The Variation of Electrical Conductivity of SmS with Temperature at Different Pressure

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Abstract **: - We have developed a theoretical model to calculate electrical parameters such as activation energy, carrier concentration, Hall constant, carrier mobility, electrical conductivity and resistivity under the effect of temperature and these parameters are used to discuss transport mechanism in SmS. Based on this analysis, we have investigated the valence transition in SmS under the effect of temperature.The variation of electrical conductivity with pressure of the SmS. which depends on the electrical resistivity. The resistivity ofSmS decreases rapidly up to 6-7 Kbar pressure, which is consistent with the electronic phase transition, observed experimentally at 6.5 Kbar pressure. The present model confirm that in SmS semiconductor to metal phase transition takes place at about 6-7 Kbar pressure. Since the value of pressure needed for the complete conversion of SmS^{2+} to Sm^{3+} is about 15 Kbar, which is higher than the transition pressure 6-7 kbar, it confirm that metallic state of SmS is intermediate valent. Again in increase in the resistivity above 7 Kbar pressure is also indicative to the metal to semiconductor phase transition at higher pressures. It again confirm that the metallic state of SmS is intermediate valent, i.e. metal to semiconductor transition in SmS. But in the present model, we found that the value of resistivity of SmS at P=11 Kbar is comparable to its value at zero pressure, it means SmS should show semiconducting behaviour at about P=11 Kbar**

Key Words : - Activation energy, carrier concentration, electrical conductivity and electrical resistivity.

INTRODUCTION :

In rare earth chalcogenides, most of the rare earth ions are trivalent with exception of Sm and Eu in the middle and Tm and Yb at the end of the series, for these ions Hund's rule of couplings becomes important and the divalent state is favoured [1]. In Sm, Eu, Tm and Yb Compounds the 4f^{n} (5d6s)^{m} and 4f^{n-1}(5d6s)$^{m+1}$ states are energetically close and may become nearly degenerate when the external parameters (pressure, temperature) are changed. Recent pressure-resistivity studies [2] on divalent rare earth chalcogenides revealed that under pressure the rare-earth ions in these compounds undergo a transformation to the trivalent state. The valance transformation from divalent to trivalent state involves the delocolization of 4f electron and its merging with conduction band at some high pressure. It has also been observed [3] that rare earth chalcogenide semiconductors were in semiconducting state when the rare earth ion was divalent and metallic when it was trivalent. We have calculated the electrical parameters associated with this valance transformation i.e. divalent to trivalent,under pressure in the case of SmS Compound, by developing a theoretical model. The results have been used to investigate electronic phase transition pressure.

THEORY

In case of Sm compounds which have no conduction electron in ground state, thermal activation process gives carriers for conduction [4]. In this process acoustic scattering dominant. In the case of acoustic scattering, the electrical conductivity σ can be calculated by using the formula [5,6].

$$\sigma = ne\mu = \frac{1}{\rho} \qquad [1]$$

Where n is the carrier concentration, e is the electrical charge, □ is the carrier mobility and □ is the electrical resistivity.

The carrier concentration n can be calculated as [7]

$$n = \frac{2\left(2\pi m^* kT\right)^{3/2}}{h^3} \exp\left(-\frac{\Delta E}{2kT}\right) \qquad [2]$$

Where m* is the carrier effective mass, ΔE is the activation energy, k is the Boltzmann's Constant, h is the Plank's Constant and T is temperature.

The effective mass m* can be expressed in terms of lattice parameter 'a' and activation energy ΔE as [8]

$$\frac{m_0}{m^*} = 1 + \frac{2\lambda^2}{m_0 a^2 \Delta E} \qquad [3]$$

Where m_0 is the electron rest mass and $\lambda^2 = \hbar^2$

The mobility can be determined by using the formula [9]

$$\mu = \frac{3\varepsilon^2}{16\pi^2 m^* \left[\ln\left(1+x\right) - \frac{x}{1+x}\right]} \left(\frac{h}{e}\right)^3 \qquad [4]$$

Where

$$x=\left(\frac{h}{e}\right)^{2}\left(\frac{e}{m^{*}}\right)\left(\frac{3N}{8\pi}\right)^{1/3}$$

[5]

and N represent the impurity concentration, is given by

$$N=\frac{n^{2}}{2\left(\frac{2\pi m^{*}kT}{h^{2}}\right)^{3/4}\exp\left(-\frac{\Delta E}{2kT}\right)}$$

[6]

The dielectric constant ε can be calculated by using formula [7].

$$\varepsilon^{2}=\frac{13.53}{\Delta E}\,\frac{m^{*}}{m_{0}}$$

[7]

From equation (1) to (7), it is clear that we need only the value of activation energy to calculate different electrical parameters.

The pressure-resistivity study [10] on samarium chalcogenides suggested a linear closing of the energy gap, expressed as

$$\Delta E(P)=\Delta E(\mathrm{P}=0)-P\,\frac{\mathrm{d}(\Delta E)}{dP}$$

[8]

Where ΔE (P=0) = E_g is the energy gap or the magnitude of the 4f-5d conduction band separation, and $\frac{\mathrm{d}(\Delta E)}{dP}=\alpha$ is the rate of closing of energy gap with pressure.

RESULT AND DISCUSSION

Using the experimental values [11-13] of E_g and □, which are (0.15ev) and $\left(-10\,\frac{mev}{kbar}\right)$ respectively for SmS, we have calculated the values of activation energy as a function of pressure, and reported in table 2, up to the pressure where energy gap becomes zero.

The lattice constant (a) of SmS has been obtained as a =2d, where d is the natural interionic distance, calculated as

d = (ionic radius of Sm^{2+} (or Sm^{3+}) + ionic radius of S^{-})

Using the values of ionic radius [14] of different ions of interest as Sm^{2+}= 1.143 A^0, Sm^{3+} =0.964$A^0$and S^-= 1.34$A^{0.}$

We have calculated the natural interionic distance d and lattice constant a for SmS in both divalent and trivalent state, and reported in table-1, The value of lattice constant of SmS, in divalent state has been compared with experimental value, and found an excellent agreement.

The value of lattice constant at different pressure are calculated as [3]

$$a(P)=a_{0}(P=0)-2(\mathrm{r}^{3+}-r^{2+})\exp\left[-\frac{\Delta E(\mathrm{P})}{kT}\right]$$

[9]

Where T = 293 K and k is Boltzmann's constant.

Using the calculated values of ΔE and a, in equations (1-7), we have obtained the values of different electrical parameters as a function of pressure, up to the pressure where energy gap reduces to zero, and reported in table-2.

The table-2 revealed that lattice constant of SmS at the pressure P= 15 Kbar, where ΔE reduces to zero, becomes adjactly equal to its value in trivalent state, It confirmed the valance transition from divalent to trivalent under pressure.

The variation of carrier concentration with pressure of SmS is shown in figure 1. This figure revealed that carrier concentration first increases linearly with the increase in pressure up to 7 Kbar and remains almost constant between 7-8 Kbar, and above 8 Kbar pressure it decreases abruptly. It is also observed that at pressure P= 14 Kbar which is lower than the pressure needed for the complete conversion of Sm^{2+} into Sm^{3+}, the carrier concentration of SmS is found much lower than the its value at zero pressure. It shows that SmS suffer semiconductor-metal electronic phase transition up to the pressure 7-8 Kbar, and above this pressure it goes back towards the semiconducting state and retain it at nearly P= 13Kbar, where carrier concentration of SmS is found to be comparable to its value at zero pressure. The smaller values of carrier concentration of SmS above 13 Kbar pressure, is indicative to the semiconductor-insulator electronic transition at high pressures.

The variation of electrical resistivity with pressure, of SmS is shown in figure 2. This revealed that the resistivity decreases rapidly up to 6-7 Kbar pressure, which is consistent with the electronic phase transition, observed experimentally at 6.5 Kbar pressure [15]. Thus the present model confirm that in SmS semiconductor to metal phase transition takes place at about 6-7 Kbar pressure. Since the value of pressure needed for the complete conversion of Sm^{2+} to Sm^{3+} is about 15 Kbar, which is higher than the transition pressure 6-7 Kbar, it confirm that the metallic state of SmS is intermediate valent, which is consistent with the discussion of Jayaraman et. al. [12, 13]. Again an increase in the resistivity above 7kbar pressure is also indicative to the metal-semiconductor phase transition at higher pressures, which is consistent with the reverse transition reported by Bucher et. al. [16]. From the present work, we found that at P=11Kbar, SmS again show semiconducting behaviour, as the resistivity of SmS is comparable to its value at zero pressure.

Table -1 Natural Interionic distance (d) and lattice parameter (a=2d) of SmS.

d/A^0,when rare earth ion is in		**a/A^0, when rare earth ion is in**		
Divalent State	**Trivalent State**	**Divalent State**	**[11]**	**Trivalent State**
2.983	2.804	5.966	5.97	5.608

Table 2: The values of electrical parameters activation energy (ΔE), lattice parameter (a), carrier effective mass (m*), carrier concentration (n), dielectric constant (ε), impurity concentration (N), carrier mobility (μ), electrical conductivity (σ) and resistivity (ρ) at different pressures of SmS

P/K bar	**ΔE /e V**	**a/ A °**	**m * /1 0^{-31} (k g)**	**n /10^{23} (m^{-3})**	**ε**	**N /1 0^{3} ^{5} (m $^{-3}$)**	**μ /1 0^{-2} (m ^{2} V^{-1}S ec $^{-1}$)**	**σ /1 0^{2} (Ω $^{-1}$ m $^{-1}$)**	**ρ /10 $^{-4}$ (Ω m)**
0	0.1	5.	2.	1.63	4.	1.	3.	1	9.7
1	5	9	3	6	8	0	94	0.	8.7
2	0.1	6	5	1.84	3	2	3.	3	5
3	4	6	9	5	3	0.	87	1	7.9
4	0.1	5.	2.	2.06	4.	9	3.	1	8
5	3	9	2	5	8	9	78	1.	7.3
6	0.1	6	4	2.29	7	1	3.	4	7
7	2	5	0	1	4	0.	70	2	6.8
8	0.1	5.	2.	2.51	4.	9	3.	1	9
9	1	9	1	9	9	6	60	2.	6.5
10	0.1	6	1	2.73	1	3	3.	5	6
11	0	4	6	4	6	0.	48	2	6.3
12	0.0	5.	1.	2.92	4.	9	3.	1	9
13	9	9	9	3	9	3	34	3.	6.3
14	0.0	6	8	3.06	6	3	3.	5	9
15	8	3	8	8	0	0.	19	7	6.6
	0.0	5.	1.	3.14	5.	9	3.	1	3
	7	9	8	3	0	0	00	4.	7.2
	0.0	6	5	3.11	0	1	2.	5	0
	6	1	6	6	5	0.	78	1	8.3
	0.0	5.	1.	2.95	5.	8	2.	1	5
	5	9	7	7	0	6	53	5.	10.
	0.0	5	1	2.63	5	7	2.	2	64
	4	9	8	2	1	0.	23	3	15.
	0.0	5.	1.	2.11	5.	8	1.	1	78
	3	9	5	5	0	3	87	5.	30.
	0.0	5	7	1.41	9	0	1.	6	75
	2	6	4	2	6	0.	44	3	11
	0.0	5.	1.	0.60	5.	7	0.	1	6.1
	1	9	4	1	1	9	89	5.	9
	0.0	5	2	-	4	0	5	6	-
	0	1	5		3	0.	-	4	
		5.	1.		5.	7		1	
		9	2		1	4		5.	
		4	6		8	5		0	
		4	9		8	0.		9	
		5.	1.		5.	6		1	
		9	1		2	9		3.	
		3	0		3	6		8	
		3	6		2	0.		8	
		5.	0.		5.	6		1	
		9	9		2	4		1.	
		1	3		7	1		9	
		7	6		2	0.		7	
		5.	0.		5.	5		9.	
		8	7		3	7		3	
		9	5		0	7		9	
		2	9		8	0.		6.	
		5.	0.		5.	5		3	
		8	5		3	0		3	
		5	7		3	2		3.	
		7	5		5	0.		2	
		5.	0.		5.	4		5	
		8	3		3	1		0.	
		0	8		4	0		8	
		4	5		7	0.		6	
		5.	0.		5.	2		-	
		7	1		3	8			
		2	9		2	9			
		5	1		6	-			
		5.	-		-				
		6							
		0							
		8							

Figure : 1

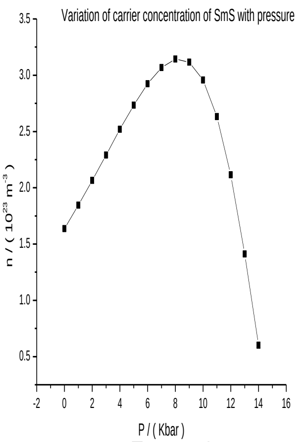
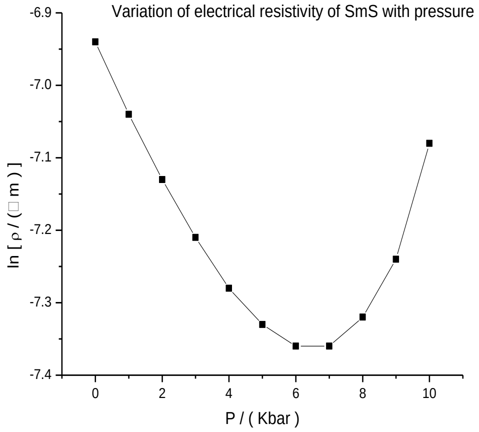


Figure : 2



CONCLUSION :

SmS undergo a valance transition from divalent to trivalent under pressure. The pressure needed to complete conversion of Sm^{2+} in to Sm^{3+} is found P=15 Kbar. The metallic state of SmS is found intermediate valent. In the process of valance transition from divalent to trivalent, SmS, undergo different types of electronic phase transition. Semiconductor to metal transition takes place at about 6-7 Kbar, metal to semiconductor at about 11 Kbar, and above P=14 Kbar, we have and above P=14 Kbar, we have predicted the semiconductor to insulator transition, All the result are compared with the exponential values and found excellent agreement between them.

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