

Effect of Te doping in MnSe: A Resistivity Study

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Abstract

We report our electrical resistivity measurements on NaCl type $MnSe_{1-y}Te_y$, $y=(0,0.3,0.4,0.5)$ as a function of temperature. All the samples show activation type behaviour and energy gap decreasing with increasing Te substitution. This has been explained on the basis of decreasing p-d hybridisation and decrease in charge transfer energy.

INTRODUCTION

Transition metal chalcogenides exhibit a large variety of optical, magnetic and transport properties. These compounds have exhibited considerable interest, as a consequence of this diversity [1]. MnSe shows interesting structural and magnetic properties. At room temperature it has NaCl type structure and orders antiferromagnetically at low temperature. It undergoes a partial structural transition to a magnetically ordered NiAs type phase at 250K [2]. Resistivity is semiconductor like with a direct energy gap of 2.0eV. MnTe on the other hand is a semiconductor with NiAs structure and an interesting crossroad material because of its non standard magnetic and electronic behaviour [1,3].

When Te is added to MnSe in increasing proportion to form solid solutions, there is a transition from NaCl to NiAs type structure. Several phase diagrams have been reported in literature [4,5,6] for this series prepared by different annealing conditions with NaCl type structure in Se rich region while NiAs type structure in Te rich region and mixed phase region for the intermediate concentrations.

We have prepared $MnSe_{1-y}Te_y$, $y=0, 0.3, 0.4, 0.5$ and MnTe with an aim of studying the effect of replacing Se atoms in MnSe by Te on the electrical properties and correlating the observed results with those obtained by photoelectron spectroscopy.

EXPERIMENTAL

The samples were prepared by mixing stoichiometric amounts of finely powdered Mn, Se, and Te pelletised, sealed in evacuated quartz ampoule below 10^{-6} Torr and given an appropriate heat treatment. MnSe was slowly to 650°C and annealed for 20 hours and furnace cooled. MnTe was annealed for 10 days at 750°C for 10 days and furnace cooled. The solid solutions were annealed at 800°C for 4 days and quenched to room temperature. The samples were characterised by X-ray diffraction and all were found to be single phase with NaCl type structure, while MnTe, ($y=0.0$) crystallised in NiAs type structure. D.C resistivity measurements were performed with standard four probe method in the temperature range between 80K and 300K.

RESULTS AND DISCUSSIONS

A plot of resistivity as a function of temperature for MnSe and MnTe is shown in Fig. 1 and Fig. 2 respectively. MnSe shows semiconducting behaviour all through the temperature range studied with resistance changing by 4 to 5 orders of magnitude. MnTe on the other hand exhibits completely different behaviour with resistance of the order of few ohms. This behaviour of MnTe resistivity is explained to be due to spin disorder scattering[7].

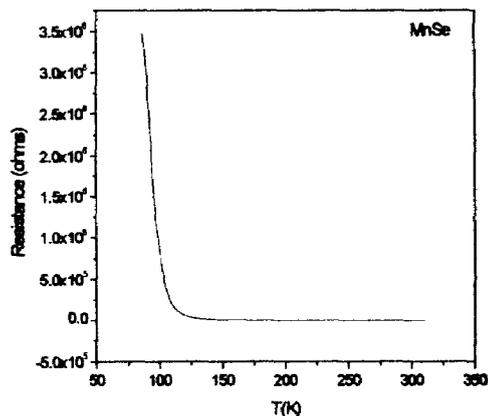


Figure 1: Resistivity behaviour of MnSe

The Te doped samples show resistivity similar to that of MnSe and is presented in Fig. 3.

Temperature dependence of resistivity can be explained by simple activation law,

$$\rho = \rho_0 \exp [E_g / 2kT]$$

The energy gap calculated from the above relation decreases with increasing Te substitution. The data on lattice parameters and calculated energy gap is presented in Table I.

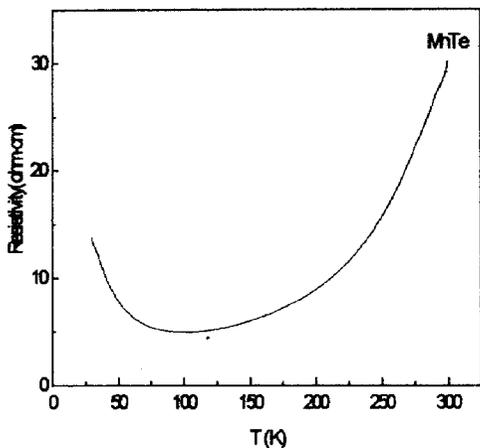


Figure 2: Resistivity versus temperature plot of MnTe

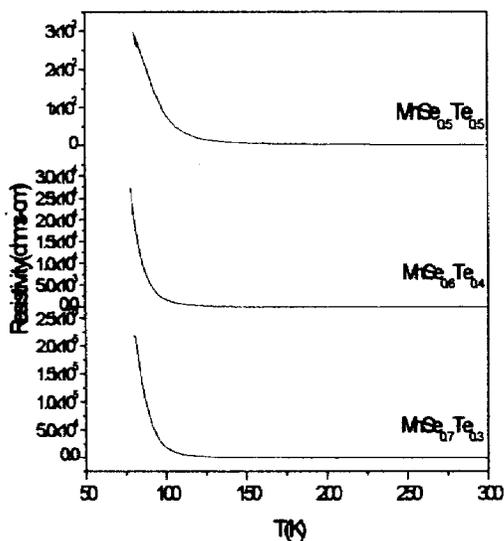


Figure 3: Resistivity plot of $MnSe_{1-y}Te_y$ solid solutions

Table I: Lattice parameters and Energy gap values for $MnSe_{1-y}Te_y$

Sample	Lattice Parameter (Å)	Energy Gap (eV)
MnSe	a=5.450	0.2463
MnTe	a=4.18, c=6.76	—
$MnSe_{0.7}Te_{0.3}$	a=5.5890	0.1835
$MnSe_{0.6}Te_{0.4}$	a=5.6385	0.1135
$MnSe_{0.5}Te_{0.5}$	a=5.6754	0.0888

H. Sato et al /8/ from their photoelectron spectroscopic studies on MnS, MnSe and MnTe have argued that the decrease in the energy gap with increasing atomic number of chalcogen to the decrease in p-d hybridisation along with decrease in ligand Mn 3d charge transfer energy. This can be understood by anion dependence of the energy level of the anion p state and the bond length between Mn and anion atom respectively. It is clear from Table I that Mn - chalcogen bond length increases with increasing Te content. Therefore the decrease in energy gap E_g with increasing Te doping is due to decrease in Mn-chalcogen hybridisation. The gap in Mn chalcogenides is between the empty Mn t_2 level and the filled hybridised AB₁ (antibonding) level /9/. Therefore as the charge transfer energy decreases the energy gap decreases and hence the value of resistivity decreases.

CONCLUSIONS

1. Resistivity measurements on $MnSe_{1-y}Te_y$ show that as Te doping increases energy gap decreases along with decrease in the order of the resistance.
2. This can be ascribed to decrease in the hybridisation between the Mn 3d and chalcogen p orbitals coupled with a decrease in the charge transfer energy.

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