CRYSTAL AND MAGNETIC STRUCTURE OF $Mn_5(Si_{1-x}Ge_x)_3$

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The system $Mn_5(Si_{1-x}Ge_x)_3$ (for x=0.15, 0.2, 0.4, 0.7) was investigated by means of X-ray diffraction,neutron diffraction; and magnetometric methods. The Curie temperature and magnetization measurements at 80 K show that the system is ferromagnetic in the concentration range $0 \le x \le 0.8$. In the neutron diffraction data crystal and magnetic structure of these compounds are determined.

1. Introduction

The study of the properties of the $Mn_5(Si_{1-x}Ge_x)_3$ system is of special interest: Mn_5Si_3 (1,2) and Mn_5Ge_3 (3-5) have the same crystal structure but their magnetic behaviour difers very much. Mn_5Si_3 is antiferromagnetic while Mn_3Ge_3 is ferromagnetic. The unit cell of the compounds is hexagonal ($D8_8$ type structure), space group is $P6_3/mcm$. The Mn atoms occupy two different crystallographic sites. The atomic positions are the following:

4 Mn in 4(d) 1/3,2/3,0,2/3,1/3,0,1/3,2/3,1/2,2/3,1/3,1/2,

6 Mn in 6(g) $x_1,0,1/4,0,x_1,1/4,x_1,x_1,1/4,\bar{x}_1,0,3/4,0,\bar{x}_1,3/4,\bar{x}_1,\bar{x}_1,3/4,$

Si or Ge in 6(g) as above (with x_2 instead of x_1)

The parameters x_1 and x_2 for Mn_5Si_3 and Mn_5Ge_3 are given in Table I.

2. Experimental Technique and Results

2.1. Magnetometric Macroscopic Measurements

Magnetic measurements were carried out in temperature range between 80 and 700 K, using a Sucksmith-type balance at a maximum field of 10 kOe, and using a vibration magnetometer(6) operated at 16 kOe field. Magnetometric measurements showed (see Fig.1) that the samples with x = 0.2,04,0.7 at low temperatures exhibits ferromagnetic

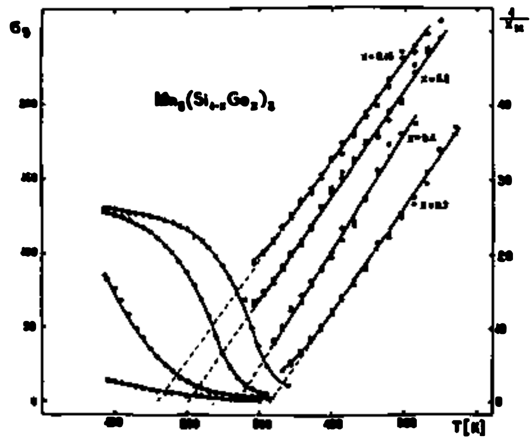

Fig. 1. Temperature dependence of the magnetization and of the inverse susceptibility of $Mn_5(Si_{1-x}Ge_x)_3$.

properties. Further increase in temperature causes a decrease in magnetization. The Curie temperature measurements were done a low field apparatus giving the initial permeability. The magnetic susceptibility of all samples at high temperatures obeys the Curie-Weiss low. From the slope of the linear part of the inverse susceptibility versus tempe-

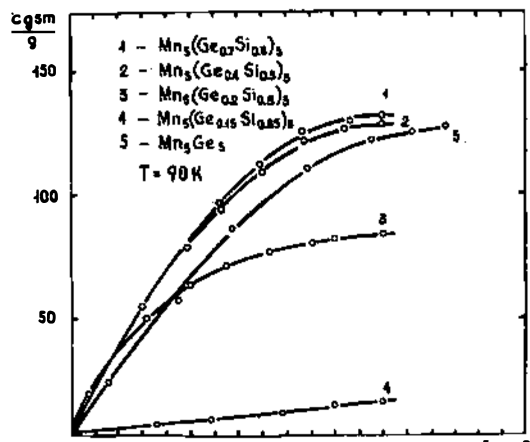

Fig.2. Magnetization curves of $Mn_5(Si_{1-x}Ge_x)_3$ at 90 K measured at magnetic fields up to 16 kOe.

rature curves, we calculated the mean effective paramagnetic moment μ_{eff}. The magnetization measurements at 90 K up to 16 kOe confirm that the system $Mn_5(Si_{1-x}Ge_x)_3$ have a ferromagnetic character in the concentration range $0 \leq x \leq 0.8$ (see Fig.2).For this concentration range,saturation values were determined by extrapolating $H_i \to \infty$ using the H_i^2 low,as shown in Table II,the mean ferromagnetic moment μ_F per Mn atom decreases slowly as the Si concentration increases.

2.2.The Crystal and Magnetic Structure Determined by Neutron Diffraction Measurements

Neutron diffraction patterns were obtained at the RA reactor of the Boris Kidrič Institute in Vinča at 80 and 290 K temperatures.The parameters x_1 and x_2 determined from nuclear reflections by the profil refinement method[7].The obtained results are presented in Table I.

Next, the magnetic structure of these compounds was determined. In the neutron diagram of these compounds at liquid nitrogen temperature no extra reflections appeared. Only an increase in the intensities of the fundamental reflections was observed, indicating that the unit cell had not changed. The analysis of the data gives the following magnetic moments:

$Mn_I=(1.7\pm0.1)\mu_B$, $Mn_{II}=(2.7\pm0.1)\mu_B$ for $Mn_5(Ge_{0.7}Si_{0.3})_3$ and
$Mn_I=(1.7\pm0.1)\mu_B$, $Mn_{II}=(2.8\pm0.1)\mu_B$ for $Mn_5(Ge_{0.4}Si_{0.6})_3$.
The magnetic moments are parallel to c-axis.

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Table I.- Structural parameters on $Mn_5(Si_{1-x}Ge_x)_3$

x	Lattice constants a (Å)	c (Å)	c/a	Volume V ($Å^3$)	Parameters x_{Mn}	$x_{Si,Ge}$	Source
0	6.898/5/	4.802/5/	0.696	197.88			
	6.911/5/	4.816/1/	0.697	199.2	0.2358	0.5992	
0.15	6.956/3/	4.858/2/	0.698	203.52			this work
0.2	6.994/7/	4.878/2/	0.698	206.51	0.2380	0.6006	-"-
0.4	7.052/8/	4.913/8/	0.697	211.50	0.2355	0.6000	-"-
0.7	7.122/6/	4.973/2/	0.698	218.50	0.2346	0.5917	-"-
1.0	7.184	5.053	0.703	225.85	0.25	0.61	
	7.175	5.062	0.705	225.68			

Table II.- Magnetic data on $Mn_5(Si_{1-x}Ge_x)_3$

x	Curie point T_c (K)	Paramagnetic Curie temperat. ^oK	Magnetization per Mn atom $\mu\|\mu_B\|$	Effective magnetic moment $\mu_{eff}\|\mu\|$	Source
0	62	-9.1		4.05	this work
0.15		160	1.3	3.4	-"-
0.2	143	203	1.66	3.6	-"-
0.4	241	270	2.00	3.4	-"-
0.7	290	314	2.17	3.3	-"-
1.0	293	342	1.85	3.42	
	300	300	2.35-2.50	3.5	