Synthesis, Structure, Magnetic and Electric Transport Properties of $W_{0.5}Si_{0.5}Te_{1.95}$

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Abstract

A new phase with the composition $W_{0.5}Si_{0.5}Te_{1.95}$has been synthesised by the standard ceramic method.X-ray diffraction studiesshow that the phase crystallizes inorthorhombic unit cell (a=21.093Å, b=8.921Å and c=7.252Å).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 naturein the temperature range 300K-500K and the conduction occurs via thermally activated mechanism.The thermal analysis suggests that the phase remains almost stable upto 873K,although there is minor mass gain above 723 K.

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

Introduction:

Binary dichalcogenides of numerous elements with composition MX_2 and their mixed analogues $M_{1-x}M'X_2$ (M and M´are different transition elements; X=S, Se or Te) are known in the literature [1, 2]. Manydichalcogenides 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 thoughtinteresting to prepare mixed chalcogenides with composition $M_{0.5}M'_{0.5}X_2$ study of theircrystal structure& follow their physical properties as function of temperature.

In the present study, synthesis of a new phase with the composition $W_{0.5}Si_{0.5}Te_{1.95}$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. The phase has been analysed for thermogravimeteric analysis (TGA) and differential thermogravimeteric analysis (DTGA).

Experiment

Synthesis

Aldrich makeTungsten (W)Silicon (Si) and Tellurium (Te) elements (purity 99.9%) havebeen used for synthesis of the new phase. The constituent elements weighed corresponding to the stoichiometry $W_{0.5}Si_{0.5}Te_{1.95}$, were mixed and homogenised by grinding in cyclohexane. The dried and homogenised mixture, pressed into pellets in hydraulicpress was placed in quartz tube and evacuated to $\sim10^{-5}$ 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 undersameconditions 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 ofthe phase ($W_{0.5}Si_{0.5}Te_{1.95}$). The theoretical value is given parenthesis.

Analysis (%)

Phase	Wo	Si	Te
$W_{0.5}Si_{0.5}Te_{1.95}$	25.21 (25.45)	3.69 (3.88)	68.89 (70.65)

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 usingCuKα and FeKα radiations[13, 14 and 15].The X- ray diffraction data are given in the Table 2, whilethe X-ray pattern, intensity, versus 2θ is drawn in the figure1.

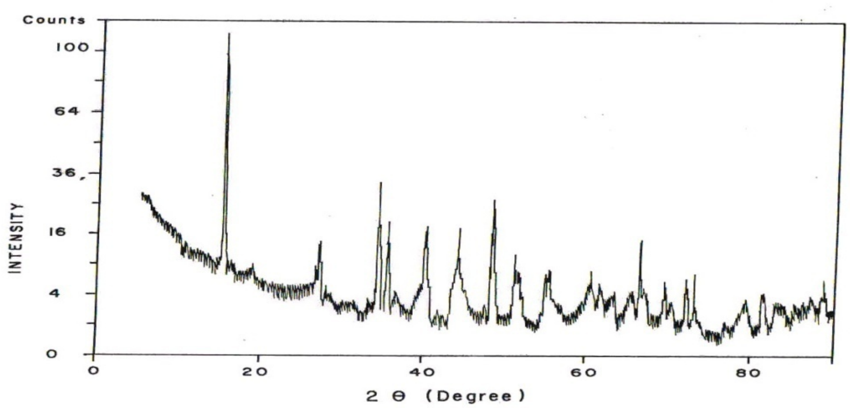

Figure 1:*X-ray Diffraction pattern of*$W_{0.5}Si_{0.5}Te_{1.95}$

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 polegaps 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 nanovoltmetermodel181 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.

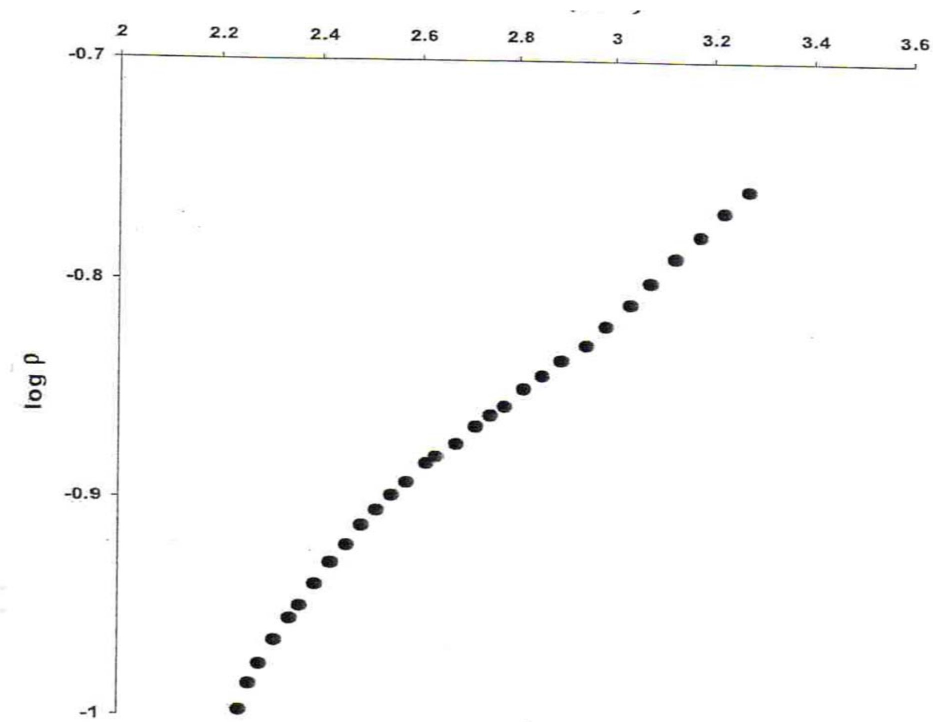

Figure 2:*Logρ versus1/T plot of $W_{0.5}Si_{0.5}Te_{1.95}$*

Thermal Analysis

The phase has been thermally analyzed for thermogravimeteric (TG) and differential thermal analysis (DTA) by Rigaku thermalAnalysis 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.

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=21.093Å, b=8.921Å and c=7.252Å). In order to determine the crystal structure, the theoreticalX-ray diffractiondata were generated by Treor (Noel *et al*., 1996) and Lazy-Pulverix analysis (Yvon *et al*., 1977). 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

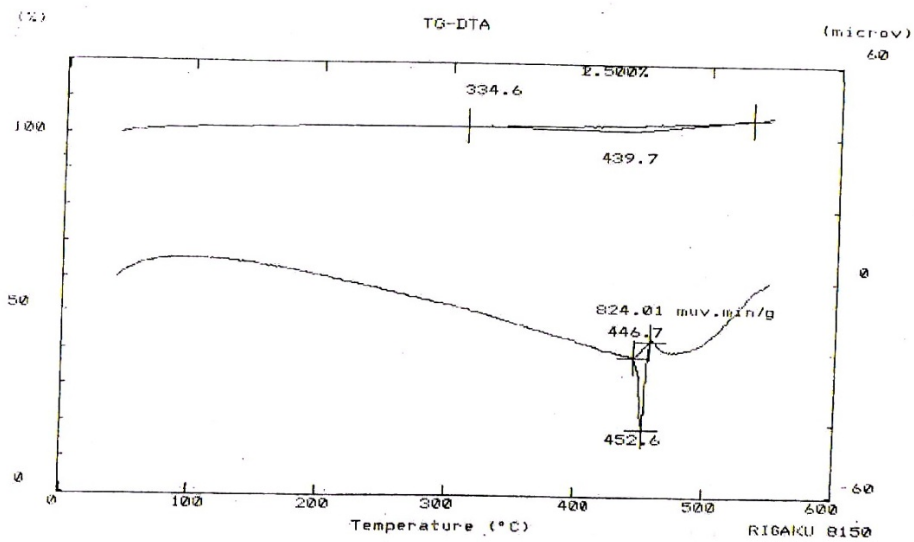

Figure 3: TG-DTA Curves of $W_{0.5}Si_{0.5}Te_{1.95}$

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Table 2: Powder X-ray Diffraction Data of $W_{0.5}Si_{0.5}Te_{1.95}$

h	k	l	d_{obs} (Å)	d_{cal}(Å)	I_{obs}
0	0	1	7.243	7.258	49.2
2	2	0	4.115	4.111	3.8
6	0	1	3.163	3.165	8.1
0	2	2	2.814	2.816	6.6
6	2	1	2.576	2.582	8.1
7	2	1	2.362	2.362	11.6
2	3	2	2.247	2.248	3.5
7	3	0	2.117	2.118	100.0
5	0	3	2.098	2.099	3.0
8	1	2	2.072	2.075	2.3
6	3	2	1.926	1.925	2.8
1	4	2	1.892	1.893	2.3
4	4	3	1.766	1.768	4.9

a= 21.093Å b=8.921Å c=7.252Å

Table 3: Specific resistance (log ρ) of $W_{0.5}Si_{0.5}Te_{1.95}$as function of temperature (K).

Temperature (K)	Specific resistanceρ (ohm cm)
446	0.100
442	0.103
437	0.105
432	0.108
427	0.110
422	0.112
417	0.114
412	0.117
407	0.119
403	0.122
398	0.124
393	0.126
388	0.128
383	0.130
379	0.131
374	0.133
369	0.136
364	0.137
360	0.138
355	0.141
350	0.143
345	0.145
340	0.148
335	0.151
330	0.154
325	0.158
320	0.162
315	0.166
310	0.170
305	0.174

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 ($W_{0.5}Si_{0.5}Te_{1.95}$), as function of temperature, is plotted in figure 2.There is a break in the slope of log ρ versus 1/T plot at around 407 K. The temperature co-efficient of resistivity in both the regions remains negative. 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.

Thermal Analysis:

The thermogravimeteric analysis (TGA) of$W_{0.5}Si_{0.5}Te_{1.95}$fig. 3 suggest that the phase remains almost stable upto 873 K, although there is minor mass gain above 723 K. The differential thermal analysis (DTA) curve of this phase shows similar thermal stability upto 719 K, beyond this temperature there is a sharp endothermic peak with peak temperature at 725.7 K.

Table 4: Magnetic and Electric Transport Parameters of ($W_{0.5}Si_{0.5}Te_{1.95}$) phase.

Phase	μ_{eff} (B.M)	μ_{theo}(B.M)	E_a(eV)
$W_{0.5}Si_{0.5}Te_{1.95}$	Diamagnetic	-	0.04 **(305-393 K)** 0.07 **(417-446K)**

Conclusion

A new phase with the composition $W_{0.5}Si_{0.5}Te_{1.95}$has been synthesised by thestandard ceramic method. On the basis of Lazy-Pulverix analysis of the X-ray diffraction data it is concluded that the phase crystallises in orthorhombic 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. The thermal analysis suggests that the phase remains almost stable upto 873K, although there is minor mass gain above 723 K.

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