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Analysis of Electrical Properties of Some Rare Earth Chalcogenides $Sm_{1-X}Eu_xS$ And $Sm_{1-x}y_xS$ Under Pressure

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ABSTRACT

The rare earth chalcogenides are some of structurally simplest materials and most of crystallize in the NaCl- type structure. In these compounds, most of rare earth ions are trivalent. Most of rare earth chalcogenides are governed by the nature of their f-electronic state. In the present paper, the study the effect of pressure on the electrical and structural properties of rare earth chalcogenides $Sm_{1-x}Eu_xS$ and $Sm_{1-x}Y_xS$. These compound are of current interest due to their potential application in the field non-liner optics, electro optic devices, composite laser. In this paper, we also developed a theoretical model to calculate the electrical parameters such as activation energy, carrier concentration, electrical resistivity, carrier mobility, electrical conductivity under the effect of pressure. The electronic phase transition are reported.

KEYWORDS : Activation energy carrier concentration, electrical resistivity and electronic phase transition.

INTRODUCTION - The rare earth Chalcogenides materials basically have structures depending on the nature of bonding. They have tetrahedral bonds and therefore form cubic or hexagonal structures [1]. They include not only covalent bonds but also ionic bonds. There are different class of semiconductors. One interesting class of semiconductor is rare earth chalcogenides. The study of rare earth monochalcogenides has received much attention because of their interesting properties and applications. They crystallize in the NaCl type structure and are semiconducting if the rare earth ion is in the divalent state and metallic if in trivalent state [2]. The atoms of all rare earth elements except Eu, Sm and Y exist in trivalent state. The divalent Eu, Sm and Y are particularly ideal as most of them are semiconducting and ionic [3, 4]. It is notable that the Samarium monochalcogenides are black semiconducting solid and they have shown continuous semiconductor to metallic transition under pressure at about 45 and 60 kbar in SmSe and SmTe respectively and discontinuous transition at 6.5 kbar in SmS [5]. These transitions in Samarium monochalcogenides can be used as a pressure sensor [6]. The rare earth chalcogenide

glasses finds applications in telecommunication devices, integrated optical systems, gas sensing and remote sensing devices [7-9]. Because of these importance, the understanding of the physical properties of these rare earth chalcogenides seems to be interesting and also requires more investigation on the effect of substitution of Eu and Y for Sm in SmS as well as the effect of pressure on these compounds. Even though, considerable information is now available on these physical properties, in many cases the data is limited. So, in this paper a theoretical model is developed for determining electrical properties of rare earth chalcogenide compounds. This theoretical study has been carried out on the systems $Sm_{1-x}Y_xS$ (x = 0.25, 0.5 and 0.7) and $Sm_{1-x}Y_xS$ (x= 0.25 and (0.75) at ambient conditions and under pressure from 0 to 16 kbar.

THEORY-

It is notable that these particular rare earth chalcogenide semiconductors are found to be in semiconducting state when the rare earth ion is divalent and metallic when it is trivalent [10]. It is reported from the magnetic susceptibility studies that for the compounds containing dipositive metal ions, the third valence electrons are highly localized in 4f levels. This would result in a full 4f shell for the ytterbium ions, half full for the europium ions and nearly half full for the samarium ions [11]. The highly localized f electrons do not contribute to the electrical conductivity [12]. The answer is in favour of acoustic scattering. In the case of acoustic scattering, the electrical conductivity σ can be calculated by using the formula [13-14].

$$\sigma = ne\mu = \frac{1}{\rho} \qquad (1)$$

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

The carrier concentration n can be calculated [15] from the carrier effective mass m* and activation energy ΔE by the expression.

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

Where k is the Boltzmann's constant, h is the Plank's constant and T is the temperature.

The effective mass m* can be given [16] in terms of lattice parameter and an activation energy ΔE as,

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

where m_0 is the electron rest mass and $\lambda^2 = \hbar^2$.The chalcogenides of Sm, Eu and Y are ionic semiconductors [17]. In ionic lattices, thermal motion and diffusion always give rise to vacant sites abandoned by one of the lattice ions or excess ions diffusing between the lattice cells. In this case, the ion is surrounded by electrostatic coulomb field which is weaker than that in a vacuum by a factor ε representing dielectric constant of the lattice [18]. An electron moving in this field is deflected from its initial path more strongly, the closer it approaches the ion, the longer it remains in the field which slows down its motion. So, the electron mobility [19] is determined by using the formula,

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

The value of x is calculated by the formula,

$$x = \left(\frac{h}{e} \right)^2 \left(\frac{e}{m^*} \right) \left(\frac{3N}{8\pi} \right)^{1/3} \qquad [5]$$

Where N represents the impurity concentration which is given by,

$$N = \frac{n^2}{2\left(\frac{2\pi m^* kT}{h^2} \right)^{3/4} \exp\left(-\frac{\Delta E}{2kT} \right)} \qquad [6]$$

The dielectric constant [20] ε is calculated by using the expression,

$$\varepsilon^2 = \frac{13.53}{\Delta E} \frac{m^*}{m_0} \qquad [7]$$

Thus, the electrical properties at ambient condition and under pressure have been calculated for $Sm_{1-x}Y_xS$ (x= 0.25, 0.5 and 0.7) and $Sm_{1-x}Y_xS$ (x=0.2 and 0.75) by using only two parameters lattice constant and activation energy.

The values of lattice constant at different pressures are calculated as [11]

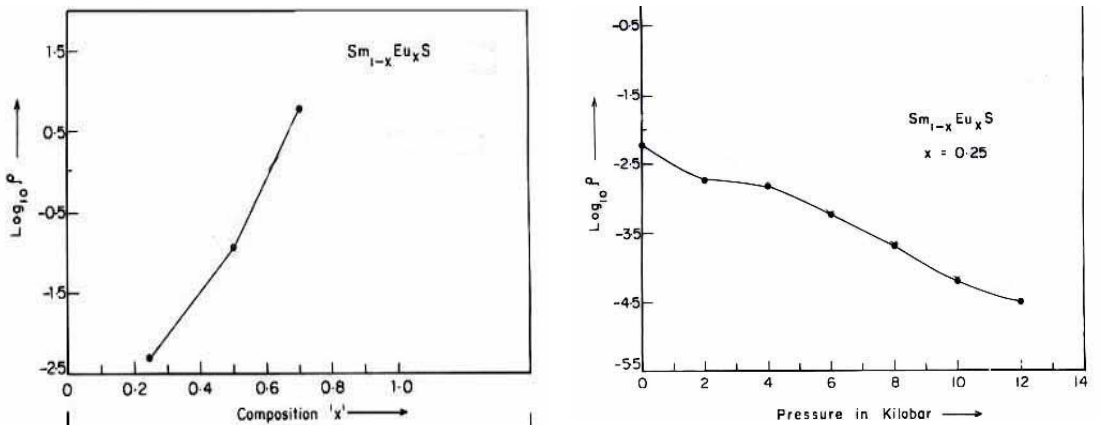
$$a(P) = a_0(P=0) - 2(r^{3+} - r^{2+})\exp\left[-\frac{\Delta E(P)}{kT}\right] \qquad [9]$$

Where T = 300 K and k is Boltzmann's constant.

Using the calculated values of ΔE and a, in equations (1-9), we have obtained the values of different electrical parameters as a function of pressure, up to the pressure where energy gap reduces to zero

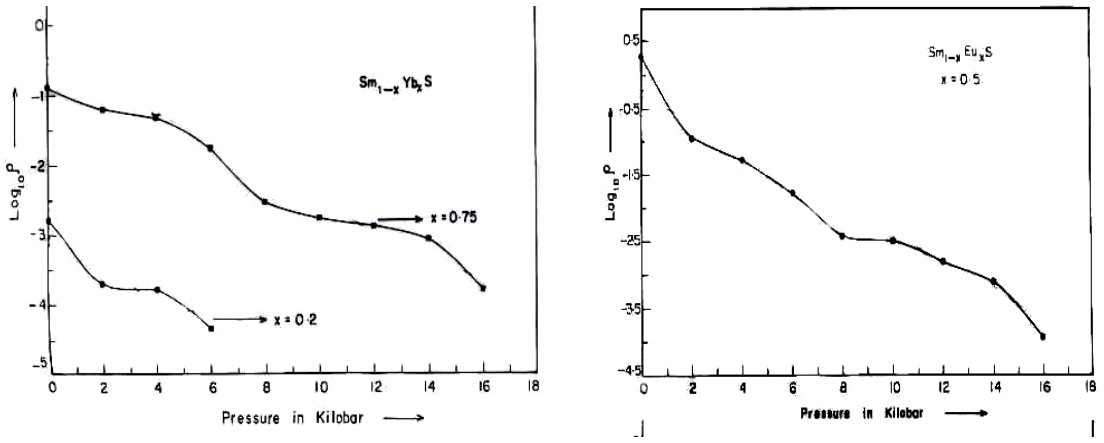
RESULT AND DISCUSSION :

The theoretical study has been made on ternary rare earth chalcogenide compounds as a function of composition x on $Sm_{1-x}Eu_xS$ (x= 0.20, 0.5 and 0.7) and $Sm_{1-x}Y_xS$ (x =0.2 and 0.75). And, the study has been extended for the same compounds under pressure from ambient to 16 kbar. Table 1 gives the values of lattice constant and activation energy used for the present study [21]. The Table 2 gives the calculated values of the electrical properties such as carrier concentration (n), carrier effective mass (m*), dielectric constant (□) and carrier mobility (□) of $Sm_{1-x}Y_xS$ (x=0.25, 0.5 and 0.7) and $Sm_{1-x}Y_xS$ (x= 0.2 and 0.75) as a function of composition x and under pressure. The electrical resistivity for $Sm_{1-x}Y_xS$ as a function of x in Fig.1a and the same as a function of a pressure for x= 0.25 for the same compound in Fig. 1b. The Figure 2a shows the theoretical electrical resistivity under pressure for $Sm_{1-x}Y_xS$ (x=0.5) and Fig 2b for $Sm_{1-x}Y_xS$ (x= 0.2 and 0.75). They are found to be in good agreement with each other. The limitation of this study is that it can be applied only to semiconductors and not to metals because of the dependence of the activation energy on the energy gap.



(a) (b)

Fig. 1 – The electrical resistivity values with the reported experimental values for $Sm_{1-x}Y_xS$ (a) as a function of x and (b) as a function of pressure for x= 0.25.



(a) (b)

Fig. 2–The electrical resistivity values with the reported experimental values as a function of a pressure for (a) $Sm_{1-x}Y_xS$ (x = 0.5) and (b) $Sm_{1-x}Y_xS$. (x= 0.2 and 0.75)

Table 1. The Values of lattice constant (a) and Activation energy (ΔEg) used for the present study [21]

Compound	**X**	**P kbar**	**a A⁰**	**Δ*Eg* eV**
	`	-	5.970	0.13
$Sm_{1-x}Y_xS$	0.50	-	5.965	0.24
(T = 300 K)	0.70	-	5.960	0.35
	0.25	0	5.970	0.180
	0.25	2	5.968	0.156
$Sm_{1-x}Y_xS$	0.25	4	5.966	0.132
(T = 300 K)	0.25	6	5.964	0.108
	0.25	8	5.962	0.084
	0.25	10	5.960	0.060
	0.25	12	5.958	0.036
	0.50	0	5.970	0.280
	0.50	2	5.969	0.256
	0.50	4	5.967	0.232
$Sm_{1-x}Y_xS$	0.50	6	5.967	0.208
(T = 300 K)	0.50	8	5.966	0.184
	0.50	10	5.964	0.160

	0.50	12	5.962	0.136
	0.50	14	5.960	0.112
	0.50	16	5.956	0.088
	0.20	0	5.900	0.90
$Sm_{1-x}Y_xS$	0.20	2	5.895	0.066
(T = 300 K)	0.20	4	5.890	0.042
	0.20	6	5.885	0.18
	0.75	0	5.759	0.240
	0.75	2	5.756	0.216
	0.75	4	5.753	0.192
	0.75	6	5.750	0.168
$Sm_{1-x}Y_xS$	0.75	8	5.746	0.144
(T = 300 K)	0.75	10	5.742	0.120
	0.75	12	5.740	0.096
	0.75	14	5.738	0.072
	0.75	16	5.735	0.024

Table 2. The calculated values of carrier concentration (n), carrier effective mass (m*), dielectric constant (□) and carrier mobility (□).

Compound	**X**	**P kbar**	**n**	**m*x10^{-31} kg.**	**□**	**□ m²v^{-1} Sec^{-1} □**
	0.25	-	2.286x10^{23}	2.125	4.928	4.949 x10^{-4}
$Sm_{1-x}Y_xS$	0.50	-	5.208x10^{22}	3.273	4.501	1.006 x10^{-4}
(T = 300 K)	0.70	-	8.683 x10^{21}	4.095	4.169	1.208 x10^{-4}
	0.25	0	1.245 x10^{23}	2.700	4.721	8.329 x10^{-3}
	0.25	2	1.531 x10^{23}	2.274	4.653	0.023
$Sm_{1-x}Y_xS$	0.25	4	2.236 x10^{23}	2.148	4.916	0.019
(T = 300 K)	0.25	6	2.808 x10^{23}	1.835	5.024	0.033
	0.25	8	2.279 x10^{23}	1.493	5.139	0.087

	0.25	10	3.381×10^{23}	1.119	5.262	0.308
	0.25	12	2.693×10^{23}	0.705	5.395	0.773
$Sm_{1-x}Y_xS$ (T = 300 K)	0.50	0	2.779×10^{23}	3.607	4.374	1.668×10^{-4}
	0.50	2	4.068×10^{23}	3.412	4.450	1.304×10^{-4}
	0.50	4	5.887×10^{23}	3.204	4.529	1.928×10^{-4}
	0.50	6	8.403×10^{23}	2.981	4.613	5.714×10^{-4}
	0.50	8	1.178×10^{23}	2.740	4.703	0.016
	0.50	10	1.612×10^{23}	2.478	4.797	0.013
	0.50	12	2.138×10^{23}	2.195	4.896	2.000×10^{-4}
	0.50	14	2.710×10^{23}	1.887	5.003	0.032
	0.50	16	3.209×10^{23}	1.550	5.005	0.162
$Sm_{1-x}Y_xS$ (T = 300 K)	0.20	0	3.101×10^{23}	1.555	5.065	0.014
	0.20	2	3.314×10^{23}	1.193	5.181	0.096
	0.20	4	2.873×10^{23}	0.796	5.304	0.145
	0.20	6	1.381×10^{23}	0.358	5.437	4.493
$Sm_{1-x}Y_xS$ (T = 300 K)	0.75	0	4.864×10^{23}	3.127	5.399	9.694×10^{-4}
	0.75	2	6.954×10^{23}	2.912	4.475	1.523×10^{-3}
	0.75	4	9.776×10^{23}	2.682	4.555	1.157×10^{-3}
	0.75	6	1.345×10^{23}	2.435	4.639	2.833×10^{-3}
	0.75	8	1.797×10^{23}	2.168	4.728	1.388×10^{-2}
	0.75	10	2.304×10^{23}	1.879	4.822	1.737×10^{-2}
	0.75	12	1.397×10^{23}	1.567	4.924	4.005×10^{-2}
	0.75	14	3.081×10^{23}	1.227	5.032	4.533×10^{-2}
	0.75	16	2.854×10^{23}	0.856	5.146	0.146

CONCLUSION :

We have perform an anylysis of the electronic phase transition in rare-earth ion substituted SmS under high pressure. The rolls of the size of substituent ion in valency transition. The Eu and Y substituted SmS ($Sm_{1-x}Eu_xS$ and $Sm_{1-x}Y_xS$). Where the a = 5.96A^0 has almost the same lattice constant $Sm_{1-x}Eu_xS$ and $Sm_{1-x}Y_xS$ at different constration of substituent ion. It is found that $4f^6$-5d energy gap increases and carrier concentration degrees with

the increase in concentration of substitution ion, and as a result the electrical resistivity increases. The present study has been restricted only to the semiconductors and not to metals. However, the theoretical study gives a reasonably good description of electrical properties as a function of composition and pressure, using only two parameters lattice constant and activation energy.

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