International Journal of
Advances in Scientific Research and Engineering (ijasre)

E-ISSN : 2454-8006

DOI: 10.31695/IJASRE.2019.33266

Volume 5, Issue 6
June - 2019

Energy Band Gap under the Effect of Temperature in Lead Sulfide (PbS)

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ABSTRACT

In the present paper, the energy band gaps with temperature have been studied in lead sulfide (PbS). The energy band gap is a linear function of temperature. The values of the energy band gap in different temperature are calculated. The calculated values are a close agreement with the experimental results.

Keywords: Energy band gap, Lead sulfide.

1. INTRODUCTION

In most semiconductors the electron–phonon interactions lead to an increase the energy band gap with decrease in temperature. In lead sulfide the reverse effect occurred due to harmonic and anhormonic contribution of electron - phonon interaction. The lead sulfide (PbS) has unique structural and electronic properties. It has wide technological applications and uses to fabricate in various optoelectronic, spintronic, thermo- electronic devices, nanoscience, nanotechnology [1–9]. The energy band gap decrease with decrease in temperature [10-14]. The larger diameter of lead sulfide made to decrease the energy band gap with decrease in temperature. The theoretical and experimental studies have been performed on their structural and electronic properties [15-24].Those properties have been studied in terms of energy band gap and harmonic and anhormonic contribution of electron-phonon interaction . The energy band gap is the function of temperature [17-25]. The calculated values are close agreement with experimental results.

2. THEORETICAL METHODOLOGY

In most of the semiconductors the electron–phonon interactions lead to an increase the energy band gap with decrease in temperature. In lead sulfide have occurred the reverse effect due to harmonic and anhormonic contribution of electron - phonon interaction.The lead sulfide (PbS) is narrow band gap semiconductor. The energy band gap is the function of temperature [21-22]. The crystal structure of lead sulfide is NaCl (B1) type. It is shown in fig 1.The coordination number of lead sulfide is 6. The electronic and structural properties were studied in terms of energy band gap with temperature [20-23]. Various experimental studies have been found the lead sulfide exhibit strongly anharmonic lattice dynamics [24].The Coulomb interaction and short range two-body interactions between lead sulfide is given by

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

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

The total energy band gap due to harmonic and anharmonic contribution of electron- phonon interaction is given by

$$\frac{\partial E_g}{\partial T}=\left(\frac{\partial E_g}{\partial T}\right)harmonic+\left(\frac{\partial E_g}{\partial T}\right)anharmonic \quad (2)$$

In eq.(2) first term be the band gap due to harmonic and second term energy band gap due to anharmonic term

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

$$[\frac{\partial E_g}{\partial T}]_{LATTICE} = (\frac{\partial E_g}{\partial a})\,(\frac{\partial a}{\partial T}) \quad (3)$$

The forbidden width is a linear function of temperature [31-33] then

$$E_g(T) = E_g(0) + \frac{\partial E_g}{\partial T}\,T \quad (4)$$

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

$\frac{\partial E_g}{\partial T}$ be the slope from the graph

The crystal structure and the variation of energy gap with temperature are shown in Fig 1 and 2 respectively. The energy band gap is the linear function of temperature. The values of energy band gap in different temperature are calculated. The calculated values are shown in table 1. Finally our calculated values are close agreement with the experimental results.

3.RESULTS AND DISCUSSION

In this method, energy band gap with temperature have been studied and calculated in lead sulfide (PbS) under the effect of temperature. The values of energy band gap in different temperature are shown in table 1. The variations of energy band gap with temperature are predicted in Fig 2.The larger diameter of lead sulfide made to decrease the energy gap with decrease in temperature under the effect of electron- phonon interaction. Our calculated parameters are close agreement with experimental result.

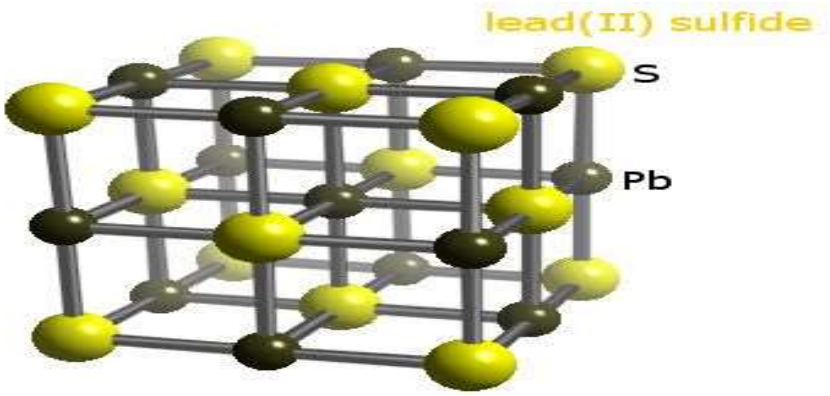

Fig 1 Crystal structure of lead sulfide (PbS)

Table 1. The values of energy band gap with temperature in lead sulfide (PbS)

Temperature (K)	Energy band gap Exp.[16]	Energy band gap Calc.
0	1.083	1.083
50	1.085	1.088
100	1.092	1.091
150	1.096	1.098
200	1.102	1.103
250	1.105	1.108
300	1.110	1.113

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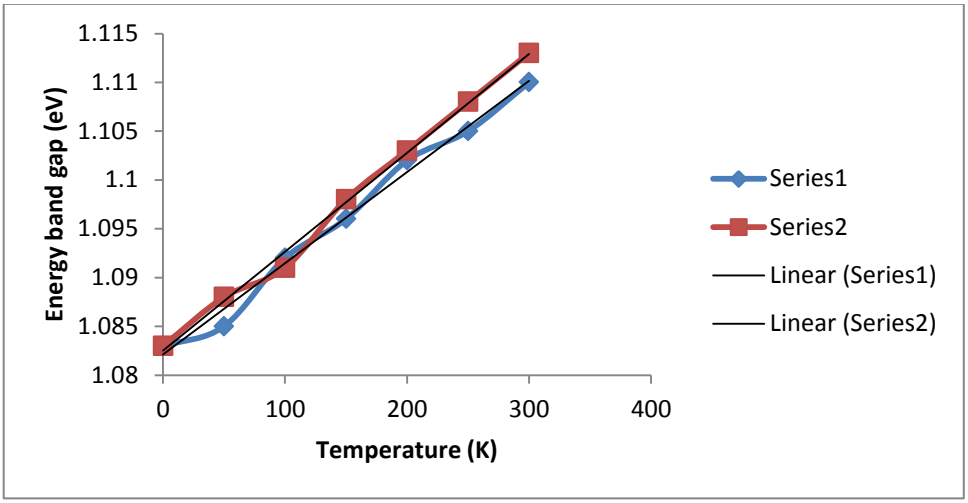

Fig.2. Energy band gap with temperature for PbS

4. CONCLUSION

In lead sulfide the reverse effect of semiconductor have occurred due to harmonic and anhormonic contribution of electron - phonon interaction. It is narrow band gap semiconductor. The energy band gap is the linear function of temperature. The calculated values of energy band gap are close agreement with the experimental result.

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