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ELECTRONIC PHASE TRANSITION IN SmTe UNDER THE EFFECT OF PRESSURE

[1]Dr. RAVINDRA KUMAR
[1]Department of Physics, Shri Ramlal Singh Mahavidhyalya Hardoi

ABSTRACT
A theoretical model is used to calculate electrical parameters such as activation energy, carrier concentration, carrier mobility, electrical conductivity and resistivity of SmTe, under the effect of pressure. The behaviour of these electrical parameters with pressure were analyzed to predict electronic phase transition pressure.
Keywords:- *Activation energy, carrier concentration, electrical resistivity and electronic phase transition.*

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 SmTe 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]

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

Where

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

and N represent the impurity concentration, is given by

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

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

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

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

$$\Delta E(P) = \Delta E(\mathrm{P} = 0) - P\frac{\mathrm{d}(\Delta E)}{dP} \qquad [8]$$

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 energy gap ΔE_g = 0.70 ev and $\alpha = -11.9\frac{mev}{Kbar}$, of SmTe in equation (8), 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. This pressure is found P=45.5 Kbar.

The lattice constant (a) of SmTe is 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 Te^-]

Using the value of ionic radius [14] of different ions of interest of Sm^{2+}= 1.143A^0, Sm^{3+} = 0.964A^0 and Te^-= 2.11A^0,

We have calculated the values of d and a for SmTe in both divalent and Trivalent state, and reported in table-1. The value of a is compared with experimental value, divalent state and found an excellent agreement between them therefore it is believed that the calculated value of a in trivalent state is also reliable.

The values of lattice constant at different pressures are calculated as [3]

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

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

The calculated values of a as function of pressure are reported in table-2.

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.

It is revealed from the table that lattice constant of SmTe at the pressure P=30 Kbar, where the energy gap reduces to zero, becomes adjactly equal to its value in trivalent state. It confirmed the valence transition from divalent to trivalent under pressure.

The variation of carrier concentration with pressure of SmTe shown in figure 1. This figure revealed that carrier concentration of SmTe remains constant up to P = 30Kbar, above this pressure up to 40 Kbar it increases slowly, and above 40 Kbar pressure it surprisingly increases rapidly and linearly upto 55 Kbar. Above this pressure it decreases abruptly. It shows that SmTe under goes semiconductor to metal transition upto 55Kbar, and above this pressure it goes back towards the semiconducting state, and expected to remain it at the pressure above 58.7 Kbar, which is nearly equal to the minimum pressure for the complete conversion of Sm^{+2} to Sm^{+3}. This discussion suggested that the metallic state of SmTe is interemediatevalent, which discussed by Svane et al. [15]. The small small concentration at zero pressure and comparable large energygap of SmTe are found to be main factors responsible for higher transition pressure for electronic phase transition.

The variation of electrical resistivity with pressure of SmTe is shown in figure-2. This figure revealed that resistivity decreases rapidly up to 50-55 Kbar, which is consistent with the electronic phase transition, as observed experimentally at about 52 Kbar [16] and observed two discontinuities in the curve at P=20 Kbar andf P= 45 Kbar, before the transition pressure [13] The rapid increases in resistivity above 55 Kbar, is indicative to that the metallic state of SmTe is intermediate valent, as the transition pressure P=50-55 Kbar is lower than the minimum pressure 58-59 Kbar, which is needed for the complete conversion of Sm^{2+} into Sm^{3+}

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

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**
3.253	3.074	6.506	6.60	6.148

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 SmTe

P /Kbar	**ΔE /eV**	**a /A°**	**m* /10^{-31} (kg)**	**n /10^{21}(m^{-3})**	**ε**	**N /10^{33} (m^{-3})**	**μ /($m^2V^{-1}Sec^{-1}$)**	**σ /10^2($\Omega^{-1}m^{-1}$)**	**ρ /10^{-3} (Ωm)**
0	0.700	6.5060	6.010	0.0125	3.571	1.62	0.86	1.72	0.58
5	0.641	5.5060	5.827	0.0384	3.674	1.57	0.90	5.55	0.18
10	0.581	5.5060	5.619	0.1190	3.790	1.54	0.94	17.92	0.056
15	0.522	5.5060	5.386	0.3591	3.915	1.53	0.96	54.95	0.018
20	0.462	5.5059	4.357	0.8563	3.743	1.38	0.76	104.6	0.0095
25	0.403	6.5059	4.047	2.4632	3.862	1.33	0.77	304.8	0.0033

30	0.343	6.5059	3.689	7.0259	3.997	1.27	0.78	873.8	0.0011
35	0.284	6.5059	3.283	18.954	4.143	1.20	0.77	2343	0.00043
40	0.224	6.5059	2.803	49.010	4.312	1.11	0.75	5880	0.00017
45	0.165	6.5054	2.857	162.060	5.071	1.12	1.06	27476	$3.63x10^{-5}$
50	0.105	6.5004	2.049	322.606	5.384	0.947	0.955	49209	$2.03 x10^{-5}$
55	0.046	6.4480	1.013	360.358	5.719	0.67	0.674	38880	$2.57 x10^{-5}$
56	0.034	6.4128	0.764	299.274	5.777	0.58	0.57	27338	$3.65 x10^{-5}$
57	0.022	6.3561	0.501	201.510	5.816	0.47	0.44	14085	$7.09 x10^{-5}$
58	0.010	6.2649	0.228	78.443	5.819	0.31	0.26	3234	$3.09 x10^{-4}$
58.5	0.004	6.2004	0.090	21.906	5.781	0.19	0.14	481	$2.1 x10^{-3}$
58.6	0.003	6.1880	0.068	14.674	5.802	0.17	0.11	271	$3.69 x10^{-3}$
58.7	0.001	6.1618	0.023	3.003	5.845	0.10	0.06	27	0.037
58.8	0.000	6.1480	0.000	0.000	-	-	-	-	-

Figure -1

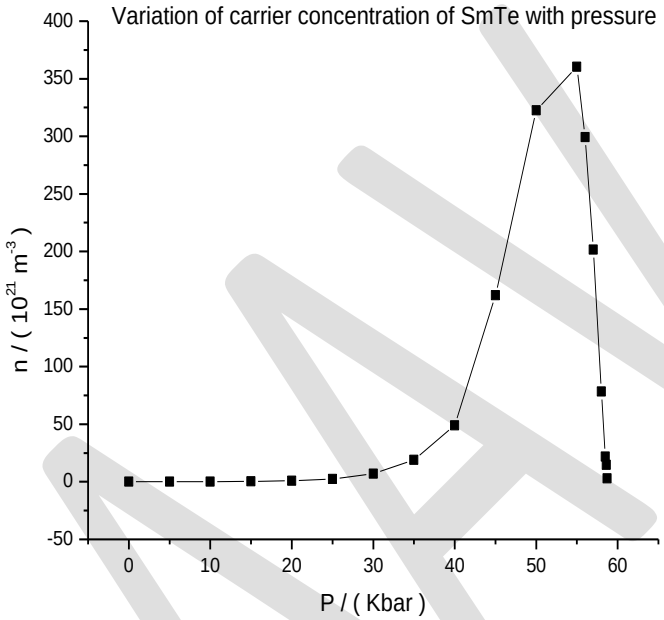
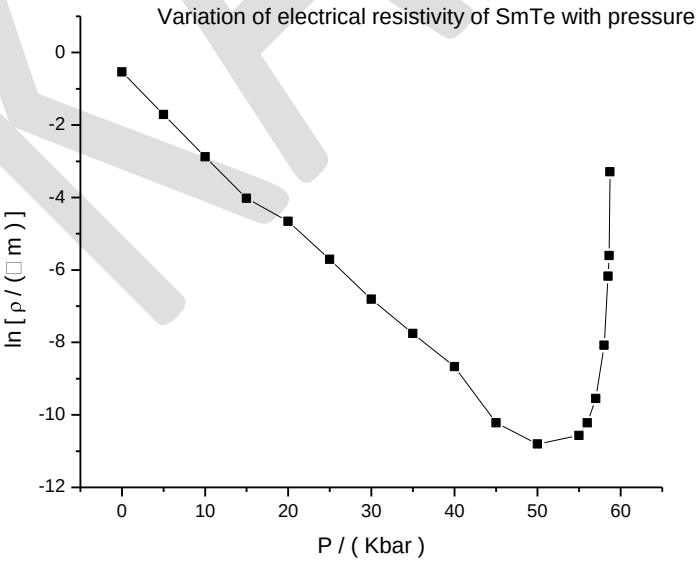


Figure -2



CONCLUSION

SmTe 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 30 Kbar. The metallic state of SmTe is found intermediate valent. In the process of valance transition from divalent to trivalent, SmTe, undergo different types of electronic phase transitions. Semiconductor to metal transition takes place at about 55-

60 Kbar, and metal to semiconductor at about 58.7 Kbar. All the result are compared with the experimental results and found excellent agreement between them.

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