Synthesis, Structure, Magnetic and Electric Transport Properties of $Mn_{0.5}Si_{0.5}Te_2$

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Abstract

A new phase with the composition $Mn_{0.5}Si_{0.5}Te_2$ has been synthesised by the standard ceramic method. X-ray diffraction studies show that the phase crystallizes with the orthorhombic unit cell (a=14.754Å, b=12.380Å and c=3.931Å). The molar magnetic susceptibility measurements as a function of temperature suggest that the phase has negative Weiss constant which shows that anti-ferromagnetic interactions are dominant. The magnetic moment (μ_{eff}) calculated from Curie constant comes out to be 6.6 B.M. The electrical resistivity measurements as a function of temperature suggest that the phase is semi-conductor in the temperature range 300K-500K and the conduction occurs via thermally activated mechanism.

Keywords: Mixed binary dichalcogenides, (XRD), molar magnetic susceptibility and electrical resistivity.

Introduction:

Binary dichalcogenides of numerous elements with composition MX_2 and their mixed analogues $M_{1-x}M'_xX_2$ (M and M′ are different transition elements; X= S, Se or Te) are known in the literature [1, 2]. Many dichalcogenides with reduced content of X are also known [3, 4]. It has been reported that structure and physical properties substantially vary with change in composition [1, 2, 3, 4]. It was thought interesting to prepare mixed chalcogenides with composition $M_{0.5}M'_{0.5}X_2$ study of their crystal structure & follow their physical properties as function of temperature.

In the present study, synthesis of a new phase with the composition $Mn_{0.5}Si_{0.5}Te_2$ has been reported. Its crystal structure has been determined from the powder X-ray diffraction data. Magnetic and electric transport properties have been studied in the temperature range 80K-300K and 300K-500K respectively.

Experiment

Synthesis

Aldrich make Manganese (Mn) Silicon (Si) and Tellurium (Te) elements (purity 99.9%) have been used for synthesis of the new phase. The constituent elements weighed corresponding to the stoichiometry $Mn_{0.5}Si_{0.5}Te_2$, were mixed and homogenized by grinding in cyclohexane. The dried and homogenized mixture, pressed into pellets in hydraulic press was placed in quartz tube and evacuated to $\sim 10^{-5}$ Torr, vacuum sealed and was heat-treated at 1048K for 72 hours. The mixture during the heat

treatment was subjected to a number of intermediate grindings, pelletizing and sealing under same conditions for the completion of the reaction. The final product was pulverized to fine powder for further investigations [5, 6, 7].

Elemental Analysis

The phase was further analyzed by atomic absorption spectrophotometry, which is one of the most prevalent methods for the trace element analysis [8, 9, 10]. The results of chemical elemental analysis [11, 12] and the atomic absorption spectrophotometry are in good agreement. The data are given in Table 1.

Table 1: Analytical data of the phase ($Mn_{0.5}Si_{0.5}Te_2$).
The theoretical value is given in parenthesis. Analysis (%)

Phase	Mn	Si	Te
$Mn_{0.5}Si_{0.5}Te_2$	9.16 (9.25)	4.63 (4.73)	85.87 (86.00)

X-ray Diffraction studies

Room temperature powder X-ray diffraction data of the product were recorded on a Stoe-powder diffraction system and a Philips diffractometer at a scanning speed 1deg/minute in the 2θ range using CuKα and FeKα radiations [13, 14 and 15]. The X- ray diffraction data are given in the Table 2, while the X-ray pattern, intensity, versus 2θ is drawn in the figure1.

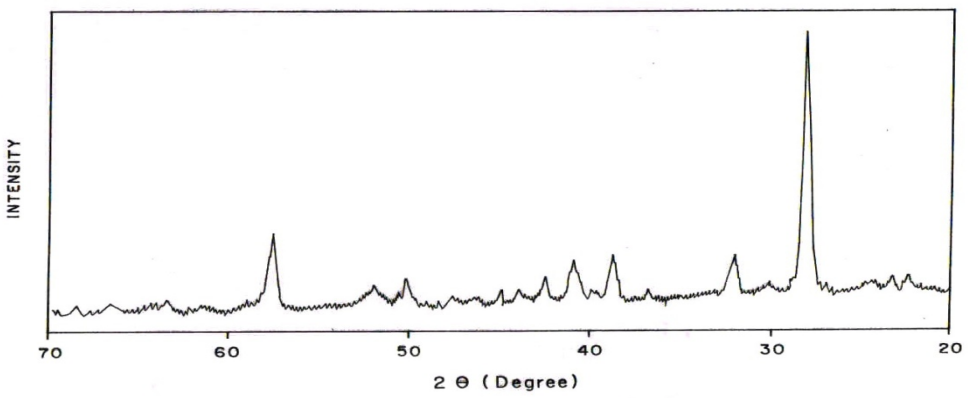

Figure 1: X-ray Diffraction pattern of $Mn_{0.5}Si_{0.5}Te_2$

Magnetic Susceptibility Measurement

Magnetic susceptibility of the powdered phase was recorded in a Faraday balance provided with Polytronic Faraday-type electromagnet and a Mettler microbalance. Specially fabricated Dewar flask of the size which could be adjusted within pole gaps of electromagnet was used for keeping liquid nitrogen,

which surrounded the phase crucible [16, 17]. The phase was held hanging in the inner tube of the Dewar flask with a fine thread. Magnetic susceptibility in the temperature range 77K-300K could be

measured by this arrangement. The data of molar magnetic susceptibility (χ_m) as a function of temperature are given in Table-3, while the inverse molar magnetic susceptibility (χ_m^{-1}) versus temperature T (K) data are plotted in figure 2.

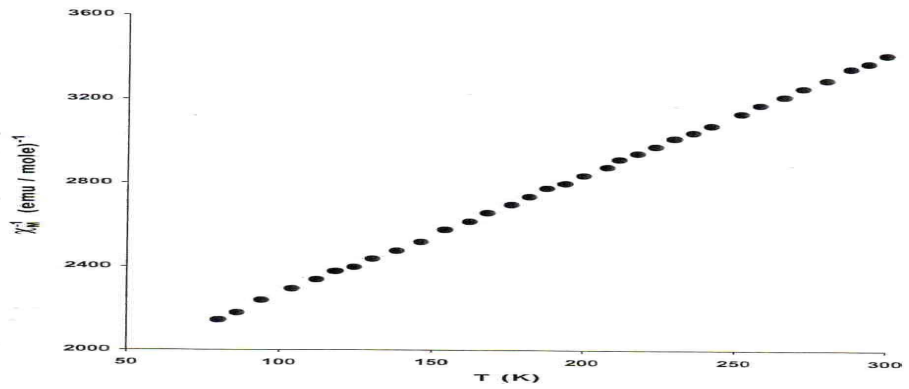

Figure 2: *χ_m^{-1} versus T plot of $Mn_{0.5}Si_{0.5}Te_2$*

Electrical Resistance study

Electrical Resistivity of thin pellet of the phase as a function of temperature in a continues flow of nitrogen was recorded by four probe method in a four probe cell, using Keithley programmable constant current supply source model 224 and nanovoltmeter model 181 for the purpose of current source and voltage measurement respectively [18,19]. The bottom surface of the pellet was kept non-conducting. The data of specific resistance (ρ) as a function of temperature are given in Table 4, while the log ρ versus 1/T data are plotted in the figure 3.

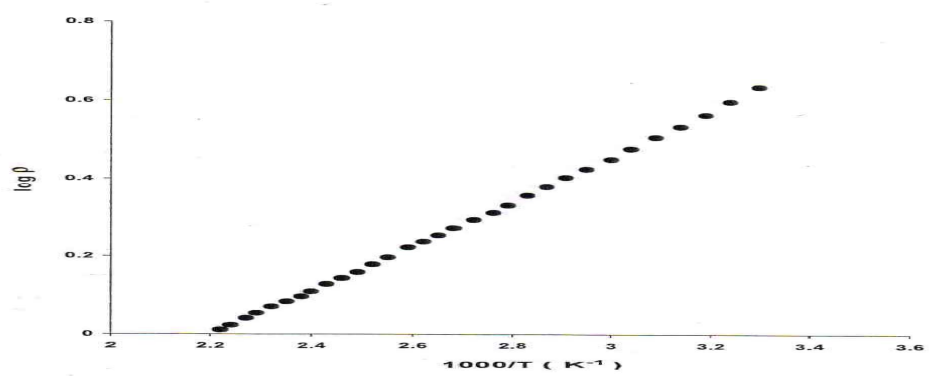

Figure 2: Log ρ versus1/T plot of $Mn_{0.5}Si_{0.5}Te_2$

Results and Discussion

Crystal Structure

The unit cell parameters of the phase were calculated from X-ray diffraction data (Table 2). The indexing of the data shows that it crystallises in the orthorhombic unit cell (a=14.754Å, b=12.380Åand

c=3.931Å). In order to determine the crystal structure, the theoretical X-ray diffraction data were generated by Treor and Lazy-Pulverix analysis. The good agreement between the observed and calculated **d** values confirms the structural parameter assignment. The data along with the assigned **h k l** values are given in the Table 2.

Table 2: Powder X-ray Diffraction Data of $Mn_{0.5}Si_{0.5}Te_2$

h	k	l	d_{obs} (Å)	d_{cal}(Å)	I_{obs}
0	2	0	6.193	6.195	5.5
0	0	1	3.934	3.934	7
1	0	1	3.801	3.802	5
4	2	0	3.175	3.171	100
1	3	1	2.796	2.797	13
1	5	0	2.442	2.443	4
5	1	1	2.320	2.320	16
5	2	1	2.206	2.206	15
2	2	2	1.817	1.817	10
1	3	2	1.761	1.763	8.5
4	3	2	1.600	1.600	29
7	3	2	1.357	1.358	8.5

a =14.754Å b = 12.380Å c = 3.931Å

Magnetic susceptibility studies

The χ_m^{-1} (molar magnetic susceptibility) versus T (temperature) values, given in Table 3 are plotted in figure 2, shows that the phase has negative Weiss constant which suggests that anti-ferromagnetic interactions are dominant and the material exhibits complex phenomenon. The magnetic moment (μ_{eff}) computed from Curie constant comes out to be 6.6 B.M and this value is slightly more than 4.90 B.M associated to the high spin Mn^{3+} ion ($t^3_{2g}\, e^1_g$). The θ and μ_{eff} values computed for the phase are given in Table-5.

Electric Transport Properties

The log of specific resistance (log ρ) versus temperature (K) values (Table 4) are plotted in the figure 3. The negative temperature co-efficient of resistivity and the values of the specific resistance show that the phase is semi-conductor in nature and the linearity of the plot shows that the electrical conduction occurs via thermal activated mechanism (Arrhenius mechanism).

Table 3: Molar magnetic susceptibility (χ_m) $Mn_{0.5}Si_{0.5}Te_2$ as function of temperature.

Temperature (K)	$\chi_m \times 10^4$ (emu / mole)
80	4.660
86	4.586
94	4.463
104	4.357
112	4.274
118	4.203
124	4.168
130	4.099
138	4.035
146	3.965
154	3.875
162	3.817
168	3.759
176	3.704
182	3.652
188	3.598
194	3.569
200	3.520
208	3.470
212	3.425
218	3.412
224	3.335
230	3.312
236	3.283
242	3.248
252	3.188
258	3.146
266	3.105
272	3.066
280	3.029
288	2.980
294	2.957
300	2.924

Table 4: Specific resistance (log ρ) of $Mn_{0.5}Si_{0.5}Te_2$ as function of temperature (K).

Temperature (K)	Specific resistance ρ (ohm cm)
450	1.029
445	1.057
440	1.102
435	1.135
430	1.182
425	1.216
420	1.255
415	1.293
410	1.351
405	1.398
401	1.448
396	1.515
391	1.577
386	1.677
381	1.736
377	1.802
372	1.883
367	1.974
362	2.059
358	2.148
353	2.278
348	2.396
343	2.546
338	2.676
333	2.835
328	3.018
323	3.222
318	3.433
313	3.673
308	3.982
303	4.353

Table 5: Magnetic and Electric Transport Parameters of $Mn_{0.5}Si_{0.5}Te_2$ phase.

Phase	μ_{eff} (B.M)	μ_{theo}(B.M)	E_a(eV)
$Mn_{0.5}Si_{0.5}Te_2$	6.66	4.90	0.12

Conclusion

A new phase with the composition $Mn_{0.5}Si_{0.5}Te_2$ has been synthesised by the standard ceramic method. On the basis of Lazy-Pulverix analysis of the X-ray diffraction data it is concluded that the phase crystallises in the orthorhombic unit cell. Magnetic study suggests that compound is antiferromagnetic. The study of electrical resistivity in the temperature range 300K-500K shows that the compound is an electrical semi- conductor and conduction occurs via thermal activated mechanism.

Acknowledgements

Thanks are due to the UGC, New Delhi for financial support, University of Delhi for thermal analysis, IIT Bombay for XRD studies and Department of Chemistry, University of Jammu, Jammu for providing requisite facilities.

References: References:

[1] Folmer J.C.W, Jellinek F. and Calis G.H.M. (1988).The Electronic Structure of Pyrites, Particularly CuS_2 and $Fe_{1-X}Cu_xSe_2$: An XPS And Mössbauer Study**,** J. Solid State Chem., 72**,** 137-144.

[2] Li Jing, Guo H.Y., Proserpio D.M. and Sironi A. (1995).Exploring Tellurides: Synthesis and Characterization of New Binary, Ternary, and Quaternary Compounds*,* J. Solid State Chem., 117**,** 247-255.

[3] Fischer P. Plambeck, Abriel W. and Urland W. (1989). Preparation and Crystal Structure of $RESe_{1.9}$ (RE = Ce, Pr), J. Solid State Chem., 78, 164.

[4] Pardo M.P., Gardette M.F., Dung N. and Flahaut J. (1991). Insertion d'oxygène dans les composés de type $Cu_{0.5}RTe_2$ et $Cu_{0.5}RTe_{1.75}$ (R = La et Nd)*,* J. Solid State Chem., 94,121-129.

[5] Huan G. and Greenblatt M. (1987*).* New $A_xNb_6Se_8$ (A= Na, K, Rb, Cu, Ag, Zn, Cd, Pb) phases with the Nb_3Te_4 structure, Mater. Res. Bull., 22, 505.

[6] Huan G. and Greenblatt M, (1991). Inorganic Syntheses, Non molecular Solids*,* Mater. Res. Bull., 22, 943.

[7] Limatta E.W. and lbers J.A. (1987*).*Synthesis, Structure, and Physical Properties of the New Layered Ternary Chalcogenide $NbNiTe_5$*,* J. Solid State Chem.,71, 384.

[8] Elwell W.T. and Gidley J.A.F., Atomic Absorption Spectrophotometry, Pergamon, 102. (1961).

[9] Robinson J.B., Atomic Absorption Spectroscopy, Marcell Dekker, New York. (1966).

[10] Khopkar S.M., Basic Concept of Analytical Chemistry, Wiley Eastern Limited. (1985).

[11] Taguchi H., Nagao M. and Shimada M. (1988). Metal-Insulator Transition in the System (Nd1−xCax) MnO2.99 (0.5 □ x □ 0.9), J. Solid State Chem., 76, 284-289.

[12] Jeffery G.H., Vogel's Text Book of Quantitative Chemical Analysis (ELBS, Longman, Essex). (1989).

[13] Yvon K., Jeitschko W. and Perthe E., Lazy Pulverix, Laboratory De Crystallographic Aux Rayons-X, Universities De Genève, Genève, Switzerland. (1977).

[14] Werner P. E., Treor - 4 Deptt. of Structural Chemistry, Arrhenius Laboratory University of Stockholm, Sweden. (1984).

[15] Noel H., Potel M., Troc R. and Shlyk. L. (1996). Crystal Structure and Physical Properties of β USe2and USe2−x Tex (x= 0.24 and 0.72), J. Solid State Chem., 126, 22-26.

[16] Selwood P.W., Magnetochemistry, (Interscience, New York), (1943).

[17] Goodenough J.B. (1963).Magnetism and the Chemical Bond (Interscience, New York).

[18] Resistivity of Semiconductors by Four Probe Method at Different Temperature Scientific Equipment and Services Roorkee 247667 U.P).

[19] Wieder H.H and Elsevier Amsterdam., Laboratory Notes on Electrical and GalvanomagneticMeasurements.67, 53-55. (1979).