Synthesis, Structure, Magnetic and Electric Transport Properties of $Zr_{0.5}Al_{0.5}Te_{1.95}$

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Abstract

A new phase with the composition $Zr_{0.5}Al_{0.5}Te_{1.95}$ has been synthesized by the standard ceramic method. X-ray diffraction studies show that the phase crystallizes with the tetragonal unit cell (a=14.628Å and c=7.146Å).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. The anomaly in the slope of Log ρ versus1/T plot changes the electrical transport property due to polymerization effect.

Keywords: Mixed binary dichalcogenides, XRD, Molar Magnetic Susceptibility, electrical resistivity.

Introduction

Binary dichalcogenides of numerous elements with composition MX_2 and their mixed analogues $M_{1-x}M'X_2$ (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 $Zr_{0.5}Al_{0.5}Te_{1.95}$ 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 Zirconium (Zr) Aluminum (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 $Zr_{0.5}Al_{0.5}Te_{1.95}$, 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 ~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 ($Zr_{0.5}Al_{0.5}Te_{1.95}$).
The theoretical value is given parenthesis. Analysis (%)

Phase	Zr	Al	Te
$Zr_{0.5}Al_{0.5}Te_{1.95}$	14.37 (14.51)	4.16 (4.29)	79.17 (81.19)

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 1degree/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.

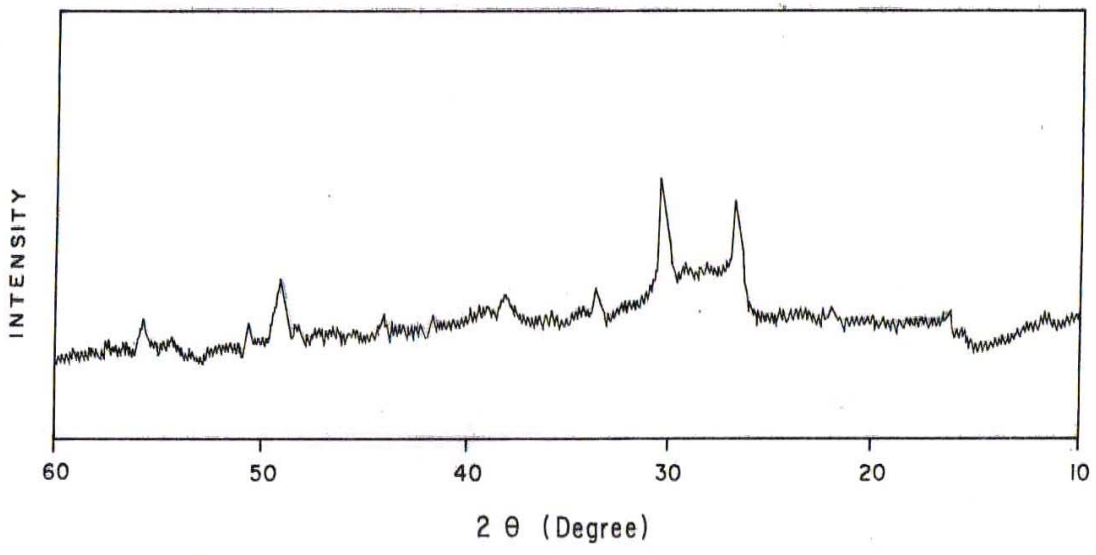

Figure 1: *X-ray Diffraction pattern of $Zr_{0.5}Al_{0.5}Te_{1.95}$*

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.

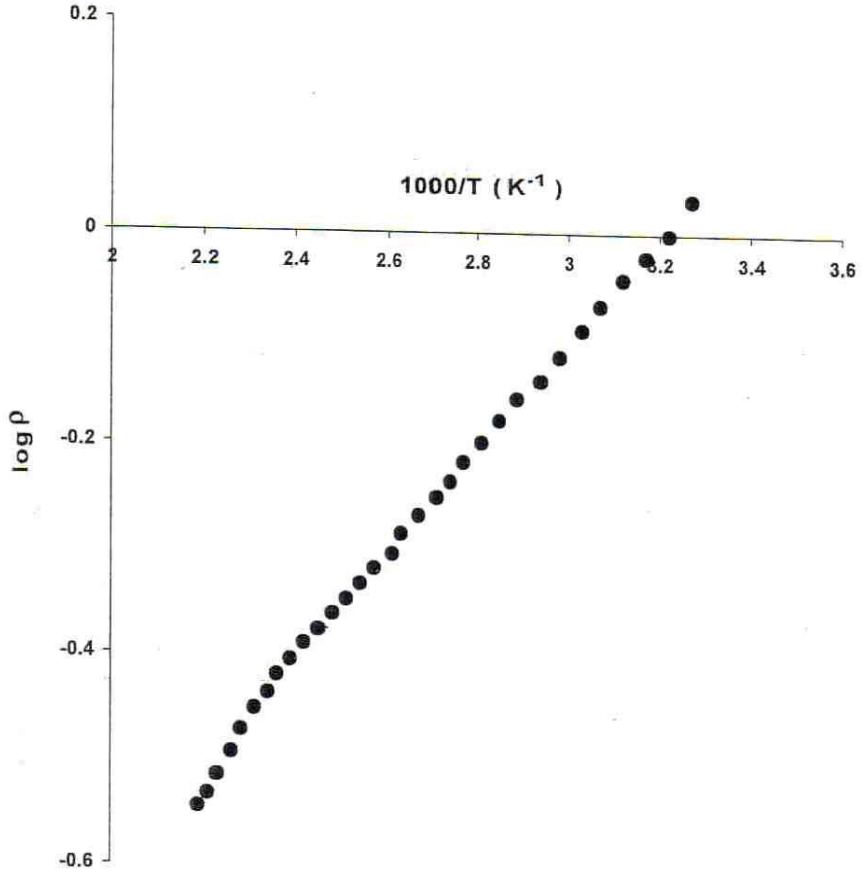

Figure 2: Log ρ Versus1/T plot of $Zr_{0.5}Al_{0.5}Te_{1.95}$

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=14.628Å and c=7.146Å.** 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 $Zr_{0.5}Al_{0.5}Te_{1.95}$

H	K	L	d_{obs} (Å)	d_{cal}(Å)	I_{obs}
2	0	0	7.314	7.320	95
1	1	2	3.375	3.379	90
4	2	1	2.978	2.976	100
3	2	2	2.682	2.683	20
6	1	0	2.404	2.406	20
6	5	1	1.813	1.813	15
6	5	2	1.658	1.660	27

a= 14.628Å c= 7.146Å

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 ρ) versus temperature (K) values (Table 3) is 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 ρ) of $Zr_{0.5}Al_{0.5}Te_{1.95}$ as function of temperature (K).

Temperature (K)	Specific resistance ρ (ohm cm)
455	0.285
452	0.293
447	0.305
442	0.321

437	0.337
432	0.353
427	0.366
422	0.380
417	0.393
412	0.407
407	0.420
403	0.435
398	0.449
393	0.465
388	0.481
383	0.496
379	0.519
374	0.539
369	0.561
364	0.581
360	0.605
355	0.633
350	0.664
345	0.697
340	0.725
335	0.765
330	0.809
325	0.854
320	0.904
315	0.950
310	1.000
305	1.079

Table3: Magnetic and Electric Transport Parameters of ($Zr_{0.5}Al_{0.5}Te_{1.95}$) phase.

Phase	**μ_{eff} (B.M)**	**μ_{theo}(B.M)**	**E_a(eV)**
$Zr_{0.5}Al_{0.5}Te_{1.95}$	Diamagnetic	-	0.10

Conclusion

A new phase with the composition $Zr_{0.5}Al_{0.5}Te_{1.95}$ 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.

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