

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

PAWAN K. SHARMA<sup>1</sup> AND INDU B. SHARMA<sup>2</sup>

<sup>1</sup>Govt. Degree College Khour, Jammu, 181203, India.

<sup>2</sup>ISCAS, Institute of Solid State and Material Science, Jammu University Campus, Jammu.

Corresponding author: drpksharma59@gmail.com

### Abstract

*A new phase with the composition  $V_{0.5}Si_{0.5}Te_2$  has been synthesized by the standard ceramic method. X-ray diffraction studies show that the phase crystallizes with the tetragonal unit cell ( $a=11.881\text{\AA}$  and  $c=9.958\text{\AA}$ ). The molar magnetic susceptibility measurements as a function of temperature suggest that the phase is diamagnetic and magnetic susceptibility is temperature independent. The electrical resistivity measurements as a function of temperature suggest that the phase is semi-conductor in nature in the temperature range 300K-500K and the conduction occurs via thermally activated mechanism.*

**Keywords:** Mixed binary dichalcogenides, XRD, Molar Magnetic Susceptibility, 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  $V_{0.5}Si_{0.5}Te_2$  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 makes Vanadium (V) 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  $V_{0.5}Si_{0.5}Te_2$ , 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

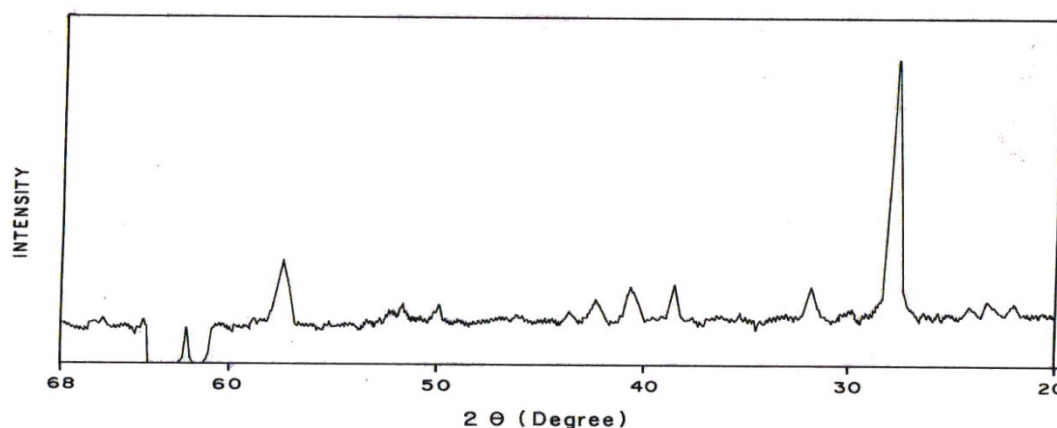
The phase was further analyzed by atomic absorption spectrophotometry, which is one of the most prevalent methods for the trace element analysis [8, 9, 10]. The results of chemical elemental analysis [11, 12] and the atomic absorption spectrophotometry are in good agreement. The data are given in Table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

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

Phase	V	Si	Te
$V_{0.5}Si_{0.5}Te_2$	8.58 (8.64)	4.65 (4.76)	86.43 (86.59)

### 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 of 1deg./minute in the  $2\theta$  range using  $CuK\alpha$  and  $FeK\alpha$  radiations [13, 14 and 15]. The X-ray diffraction data are given in the Table 2, while the X-ray pattern, intensity, versus  $2\theta$  is drawn in the figure1.



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

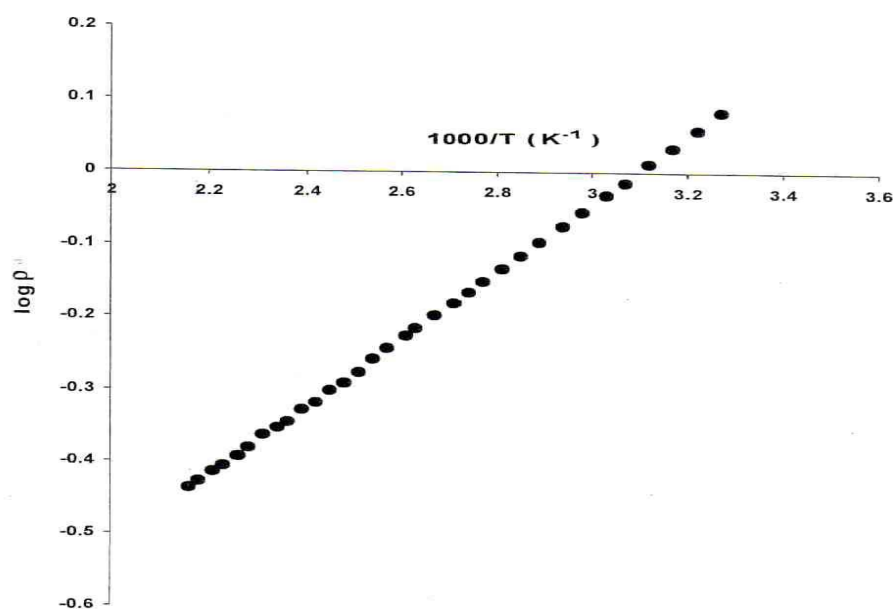
### Magnetic Susceptibility Measurement

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.

### ***Electrical Resistance study***

Electrical Resistivity of thin pellet of the phase as a function of temperature in a continuous flow of nitrogen was recorded by four probe method in a four probe cell, using Keithley programmable constant current 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 ( $\rho$ ) as a function of temperature are given in Table 4, while the  $\log \rho$  versus  $1/T$  data are plotted in the figure 2.



**Figure 2:** *Log  $\rho$  versus  $1/T$  plot of  $V_{0.5}Si_{0.5}Te_2$*

## **Result 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 crystallizes in the tetragonal unit cell with  $a=11.881\text{\AA}$  and  $c=9.958\text{\AA}$ . In order to determine the crystal structure, the theoretical X-ray diffraction data were generated by Treor and Lazy-Pulverix analysis. The  $d_{\text{cal}}$  values computed from data are in good agreement with the experimental interplanar distances. The data along with the assigned  $h k l$  values are given in the Table 2.

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

H	K	L	$d_{obs}$ (Å)	$d_{cal}$ (Å)	$I_{obs}$
2	0	2	3.817	3.819	7
3	0	1	3.677	3.683	6
1	0	3	3.197	3.199	100
3	3	0	2.805	2.802	13
3	2	3	2.338	2.340	15
4	0	3	2.216	2.215	14
5	4	1	1.824	1.825	6
6	3	0	1.771	1.772	6
4	4	4	1.605	1.606	23

$$a = 11.881 \text{ \AA}$$

$$c = 9.958 \text{ \AA}$$

### *Magnetic susceptibility studies*

The molar magnetic susceptibility measurements as a function of temperature suggest that the phase is diamagnetic and magnetic susceptibility is temperature independent.

### *Electric Transport Properties*

The log of specific resistance ( $\log \rho$ ) versus temperature (K) values (Table 3) are plotted in the figure 2. The negative temperature co-efficient of resistivity and the values of the specific resistance suggest that the phase is semi-conductor in nature and the linearity of the plot shows that the electrical conduction occurs via thermal activated mechanism.

**Table 3:** Specific resistance ( $\log \rho$ ) of  $V_{0.5}Si_{0.5}Te_2$  as function of temperature (K).

	Temperature (K)	Specific resistance $\rho$ (ohm cm)
1.	462	0.366
2.	457	0.374
3.	452	0.386
4.	447	0.392
5.	442	0.404
6.	437	0.416
7.	432	0.434
8.	427	0.443
9.	422	0.452
10.	417	0.470
11.	412	0.481

12.	407	0.501
13.	403	0.512
14.	398	0.529
15.	393	0.553
16.	388	0.572
17.	383	0.594
18.	379	0.607
19.	374	0.635
20.	369	0.659
21.	364	0.682
22.	360	0.707
23.	355	0.736
24.	350	0.768
25.	345	0.802
26.	340	0.843
27.	335	0.882
28.	330	0.929
29.	325	0.996
30.	320	1.032
31.	315	1.850
32.	310	1.150
33.	305	1.217

**Table3:** Magnetic and Electric Transport Parameters of ( $V_{0.5}Si_{0.5}Te_2$ ) phase.

Phase	$\mu_{\text{eff}}$ (B.M)	$\mu_{\text{theo}}$ (B.M)	$E_a$ (eV)
$V_{0.5}Si_{0.5}Te_2$	Diamagnetic	-	0.09

## Conclusion

A new phase with the composition  $V_{0.5}Si_{0.5}Te_2$  has been synthesized by the standard ceramic method. On the basis of Lazy-Pulverix analysis of the X-ray diffraction data it is concluded that the phase crystallizes in the tetragonal unit cell. The molar magnetic susceptibility measurements as a function of temperature suggest that the phase is diamagnetic and magnetic susceptibility is temperature independent. 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:

- [1] Folmer J.C.W, Jellinek F. and Calis G.H.M. (1988). The Electronic Structure of Pyrites, Particularly  $\text{CuS}_2$  and  $\text{Fe}_{1-x}\text{Cu}_x\text{Se}_2$ : An XPS and Mossbauer 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  $\text{RESe}_{1.9}$  (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  $\text{Cu}_{0.5}\text{RTe}_2$  et  $\text{Cu}_{0.5}\text{RTe}_{1.75}$  (R = La et Nd), *J. Solid State Chem.*, 94, 121-129.
- [5] Huan G. and Greenblatt M. (1987). New  $\text{A}_x\text{Nb}_6\text{Se}_8$  (A = Na, K, Rb, Cu, Ag, Zn, Cd, Pb) phases with the  $\text{Nb}_3\text{Te}_4$  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 Ibers J.A. (1987). Synthesis, Structure, and Physical Properties of the New Layered Ternary Chalcogenide  $\text{NbNiTe}_5$ , *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  $(\text{Nd}_{1-x}\text{Ca}_x)\text{MnO}_{2.99}$  ( $0.5 \leq x \leq 0.9$ ), *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  $\beta$  USe<sub>2</sub> and USe<sub>2-x</sub> 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 Galvanomagnetic Measurements. 67, 53-55. (1979).