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

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Abstract

A new phase with the composition $V_{0.5}Al_{0.5}Te_2$ has been synthesised by the standard ceramic method. X-ray diffraction studies show that the phase crystallizes in tetragonal unit cell (a=12.592Å and c=9.990Å). 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. Anomaly at around 422 K, shows that a phase transformation occurs. The thermal analysis suggests that above 673 K there is 9.8% mass gain and at low temperature (423.3K), there is phase transformation which results polymerisation process.

Keywords: Mixed binary dichalcogenides, XRD, electrical resistivity, TG-DTA.

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 $V_{0.5}Al_{0.5}Te_2$ 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. The phase has been analysed for thermogravimeteric analysis (TGA) and differential thermogravimeteric analysis (DTGA).

Experiment

Synthesis

Aldrich make Vanadium (V) Aluminium (Al) and Tellurium (Te) elements (purity 99.9%) have been used for synthesis of the new phase. The constituent elements weighed corresponding to the stoichiometry $V_{0.5}Al_{0.5}Te_2$, were mixed and homogenised by grinding in cyclohexane. The dried and

homogenised mixture, pressed into pellets in hydraulic press was placed in quartz tube and evacuated to ~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 pulverised to fine powder for further investigations [5, 6, 7].

Elemental Analysis

The phase was further analysed 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 ($V_{0.5}Al_{0.5}Te_2$).
The theoretical value is given parenthesis. Analysis (%)

Phase	V	Al	Te
$V_{0.5}Al_{0.5}Te_2$	8.57 (8.65)	4.53 (4.58)	86.64 (86.75)

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 2θ range using Cu$K\alpha$ and Fe$K\alpha$ 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.

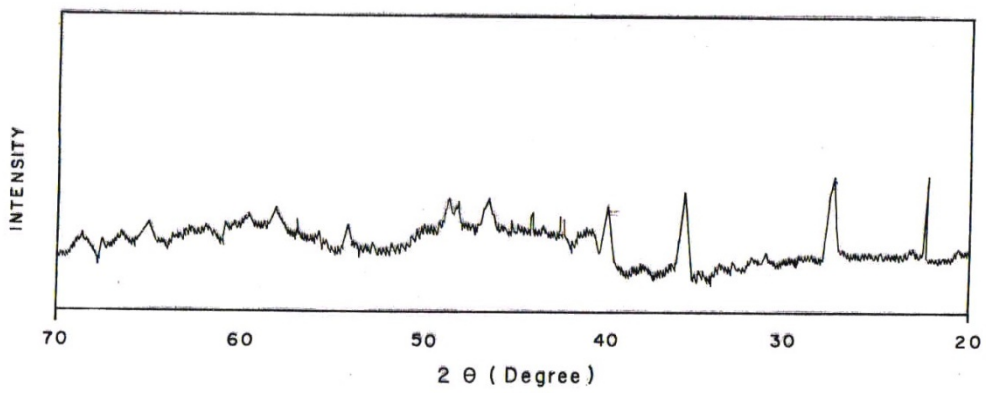

Figure 1: *X-ray Diffraction pattern of $V_{0.5}Al_{0.5}Te_2$*

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 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 2.

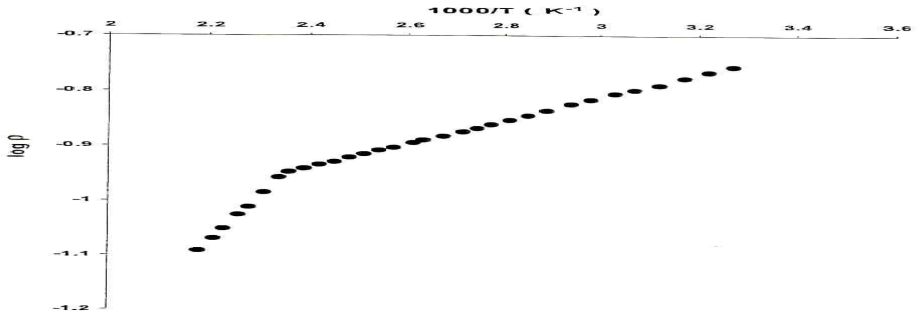

Figure 2: *Log ρ versus1/T plot of $V_{0.5}Al_{0.5}Te_2$*

Thermal Analysis

The phase has been thermally analyzed for thermogravimeteric (TG) and differential thermal analysis (DTA) by Rigaku thermal Analysis System 8150, provided with a microprocessor, in the temperature range 300K- 873K at the heating rate of 10 deg./min in continuous flow of nitrogen [20, 21]. The TG and DTA plot is given in figure 3.

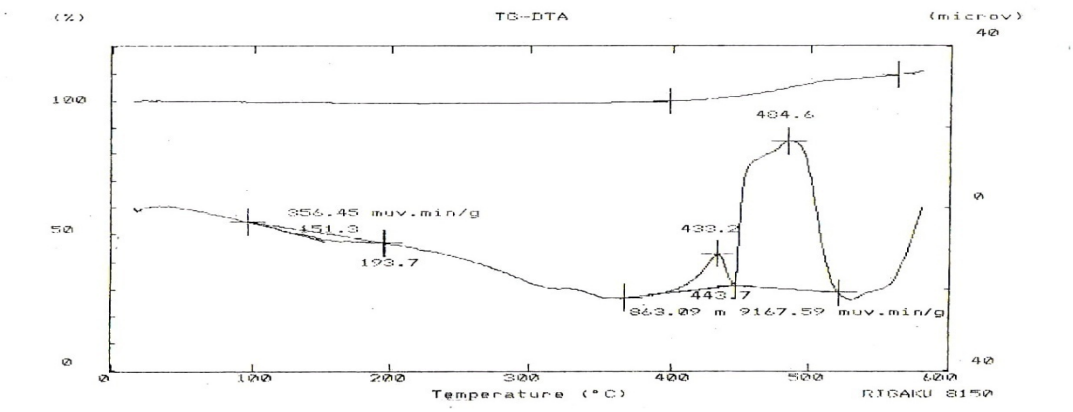

Figure 3*: TG-DTA Curves of $V_{0.5}Al_{0.5}Te_2$*

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 orthorhombic unit cell (a=12.592Å and c=9.990Å). In order to determine the crystal structure, the theoretical X-ray diffraction data were generated by Treor and Lazy-Pulverix analysis. The $\mathbf{d_{cal}}$ 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 $V_{0.5}Al_{0.5}Te_2$

h	k	l	d_{obs} (Å)	d_{cal}(Å)	I_{obs}
3	0	1	3.866	3.872	22
1	0	3	3.220	3.221	100
4	2	0	2.813	2.817	72
5	2	0	2.338	2.340	83
4	4	0	2.227	2.227	28
0	5	0	1.972	1.974	22
2	2	5	1.824	1.824	28
5	0	4	1.774	1.774	16
8	2	0	1.527	1.528	22

a= 12.592Å c= 9.990Å

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 electrical resistivity of the phase ($V_{0.5}Al_{0.5}Te_2$), as function of temperature, is plotted in figure 2. The negative temperature co-efficient of resistivity and the values of the specific resistance (Table.3) suggest that the phase is semi-conductor in nature and the electrical conduction occurs via thermal activated mechanism. However, the slope of the plot shows an anomaly around 422K which suggests that a phase transformation occurs and it could be assigned to the polymerisation of telluride.

Thermal Analysis:

The thermogravimeteric analysis (TGA) of $V_{0.5}Al_{0.5}Te_2$ fig. 3 suggests that there is almost no mass change upto 673 K and beyond this temperature there is 9.8% mass gain. The differential thermal

analysis (DTA) exhibits a broad endothermic peak with peak temperature 423.3 K. Between 673 and 783 K the material undergoes to exothermal peaks. During the broad endothermic peak at 423.3 K, the mass of the sample remains constant which suggests that this transition is associated with phase transformation which in this case considered to be the polymerisation process associated with $V_{0.5}Al_{0.5}Te_{2.}$

Table 3: Specific resistance (log ρ) of $V_{0.5}Al_{0.5}Te_2$ as function of temperature (K).

Temperature (K)	Specific resistance ρ (ohm cm)
457	0.080
452	0.085
447	0.088
442	0.094
437	0.097
432	0.103
427	0.110
422	0.112
417	0.114
412	0.116
407	0.117
403	0.119
398	0.121
393	0.123
388	0.124
383	0.127
379	0.129
374	0.131
369	0.133
364	0.135
360	0.137
355	0.140
350	0.142
345	0.145
340	0.149
335	0.152
330	0.156
325	0.159
320	0.162
315	0.167
310	0.171
305	0.175

Table4: Magnetic and Electric Transport Parameters of ($V_{0.5}Al_{0.5}Te_2$) phase.

. Phase	μ_{eff} (B.M)	μ_{theo}(B.M)	E_a(eV)
$V_{0.5}Al_{0.5}Te_2$	Diamagnetic	-	0.04 **(305-422 K)** 0.17 **(427-457K)**

Conclusion

A new phase with the composition $V_{0.5}Al_{0.5}Te_2$ 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 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. Anomaly at around 422 K, shows a phase transformation. The thermal analysis suggests that above 673 K there is 9.8% mass gain and at low temperature (423.3K) there is transition associated with phase transformation which results the polymerisation process.

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.

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