compound $PrMnSb_2$ was prepared by melting together of the stoichiometric amounts of the constituent elements in a radio frequency induction furnace under a continuous flow of argon gas. The sample was turned over and melted several times. Subsequently, it was annealed at 850 °C for seven days and furnace cooled to room temperature. Powder x-ray diffraction patterns were obtained using Cu $K\alpha$ radiation. Magnetization measurements on $PrMnSb_2$ were carried out in the temperature range of 5–400 K and in applied fields up to 55 kOe using a SQUID magnetometer (quantum design). Magnetization-field hysteresis loops were also recorded at various temperatures. Neutron diffraction patterns were obtained at temperatures of 300, 200, 70, and at 10 K, using the high resolution powder neutron diffractometer at the University of Missouri Research Reactor Facility with neutrons of wavelength 1.4875 Å.

III. RESULTS AND DISCUSSION

Powder x-ray diffraction studies reveal that $PrMnSb_2$ is nearly single phase with a small amount of PrSb. This is also verified from neutron diffraction studies. Rietveld refinement of the room temperature neutron diffraction data yields about 8% PrSb by weight. The $PrMnSb_2$ compound crystallizes in the tetragonal $ZrCuSb_2$ type structure. The lattice parameters and other structural details are given in Table I. Refinement of the site occupancies also suggests some Mn deficiency consistent with the earlier observation that these compounds form with reduced Mn content.[1] In this article, we will continue to refer to this compound by its nominal stoichiometry.

Figure 1 shows the plot of magnetization versus temperature for $PrMnSb_2$ measured in an applied field of 5 kOe. Two magnetic transitions are clearly visible—one at around 175 K and the other around 35 K (along with a broad shoulder). It is reasonable to attribute the higher of the two tran-

a)Electronic mail: zc58f@mizzou.edu

TABLE I. Lattice parameters and magnetic moment values in $PrMnSb_2$. Uncertainty on each quantity are given in parentheses.

Temp.	10 K		70 K		200 K		300 K	
a (Å)	4.29794(23)		4.29897(25)		4.308132(22)		4.31516(25)	
c (Å)	10.68809(58)		10.69018(59)		10.69847(63)		10.70586(63)	
χ^2	2.76		2.59		2.61		2.88	
Mn_vac %	10.3(8)%		10.3(8)%		10.3(8)%		10.3(8)%	
wt. frac.	91.9(15)%		91.90(15)%		91.9(15)%		91.9(15)%	
wt. frac. PrSb	8.1(5)%		8.1(5)%		8.1(5)%		8.1(5)%	
Propagation	(0,0,0.5)		(0,0,0.5)		(0,0,0)		(0,0,0)	
	$M_z(\mu_B)$	$M_{xy}(\mu_B)$	$M_z(\mu_B)$	$M_{xy}(\mu_B)$	$M_z(\mu_B)$	$M_{xy}(\mu_B)$	$M_z(\mu_B)$	$M_{xy}(\mu_B)$
Pr(1/4,1/4, 0.73)	−0.899(48)	0.261(14)						
Pr(3/4,3/4, −0.73)	−0.899(48)	−0.261(14)						
Mn(3/4,1/4, 0)	1.893(41)	2.965(65)	1.338(24)	2.729(48)				
Mn(1/4,3/4, 0)	1.893(41)	−2.965(65)	1.338(24)	−2.729(48)				

sitions to the magnetic ordering of the Mn moments while the lower transition may possibly be due the ordering of the Pr moments. The peaks in the magnetization data suggest these to be transitions to the antiferromagnetic state. No other transition is visible in the temperature range of 5–400 K. Sologub *et al.*[1] reported a magnetic transition at about 390 K in their $PrMn_{0.82}Sb_2$ sample. However, none are seen at that temperature in our sample.

Figure 2 shows the magnetization (M) applied field (H) hysteresis loops at various temperatures in applied fields up to 55 kOe. At 5 K, where both Pr and Mn moments are presumed to be magnetically ordered, the $M-H$ loop deviates only slightly from linear variation expected for an antiferromagnetic ordering of the moments. The small deviation from linearity may be either due to canting of moments or due to the onset of applied field-induced spin reorientation. The $M-H$ loop at 100 K (where only Mn moments are ordered) is a straight line typical of antiferromagnetic systems. The $M-H$ loops at 250 and 400 K largely exhibit a straight-line behavior on which a very small ferromagnetic component is superposed. At present it is not clear whether the

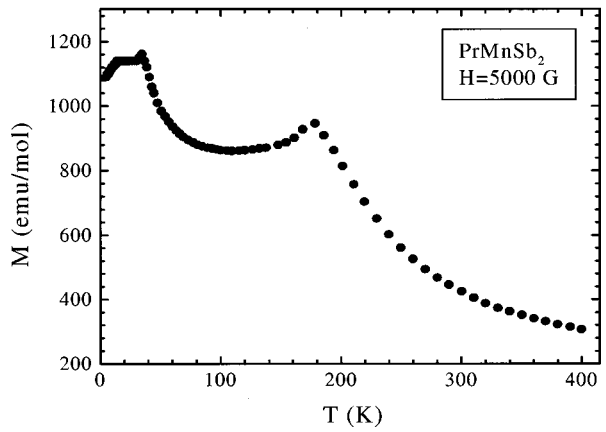

FIG. 1. Magnetization vs. temperature for $PrMnSb_2$ in an applied field of 5 kOe.

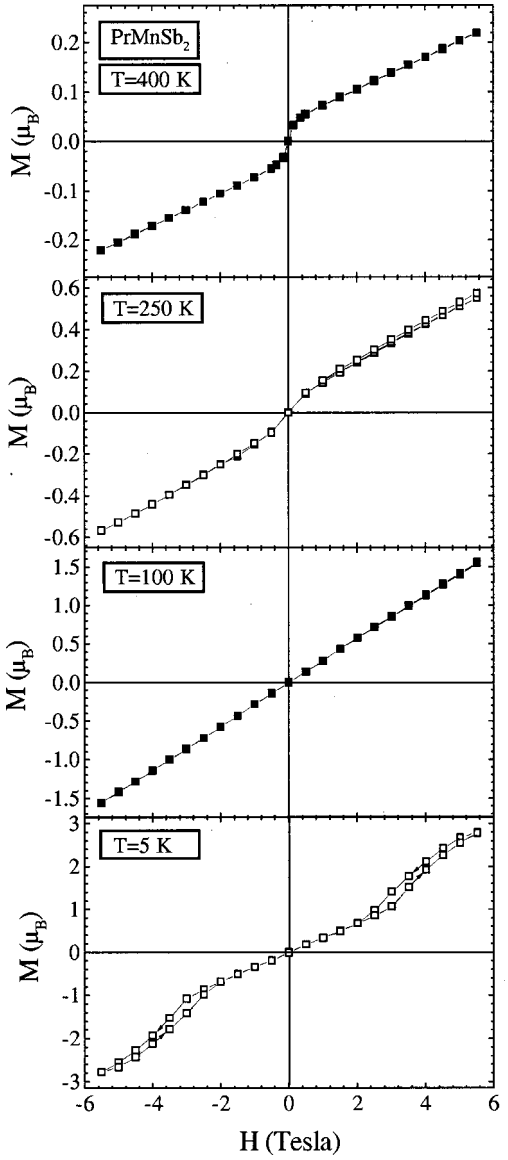

FIG. 2. Magnetization-field hysteresis plots for $PrMnSb_2$ at various temperatures.

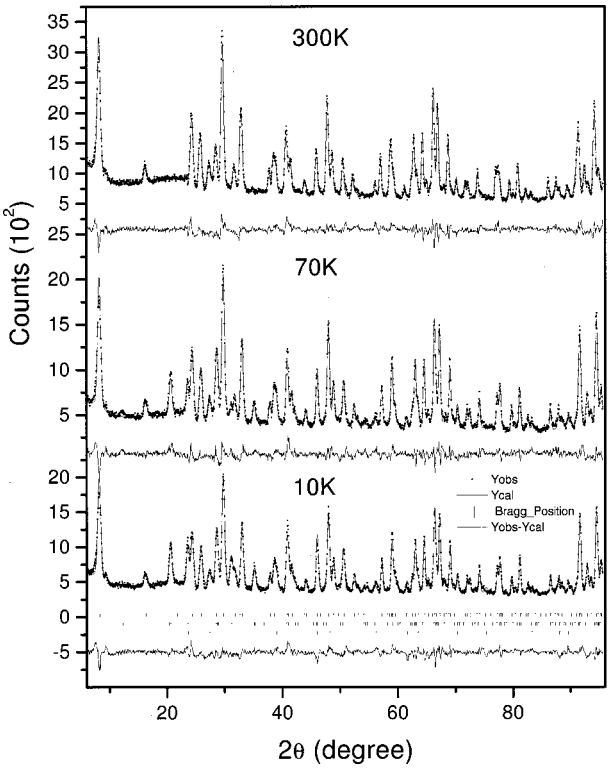

FIG. 3. Refined powder diffraction patterns for $PrMnSb_2$ at various temperatures. The upper tic mark is nuclear structure of $PrMnSb_2$, middle is antiferromagnetic phase of $PrMnSb_2$, and lower is nuclear structure of PrSb.

ferromagnetism is intrinsic or due to the presence of some impurity phases. Formation of PrSb as an impurity phase in $PrMnSb_2$ suggests that a very small amount of MnSb phase may also be present in this compound (based on stoichiometry). The MnSb phase is known to order ferromagnetically with a Curie temperature of about 573 K (Ref. 2) and its presence may lead to some nonlinearity in the $M-H$ curves at 250 and 400 K. Extension of magnetization studies to higher temperatures is desirable.

The 300 K neutron diffraction (ND) pattern can be analyzed without any magnetic moment on Mn ions. The 10 and 70 K data show several extra peaks, see Fig. 3, which indicated the antiferromagnetic ordering. The magnetic structure is modeled with propagation vector (0,0,0.5). This doubles the unit cell along *z*. Each magnetic site in the lower half of the magnetic unit cell has a counterpart in the upper half with antiparallel alignment. Analysis of the 70 K ND pattern yields a magnetic structure in which Mn ion moments are antiferromagnetically ordered and have a value of $\sim 3\mu_B$. The 10 K diffraction pattern is analyzed on the basis of magnetic ordering of both the Pr and the Mn moments. The magnetic ordering appears more complex (Fig. 4) with Pr and Mn sublattices ordered antiferromagnetically (with different canting angles) and with moment values of $\sim 3.5\mu_B$ at the Mn site and $0.94\mu_B$ at the Pr site. The results of structural and magnetic refinements are largely summarized in Table I.

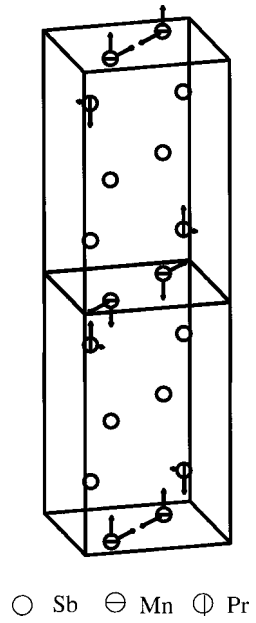

FIG. 4. Magnetic structure of PrMnSb at 10 K. The magnetic unit cell is doubled along the *c* axis with respect to the crystallographic cell.

[1] O. Sologub, K. Hiebl, P. Rogl, and O. Bodak, J. Alloys Compd. **227**, 40 (1995).
[2] See, for instance, W. Reimers, E. Hellner, W. Treutmann, and G. Heger, J. Phys. C **15**, 3597 (1982).