LEC Journal 2024, 6(1): 45-49
ISSN: ISSN: 2565-5205 (print)

Research Article

STUDY OF COMPRESSIBILITY AND ATOMIC RADIUS OF LEAD SULFIDE (PBS)

D. R. Adhikari[1, *], S. K. Adhikari[2] and S. P. Baral[3]

[1]Graduate School of Science and Technology, Central Department of Physical and Mathematical Sciences , Mid- West University, Birendranagar, Surkhet Nepal
[2]Department of Physics,Birendra Multiple Campus,Bharatpur, Chitwan(Tribhuvan University) Nepal.
[3]Department of Physics,Amrit Science Campus , Thamel,Kathmandu (Tribhuvan University) Nepal.
E-mail: dipak74adhikari@gmail.com

Received: 17th Sept., 2023 Revised: 29th Dec., 2023 Accepted: 15th Jan, 2024

Abstract

The purpose of the paper is to study the relationship between temperature and various physical properties of Lead Sulfide (PbS) such as atomic radius, nanoparticle size, compressibility, energy band gap, and density. It is noted that PbS has a narrow band gap at low temperatures and acts as a semiconductor. The atomic radius is found to be linearly dependent on temperature. The size of the nanoparticle is influenced by the energy band gap and the effective mass of electrons and holes in the material. The unique properties of PbS have various applications in the fields of optoelectronics, thermo-electronics, and nanotechnology. We have used various parameters to calculate the atomic radius, bulk modulus, nanoparticle size, and compressibility, which play an important role in recent technologies and devices. The results are in good consistent with experimental data.

Keywords: Lead sulfide, atomic radius and compressibility

1. Introduction

The lead sulfide (PbS) is narrow band gap (0.2-0.4 eV) semiconductor at lower temperature. The lead sulfide (PbS) has unique structural and electronic properties[1, 2]. It has wide technological applications and uses to fabricate in various optoelectronic, spintronic, thermo-electronic devices, nanoscience, nanotechnology[3,4]. The theoretical and experimental studies have been performed on their structural and electronic properties .Those properties have been studied in terms of atomic radius, nanoparticle size, energy band gap and compressibility. The atomic radius and energy band gap are function of temperature [5,6]. The calculated values are compared with experimental results.

2. Theoretical Methodology

The lead sulfide (PbS) is narrow band gap semiconductor. The energy band gap and atomic radius are the function of temperature [7,8]. The crystal structure of lead sulfide is NaCl (B1) type.The coordination number of lead sulfide is 6. The electronic and structural properties were

studied in terms of atomic radius, and energy band gap with temperature. Various experimental studies have been found the lead sulfide exhibit strongly anharmonic lattice dynamics[9,10].The Coulomb interaction and short range two-body interactions between lead sulfide is given by

$$U_{ij}= \frac{Q_i Q_j}{R_{ij}} + Xe^{\frac{-R_{ij}}{\rho}} - \frac{D_6}{R_{ij}^6} \quad (1)$$

In equation (1), The first term describe the long range coulomb interaction between two charges .The second term indicates the repulsive potential. Third term represent the dipole- dipole interaction Abuckingham potential. Where X , ρ and D_6 are fitting parameters but the short range cation –cation interactions are ignored. The thermodynamics the enthalpy in lead sulfide NaCl (B1) structure is given by

$$H=E+PV \quad (2)$$

The Gibbs free energy is given by

$$G=H-TS \quad (3)$$

According to the Classical Heisenberg Model,the Hamiltonian is given by

$$H= -\frac{1}{2}\sum \vec{S}_i \left(J_1 \sum_j^{nn} \vec{S}_j + J_2 \sum_j^{nnn} \vec{S}_j\right) \quad (4)$$

With normalized spin vectors $\vec{S}_i$ and $\vec{S}_j$ and where summation over nearest neighbor and next nearest neighbor.

The energy gap is related with temperature and lattice parameter by following relation

$$\left[\frac{\partial E_g}{\partial T}\right]_{LATTICE} = \left(\frac{\partial E_g}{\partial a}\right)\left(\frac{\partial a}{\partial T}\right) \quad (5)$$

The forbidden width is a linear function of temperature [11,12] then

$$E_g(T) = E_g(0)+\frac{\partial E_g}{\partial T}T \quad (6)$$

$E_g(0)$ be the energy at absolute zero

The atomic radius of lead sulfide is the function of temperature then

$$R(T) = A + BT + CT^2 \quad (7)$$

Where A, B and C are the fitting parameter.

The lattice parameter in term of atomic radius is given by following relation

$$a(T) = 2\sqrt{2}\ \mathrm{R(T)}$$

The lattice parameter for any composition of lead sulfide is given by,

$$a = (1-x)a_{Pb-S} + xa_{Pb-S} \quad (8)$$

a_{Pb-S} be the lattice parameter of lead(Pb) and (S) compound.

The bulk modulus

$$B_0 = \left(\frac{V\partial^2 E}{\partial V^2}\right)_{V_0} \quad (9)$$

Again,the value of B bulk modulus (B_0) in term of C_{11} an C_{12} is given by

$$B_0 = \frac{C_{11}+2C_{12}}{3} \quad (10)$$

The compressibility K = $1/B_0=\frac{3}{C_{11}+2C_{12}}$

The particle size of lead sulfide (PbS) has been calculated by effective mass of hole and electron. Now the carrier effective mass of hole is given by

$$m_h = 1.44m_e \quad (11)$$

Where, m_e be the carrier effective mass of electron,

Generally, electrons and holes are in conduction band and valence band respectively. Both are

achieved the lowest energy of an optical transition from valence band to conduction band then the expression for the radius of nanoparticle is given by

$$R^{+2} = \frac{h^2}{8(\Delta E - \Delta E_g)}\left[\frac{1}{m_e} + \frac{1}{m_h}\right] \quad (12)$$

Where, ΔE be the energy gap at 4.2 K and 300 K respectively, $\Delta E_g energy gap at 0K$

The crystal structure and the variation of lattice parameter with temperature are shown in Fig 1 and 2 respectively. The lattice parameter is the linear function of temperature. The value of atomic radius and nanoparticle are calculated. The calculated atomic radius, nanoparticle size and compressibility are shown in table 1. Finally our calculated values are close agreement with the experimental results.

3. Results and Discussion

In this method, the atomic radius, nanoparticle size, compressibility, energy band gap and density have been studied in lead sulfide (PbS) .The atomic radius and nanoparticle size in lead sulfide has been calculated and studied under the effect of temperature. We have calculated atomic radius with help of fitting parameter, nanoparticle size and compressibility of lead sulfide (PbS) . The values of atomic radius, nanoparticle size, bulk modulus, energy band gap and compressibility are shown in table 1. The variations of lattice parameter with temperature are predicted in Fig 1. Our calculated parameters are close agreement with experimental result.

Table 1. The values of atomic radius, energy band gap, nanoparticle size and compressibility of lead sulfide (PbS)

Temperature K	PbS $R(t) = \frac{a}{2\sqrt{2}}$ A=2.082 (Å) B=0.367×$10^{-4}(\text{ÅK}^{-1})$ C=2.938×$10^{-8}(\text{ÅK}^{-2})$ Calc. Exp.[7-12]	Compound- PbS (Lead Sulfide)	
0	2.082	Energy gap $(\Delta E_g)at0K$ Exp.[16]	0.290
4	2.082	Energy gap $(\Delta E_g)at4K$ eV	0.20
75	2.085	Particle Size (R) nm	5.42
150	2.088	Energy gap $(\Delta E_g)at$ 300K eV	0.26
225	2.091	Particle Size (R) nm	9.39
300	2.095	Density kg/m^3	7.61
375	2.100	Bulk modulus	50.33
400	2.101	Compressibility	.019

525	2.109	C_{11}	124
600	2.114	C_{12}	14

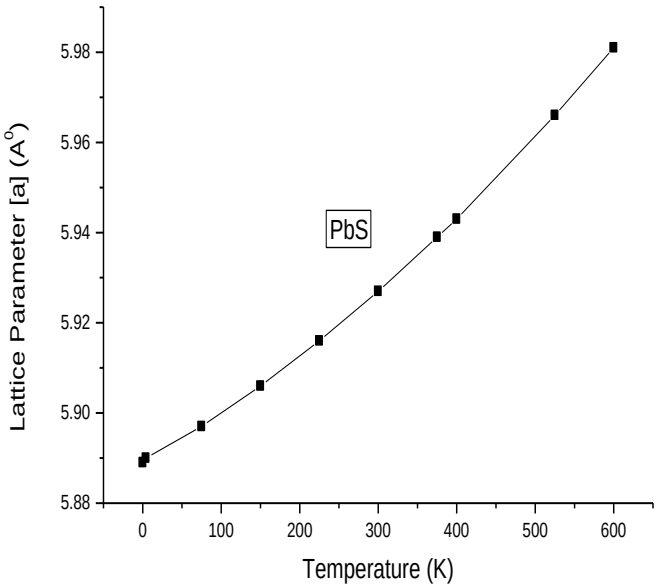

Fig.2. Lattice parameter with temperature for PbS

References

[1] A. Paul and G. Klimeck, "Atomistic study of electronic structure of PbSe nanowires," Applied Physics Letters, **98**, 21, (2011). Article ID 212105.

[2] A. Grzechnik and K. Friese. "Pressure-induced orthorhombic structure of PbS," Journal of Physics Condensed Matter, **22**, 9, (2010). Article ID 095402.

[3] G. Rousse, S. Klotz, A. M. Saitta et al., "Structure of the intermediate phase of PbTe at high pressure," Physical Review B, **71**, 22, (2005). Article ID 224116.

[4] S. V. Ovsyannikov, V. V. Shchennikov, A. Y. Manakov et al., "High-pressure X-ray diffraction study of ternary and nonstoichiometric PbTe and PbSe crystals," Physica Status Solidi (B) Basic Research, **244**, 1, 279–284, (2007).

[5] R. J. Ellingson, M. C. Beard, J. C. Johnson, P. Yu, O. I. Micic, A. J. Nozik, A. Shabaev, and A. L. Efros, "Highly efficient multiple exciton generation in colloidal PbSe and PbS quantum dots," Nano Lett. **5**, 865–871 (2005).

[6] Y. Bencherif, A. Boukra, A. Zaoui, and M. Ferhat, "Highpressure phases of lead chalcogenides," Materials Chemistry and Physics, **126**, 3, 707–710 (2011).

[7] Z. M. Gibbs, H. Kim, H. Wang, R. L. White, F. Drymiotis, M. Kaviany, and G. Jeffrey Snyder, "Temperature dependent bandgap in

PbX(X=S,Se,Te)", Applied Physics Letters 103. (2013).

[8] J. P. Heremans, V. Jovovic, E. S. Toberer, A. Saramat, K. Kurosaki, A. Charoenphakdee, S. Yamanaka, and G. J. Snyder, "Galv. properties and electronic structure of iron doped PbTe" ,Science **321**, 554, (2008) .

[9] Z. T. Tian, J. Garg, K. Esfarjani, T. Shiga, J. Shiomi, and G. Chen, "Entropically stabilized local dipole formation in lead chalcogenides", Phys. Rev. B 85, (2012).

[10] E. S. Bozin, C. D. Malliakas, P. Souvatzis, T. Proffen, N. A. Spaldin, M. G. Kanatzidis, and S. J. L. Billinge, "Entropically stabilized local dipole formation in lead chalcogenides", Science **330**, 1660, (2010).

[11] A. J. Miller, G. A. Saunders, and Y. K. Yogurtcu, "Pressure dependence of elastic constants of PbTe and SnTe", J. Phys. C **14**, 1569, (1981).

[12] R. Dornhaus, G. Nimtz, and B. Schlicht, "Thermal physics of lead chalcogenides PbS, PbSe and PbTe from first principles" ,Springer Tr Mod Phys **98**, R5, (1983).