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

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Abstract

A new phase with the composition $Mo_{0.5}Si_{0.5}Te_2$has been synthesized by the standard ceramic method. X-ray diffraction studies show that the phase crystallizes in orthorhombic unit cell (a=16.926Å, b=14.129Å and c=7.007Å).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 thermal analysis suggests that the phase remains stable up to 623K and above this temperature there is mass gain of 3.2 %.
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]. 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 $Mo_{0.5}Si_{0.5}Te_2$ 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. The phase has been analyzed for thermogravimeteric analysis(TGA) and differential thermogravimeteric analysis (DTGA).

Experiment

Synthesis

Aldrich make Molybdenum (Mo) Silicon (Si) and Tellurium (Te) elements (purity 99.9%) have been used for synthesis of the new phase. The constituentelements weighed corresponding to the stoichiometry $Mo_{0.5}Si_{0.5}Te_2$, 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

~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 undersame 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 ofthe phase ($Mo_{0.5}Si_{0.5}Te_2$). The theoretical value is given in parenthesis.

	Analysis (%)		
Phase	**Mo**	**Si**	**Te**
$Mo_{0.5}Si_{0.5}Te_2$	15.01 (15.12)	4.29 (4.42)	80.03 (80.45)

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].TheX- ray diffraction data are given in the Table 2, whilethe X-ray pattern, intensity, versus 2θ is drawn in the figure1.

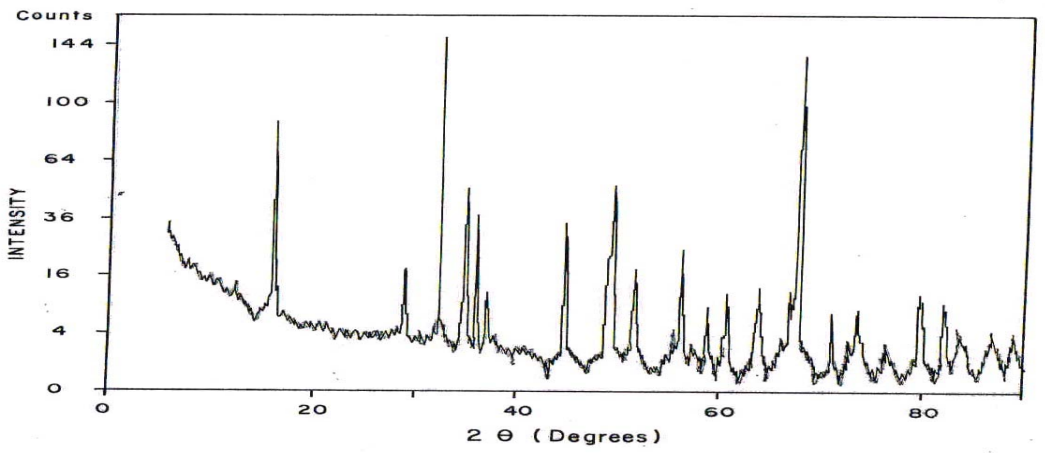

Figure 1:X-ray Diffraction pattern of $Mo_{0.5}Si_{0.5}Te_2$

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 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 figure2.

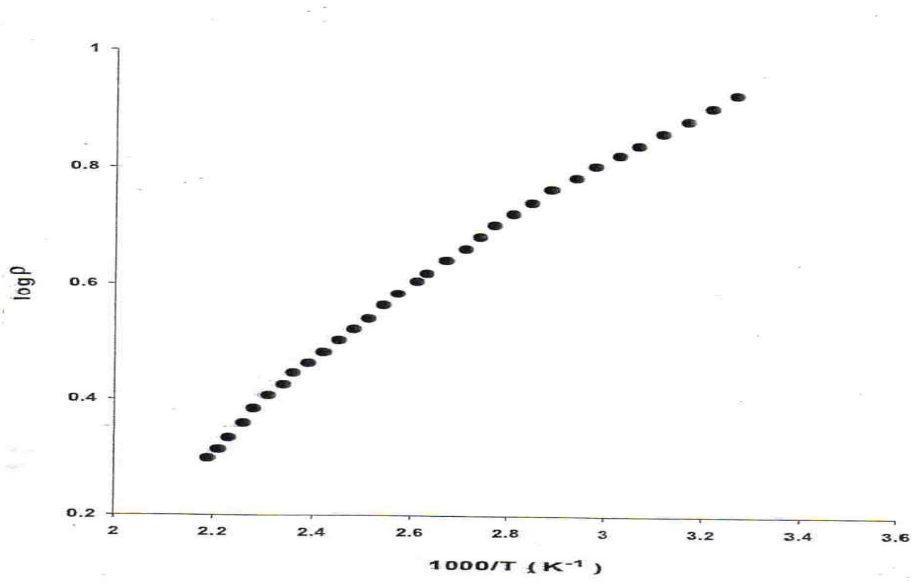

Figure 2: Log ρ versus1/T plot of $Mo_{0.5}Si_{0.5}Te_2$

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.

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 crystallizes in orthorhombic unit cell (a=16.926Å, b=14.129Å and c=7.007Å). 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.

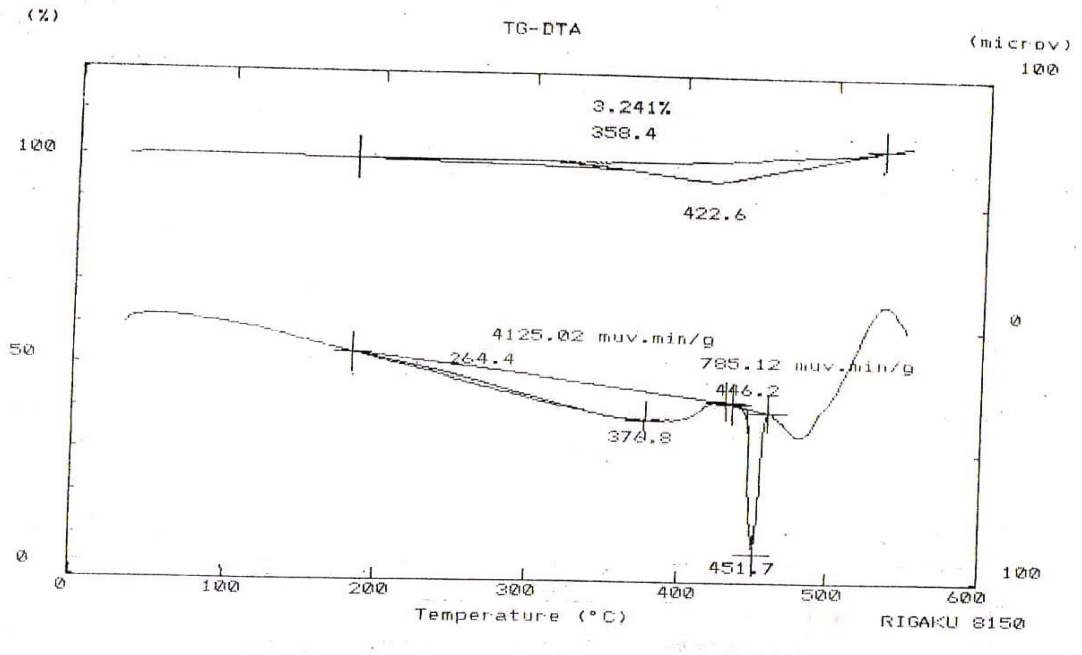

Figure 3: TG-DTA Curves of $Mo_{0.5}Si_{0.5}Te_2$

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 logs of specific resistance (log ρ) 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 electrical conduction occurs via thermal activated mechanism. The plot(log ρ versus K) given in fig. shows that there is an anomaly at around 369 K which changes electrical transport property due to polymerization effect.

Thermal Analysis:

The thermogravimeteric analysis (TGA) of $Mo_{0.5}Si_{0.5}Te_2$(fig.3) suggests that the phase remains stable upto 623K and above this temperature there is mass gain of 3.2 %. The differential thermal analysis (DTA) curve of this phase does not show any peak upto 719 K, but between 719 and 728 K there is a sharp endothermic peak with peak temperature at 724.7 K.

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

h	k	l	d_{obs} (Å)	d_{cal}(Å)	I_{obs}
0	2	0	7.067	7.069	47.2
0	0	1	7.012	7.135	32.8
4	1	1	3.515	3.511	89.6
0	0	2	3.505	3.506	71.8
0	1	2	3.412	3.403	0.5
2	0	2	3.241	3.239	23.9
4	3	0	3.149	3.150	23.1
5	2	0	3.060	3.055	4.2
3	4	0	2.988	2.996	2.3
3	1	2	2.912	2.914	1.1
5	3	1	2.561	2.561	18.9
0	6	0	2.356	2.356	12.3
0	0	3	2.338	2.337	24.6
0	6	1	2.232	2.333	9.3
2	6	1	2.158	2.160	7.1
0	3	3	2.092	2.094	3.1
3	2	3	2.063	2.065	14.6
2	3	3	2.029	2.033	0.8
5	0	3	1.924	1.924	6.7
7	5	0	1.839	1.838	5.2
4	7	1	1.763	1.764	6.0
6	6	1	1.750	1.751	70.5
9	3	0	1.745	1.747	41.1
3	7	2	1.671	1.671	2.3
7	6	1	1.640	1.641	1.1
4	0	4	1.620	1.619	3.9
3	3	4	1.575	1.577	1.5
7	4	3	1.517	1.518	6.0
6	1	4	1.479	1.481	3.4
11	2	1	1.470	1.471	100.0
8	7	0	1.459	1.461	3.1
10	3	2	1.449	1.451	3.6
7	7	2	1.416	1.418	2.6

a = 16.926Å b=14.129Å c=7.007Å

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

Temperature (K)	Specific resistanceρ (ohm cm)
456	1.999
452	2.066
447	2.164
442	2.294
437	2.429
432	2.559
427	2.674
422	2.811
417	2.922
412	3.050
407	3.206
403	3.346
398	3.486
393	3.681
388	3.848
383	4.049
379	4.186
374	4.409
369	4.619
364	4.845
360	5.075
355	5.301
350	5.542
345	5.842
340	6.109
335	6.415
330	6.711
325	6.971
320	7.319
315	7.685
310	8.073
305	8.520

Table 4: Magnetic and Electric Transport Parameters of ($Mo_{0.5}Si_{0.5}Te_2$) phase.

Phase	μ_{eff} (B.M)	μ_{theo}(B.M)	E_a(eV)
$Mo_{0.5}Si_{0.5}Te_2$	Diamagnetic	-	0.09 **(305-350 K)** 0.15 **(407-456K)**

Conclusion

A new phase with the composition $Mo_{0.5}Si_{0.5}Te_2$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 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. Anomaly at around 369K, changes electrical transport property due to polymerization effect. The thermal analysis suggests that the phase remains stable up to 623K.

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