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Neutron Diffraction Study of MnTe

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Abstract

We report our neutron diffraction studies at low temperature on MnTe. The low temperature data indicates presence of another crystallographic phase along with the high temperature antiferromagnetic hexagonal phase. This low temperature phase also orders magnetically and is responsible for the increase in susceptibility of MnTe.

INTRODUCTION

MnTe an antiferromagnetic p-type semiconductor crystallizes in the hexagonal NiAs type structure with direct band gap of 1.3eV. Its crystal structure supports metallic conductivity but its magnetic and electronic behaviour show properties similar to those of NaCl type chalcogenide magnetic insulator /1,2/. Low temperature resistivity and susceptibility measurements on MnTe revealed a possibility of structural transition/3/. Electrical resistivity showed a semiconductor like behaviour below 100K and d.c. susceptibility exhibited a sharp rise at around 83K indicating a ferromagnetic like transition. In order to understand the magnetic and the chemical structure of MnTe at low temperature we have carried out neutron diffraction experiments and the preliminary results are reported here.

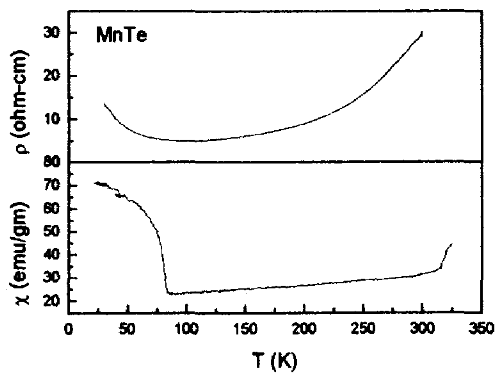

Figure 1: Electrical resistivity and d.c. susceptibility of MnTe.

EXPERIMENTAL

MnTe was prepared by taking stoichiometric amounts of Mn and Te and enclosed in quartz ampoule below 10^{-6} Torr. The quartz ampoule was given a heat treatment for 10 days at 750°C. X-ray diffractogram showed the sample to be single phase with NiAs structure and the lattice parameters were calculated to be a = 4.190Å and c = 6.751Å. Electrical resistivity was measured using standard four probe technique. DC susceptibility measurements were performed on a Faraday balance. Neutron diffraction experiments were carried out in the temperature range 10-300K and at a wavelength of 1.242Å using the Profile Analysis Diffractometer at Dhruva.

RESULTS AND DISCUSSION

A plot of resistivity and d.c susceptibility for MnTe is shown in figure 1. The positive coefficient of resistivity below T_N (310K) is due to spin disorder scattering with a large contribution from influence of magnon drag /4/. Below 100K the resistivity shows a negative temperature coefficient. The d.c. susceptibility exhibits a sudden drop at 310K indicating an antiferromagnetic order /4/ and a sharp rise below 80K suggestive of a ferromagnetic like order /3/. There is no report of any structural transition below 80K in MnTe. However a zinc blend phase for MnTe has been reported in 1μ thick films /5/. In order to study the low temperature structure and the nature of magnetic order, neutron diffraction experiments have been carried out. Neutron diffraction pattern of MnTe at room temperature is presented in figure 2.

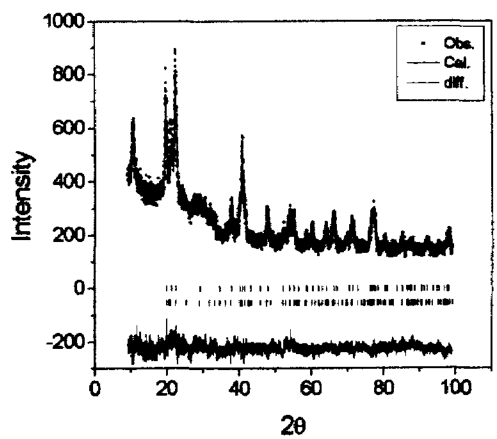

Figure 2: Neutron diffraction pattern of MnTe at RT

The pattern could be fitted well with two-phase refinement – nuclear and magnetic phases of MnTe. The fitting results are quite satisfactory and are summarized in Table I.

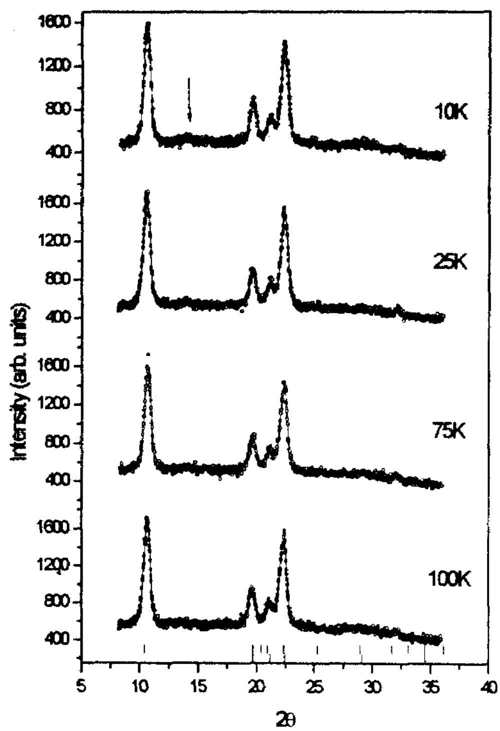

Figure 3: Neutron diffraction patterns at 10, 25, 75 and 100K

Table I: Structural Parameters of MnTe at Room Temperature

Atom	Position	Temp. Factor ($Å^2$)	Occupancy
Mn	0,0,0	0.47± 0.04	0.09± 0.001
Te	1/3,2/3,1/4	0.80± 0.07	0.08± 0.002
a=4.18± 0.04 Å, c=6.76± 0.05 Å, $c_{(mag)}$=13.65± 0.07 Å			
Magnetic Moment / Mn atom = 0.97± 0.01 μ_B			
R_p=5.9 R_{wp}=7.46 R_{exp}=6.48			
Bragg R =14.7		Magnetic R =14.7	

These parameters were used as input to refine the neutron diffraction data at low temperatures. The magnetic moment is seen to increase from 0.97μ_B (at RT) to 2.17μ_B (at 10K) with the decrease in temperature. The Mn spins are aligned in the basal plane and these planes are stacked antiferromagnetically along the c-axis. The neutron diffraction patterns at few representative temperatures are shown in figure 3. A careful inspection of the plots indicates that below 75 K there is a peak at around 2θ = 14° which grows in intensity with decreasing temperature. It may be noted that this peak cannot be indexed in the NiAs phase. In addition, at about 2θ = 32° there also seems to be a mismatch between the calculated and observed data points below 75K. This correlates well with the increase in susceptibility below 80K. MnTe seems to undergo a structural transition to a zinc blend phase that has been hitherto reported only in thin films/5/ and this zinc blend phase orders ferromagnetically below 80K.

CONCLUSIONS

1. Low temperature neutron diffraction study indicates that MnTe orders antiferromagnetically along c-axis with Mn spins aligned ferromagnetically in the basal plane.
2. There seems to be a structural and magnetic transition at low temperatures that could account for the sudden rise in susceptibility.

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