

Magnetic and Electronic Transition in Samarium Chalcogenides

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ABSTRACT

In the present paper, we have been studied the magnetic and electronic transition in samarium chalcogenides [(SmX, X=S, Se and Te)] under the effect of pressure. We have reviewed relaxation time mean free path, magnetic susceptibility, electronic polarizability and dielectric constant by simple calculation. Our calculated values are close agreement with the experimental results.

Keywords: Magnetic Susceptibility, Electronic Polarizability, Dielectric Constant, Samarium Chalcogenides.

I. INTRODUCTION

The magnetic and electronic phase transitions have been studied in samarium chalcogenides [(SmX, X=S, Se and Te)]. The notable property of samarium chalcogenides is found to be in semiconducting and metallic. They have used in various practical application on the field of electro-optic component, electronics, telecommunications devices, integrated optical systems and remote sensing devices [1]. They have shown NaCl to CsCl phase transition at high pressure. The energy band gap has reduced at high pressure [2-4]. There were two kinds of transitions in SmS, a semiconductor-metal transition and a magnetic transition from the paramagnetic state to the antiferromagnetic ordered state. The magnetic transition [(SmX, X=S, Se and Te)] have occurred pseudo-gap in the metallic state and revealed paramagnetic behavior. It has shown the non-magnetic semiconducting state due to different lattice behavior and discontinuous transition at 6.5kbar [5-7].

The magnetic property have been applied electronic devices and biological systems such as GMR {(Giant magneto resistance) Magnetic field Sensor} and LED [8]. The SmS is used as a new kind of non-volatile memory and pressure induced semiconductor to metal transition occurred due to conversion of Sm²⁺ to Sm³⁺ (divalent to trivalent) of samarium ion [8-12]. The relaxation time and mean free path are helpful to understand the electrical conductivity under the effect of temperature. The calculated Fermi parameter and other parameters are shown in Table 1, 2 and 3 respectively. The calculated values are compared with the experimental results.

II. THEORETICAL CALCULATION

The samarium chalcogenides have occurred two kind of transition. One side semiconductor to metal transition, other sides have predicted the magnetic transition or paramagnetic state to the antiferromagnetic ordered state. SmS have shown a pseudo-gap in the metallic state and paramagnetic behavior in non-magnetic semiconducting state. The magnetic transition from the paramagnetic state at lower pressures to the antiferromagnetic ordered state at higher pressure. The Magnetic susceptibility is given by

$$\chi = 8 N \mu_m B^2 / k_B T \quad (1)$$

Where, μ_m be the molecular magnetic moment, N be the number of molecules, k_B be the Boltzmanns constant, B be the magnetic field and T be the temperature then,

$$k_B T = \approx (E_{j=1} - E_{j=0})$$

Now, the magnetic susceptibility in term of energy is given by

$$\chi = 8 N \mu_m B^2 / (E_{j=1} - E_{j=0}) \quad (2)$$

The magnetic properties with localized magnetic moments in term of Curie temperature and paramagnetic transition temperature T_p may be expressed in term of coordination number and exchange interaction can be expressed as

$$T_c = T_p = \frac{2(J+1)S^2}{3jk} z E_{ij} \quad (3)$$

Where, z be the coordination number of the system, J and S are quantum numbers of total angular and spin moments, E_{ij} = be exchange interaction between i and j and exchange interaction in term of Heisenberg can be expressed as,

$$H_{ij} = -2 E_{ij} \vec{S}_i \cdot \vec{S}_j \quad (4)$$

\vec{S} be the spin angular momentum, differentiating on pressure of the curie temperature is given by

$$\frac{dT_c}{dP} = \frac{dT_p}{dP} = \frac{2(J+1)S^2}{3jk} z \frac{dE_{ij}}{dP} \quad (5)$$

Using Hook's law in the form of $dV/V = K dP$, Then

$$\frac{d \ln T_c}{d \ln V} = \frac{d \ln T_p}{d \ln V} = \frac{d \ln E_{ij}}{d \ln V} \quad (6)$$

The samarium chalcogenides have shown pressure-induced transition from the semiconducting to the metallic state [14-17]. It is also called the black-golden transition; this appears at about 6.5 kbar at room temperature [14, 16-20]. The total energy in a crystal is given by

$$E_T = E_T^0 + P(V - V_0) + E_{elastic} \quad (7)$$

E_T^0 be the total energy in unstrained crystal, V_0 be the volume of crystal in initial state, V be volume of strained lattice, P be the pressure and $E_{elastic}$ be the elastic energy

Now the value of pressure P is given by

$$P = \left[\frac{\partial E_T^0}{\partial V} \right]_{V=V_0} \quad (8)$$

Elastic energy is given by

$$E_{elastic} = V/2 C_{ijkl} \epsilon_{ij} \epsilon_{kl} \quad (9)$$

For two suffix notations, $E_{elastic}$ is given by

$$E_{elastic} = V/2 C_{ij} \epsilon_i \epsilon_j \quad (10)$$

$$C_{ij} = \left[\frac{1}{V_0} \frac{\partial^2 E}{\partial \epsilon_i \partial \epsilon_j} \right]_{\epsilon = 0} \quad (11)$$

An electronic polarizability in term of dielectric constant is given by

$$\alpha = \frac{(\kappa - 1)M}{(\kappa + 2)D} \quad (12)$$

Where, M be the molecular weight, D be the density and κ be the dielectric constant of material

The dielectric constant in term of energy gap is given by

$$\kappa^2 = \frac{1.49 \times 10^{-31}}{\Delta E} m^* \quad (13)$$

The mean free path of the carriers λ is given by

$$\lambda = 2\tau v_{rms} \quad (14)$$

Where τ is relaxation time which is given by

$$\tau = \mu m^* / e = \lambda / v_f \quad (15)$$

Where v_{rms} is the root mean square velocity of the carrier and m^* is the carrier effective mass and the Fermi energy is given by

$$E_f = \frac{\hbar^2}{2m^*} k_f^2 \quad (16)$$

The carrier effective mass of hole is given by

$$m_h^* = 1.44m_e^*$$

And the Fermi temperature is given by

$$T_f = E_f / k_B \quad (17)$$

Where k_B is the Boltzmann constant.

The variation of band gap of samarium chalcogenides due to the localized f- level is given by

$$\Delta\epsilon_f = E(f^6d) - E(f^7) \quad (18)$$

Where $E(f^6d)$ the valance band is maximum and $E(f^7)$ is the conduction band minimum. The trivalent – divalent energy difference is given by

$$\Delta E = E(f^5) - E(f^6) \quad (19)$$

Where $(E(f^5))$ is the energy level of (f^5) level and $E(f^6)$ is the energy level of f^6 level.

The pressure and temperature dependence mean free path is given by

$$\lambda = K_T T / \sqrt{2} \pi p d_m^2 \quad (20)$$

Where p is the pressure and d_m is the molecular diameter

The electrical conductivity in term of Fermi velocity can be expressed as

$$\sigma = \frac{\lambda n e^2}{m v_f} \quad (21)$$

Where λ and v_f are the mean free path and Fermi velocity of carriers respectively.

The Fermi velocity of carriers is given by

$$v_f = \frac{\hbar k_f}{m} \quad (22)$$

Where, k_f is the radius of the fermi sphere which is given by

$$k_f = (3\pi^2 n)^{1/2} \quad (23)$$

Where, $n = N/V$ is the carrier density

The electrical conductivity in term of Fermi sphere can be expressed as

$$\sigma = \frac{\lambda S_f e^2}{\frac{3\pi^3 \hbar}{2\pi}} \quad (24)$$

Where S_f is the area of free carrier Fermi sphere given by

$$S_f = 4\pi k_f^2 \quad (25)$$

The calculated values of Fermi parameter and magnetic transition parameter are given in table1, 2, and 3. The graph plotted frictional volume versus pressure have shown in fig. 1 due to pressure induced semiconductor to metal transition occurred due to conversion of Sm^{2+} to Sm^{3+} (divalent to trivalent) of samarium ion

III.CONCLUSIONS

In this method relaxation time, mean free path and electrical conductivity of samarium chalcogenides have been calculated. From equation (1) to equation (3) we have described the magnetic susceptibility, Curie temperature and paramagnetic temperature. The value of relaxation time, conductivity and mean free path is shown in table 1. Equation (7) ,(12) and (13) have shown the energy, electronic polarizability and dielectric constant of given chalcogenides. The equation (14) to (35) have indicated the Fermi parameters.

The relaxation time and mean free path are helpful to understand the electrical conductivity. SmS presents a pseudo-gap in the metallic state and shows paramagnetic behavior, while it is non-magnetic in the semiconducting state. This has revealed by measuring the magnetic susceptibility. Using above equations we have calculated the different parameter of given chalcogenides. Those calculated values are shown in table1, 2 and3. The graph plotted frictional volume versus pressure have shown in fig. 1 due to pressure induced semiconductor to metal transition occurred due to conversion of Sm^{2+} to Sm^{3+} (divalent to trivalent) of samarium ion. The magnetic transition from the paramagnetic state at lower pressures to the antiferromagnetic ordered state at higher pressure. The calculated values are close agreement with the experimental results.

Table 1: The Fermi parameter of samarium chalcogenides

Compounds	Relaxation time sec. 10^{-16}	Mean free path Calc. meter. 10^{-11}	Conductivity Calc $\Omega^{-1} m^{-1} 10^{-2}$
SmS	0.11	0.25	0.67
SmSe	7.19	0.16	6.90
SmTe	2.93	6.52	13.18

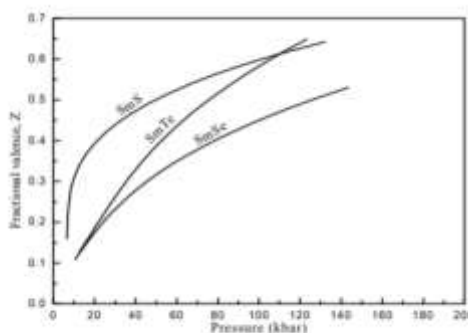


Fig.1. Fractional valence Vs Pressure

Table 2: The values of magnetic susceptibility, electronic polarizability and dielectric constant.

Compound	Magnetic susceptibility $Emu/mole * 10^{-3}$	Electronic polarizability	Dielectric constant
SmS (paramagnetic)	9.48	7.19	Exp.6.48 at p=0, calc.5.16.
SmSe (paramagnetic)	7.90	6.75	Exp.6.74 at p=0, Calc.4.1
SmTe (paramagnetic)	7.16	11.59	Exp.7.20 at p=0, Calc.3.01

Table 3:Exp. value of carrier effective mass Energy band gap carrier effective mass of hole.

Compound	Carrier effective mass(m^*)kg at P=0 EXP.	Mass of hole $m_h^* = 1.44 m^*$ Calc..	Exp. ΔE in eV
SmS (paramagnetic)	1.43	2.07	0.40
SmSe (paramagnetic)	4.70	6.77	0.40
SmTe (paramagnetic)	4.61	6.63	0.46

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