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

E-ISSN : 2454-8006

DOI: 10.31695/IJASRE.2019.33208

Volume 5, Issue 5
May - 2019

Study of Thermodynamic Parameter and Elastic Constants in Lead Chalcogenides

Dipak Raj Adhikari[1], S.K.Adhikari [2] and Hari Prasad Lamichhane[3]

1. Department of Physics, Amrit Science Campus, Tribhuvan University

2. Department of Physics, Birendra Multiple Campus, Tribhuvan University

3. Central Department of Physics, Tribhuvan University

Nepal

ABSTRACT

In the present paper, we have been studied the elastic constants of lead chalcogenides [(PbX, X= Se and Te)] with help of lattice constants. The elastic constant such as Young's modulus, bulk modulus, shear modulus and Poisson ratio in lead chalcogenides [(PbX, X= Se and Te)] are calculated. The calculated values are a close agreement with the experimental results.

Keywords: Lead chalcogenides, lattice constant, Elastic constant.

I. INTRODUCTION

The Mechanical properties of PbSe and PbTe are shown the n-type and p-type semiconductor in the NaCl Structure. The PbSe and PbTe are used in thermoelectric devices due to their brittle nature. They have unique structural and electronic properties. They have wide technological applications and used to fabricate in various optoelectronic, spintronic, thermo- electronic devices, nanoscience, nanotechnology [1–9]. The lead chalcogenides (Pb X, X=Se and Te) are narrow band gap (0.2-0.4 eV) semiconductors at lower temperature. The theoretical and experimental studies have been performed on their mechanical properties and typically has a lower hardness [10–17].Those properties have been explained in terms of elastic constant [17].The elastic constant such as Young's moduli (Y),bulk moduli (B),shear moduli (G) and Poisson ratio (σ) in lead chalcogenides [(PbX, X= Se and Te)] are calculated with help of lattice constants and using the Reuss-Voigt-Hill method [18-20] . The calculated values are close agreement with the experimental results.

2. THEORETICAL CALCULATION

The elements selenium, and tellurium are called chalcogens and their compounds are referred as chalcogenides.The crystal structure of lead chalcogenide is NaCl (B1) type. The coordination number and bond between lead (Pb) and chalcogen{X= Se,Te}are 6 and ionic respectively. The mechanical properties were studied in terms of lattice constant and Reuss-Voigt-Hill method [18-20]. Various experimental studies have been found the lead chalcogenides exhibit strongly anharmonic lattice dynamics [21]. The thermodynamics the enthalpy in NaCl (B1) structure is given by

$$H=E+PV \quad (1)$$

The Gibbs free energy is given by

$$G=H-TS \quad (2)$$

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

$$\mathcal{H}= -\frac{1}{2}\sum \vec{S}_i \left(J_1 \sum_j^{nn} \vec{S}_j + J_2 \sum_j^{nnn} \vec{S}_j\right) \quad (3)$$

With normalized spin vectors $\vec{S}_i$ and $\vec{S}_j$ and where summation over nearest neighbor and next nearest neighbor.
The energy differences in term of J_1 and J_2 are given the following relation,

$\Delta E_1 = 8J_1$

$\Delta E_2 = 6J_1 + 6J_2$

The enthalpy of lead chalcogenide crystal is defined as

$$H \approx H_{ELEC} + H^0_{VIB} + H_{VIB}(T) + H_{ROT}(T) + H_{TRANS}(T) + RT \quad (4)$$

$where,$ H_{ELEC} be the electronic component of enthalpy, H^0_{VIB} be the vibrational component of enthalpy (main State), $H_{VIB}(T)$ be the vibrational component of enthalpy, $H_{ROT}(T)$ be the rotational component of enthalpy, $H_{TRANS}(T)$ be the trans. component of enthalpy, R be the universal gas constant and T be the temperature.

The entropy of the crystal is the sum of following component ,

$$\Delta S = S_{TRANS} + S_{VIB} + S_{ELECT} - nR[\ln(nN_0) - 1] \quad (5)$$

Where, N_0 be the Avogadro constant and N be the number of moles in molecules.

The Gibbs free energy of the crystal in term entropy of individual members of molecules reagent Pb and X=(Se and Te) then,

$$\Delta G = H_{Pb} - H_X + \frac{1}{2}\sum_{i\varepsilon Pb} h\nu_i - \frac{1}{2}\sum_{j\varepsilon X} h\nu_j - T\,(S^{Pb}_{VIB} - S^{X}_{VIB} + S^{Pb}_{ROT} - S^{X}_{ROT} + S^{Pb}_{TRANS} - S^{X}_{TRANS}) \quad (6)$$

Where, H_{Pb} be the enthalpy of lead, H_X be the enthalpy of chalcogen[X=Se and Te], S^{Pb}_{VIB} be the entropy of lead due to vib. component, S^{X}_{VIB} be the entropy of chalcogen due to vib. component, S^{Pb}_{ROT} be the entropy of lead due to rot. component,S^{X}_{ROT} be the entropy of chalcogen due to rot. component,S^{Pb}_{TRANS} be the entropy of lead due to trans. Component and S^{X}_{TRANS} be the entropy of chalcogen due to trans. component.

The mechanical properties in term of elastic constant such as bulk modulus (B) is given by

$$B = \frac{1}{3}(c_{11} + 2\,c_{12}) \quad (7)$$

Where, c_{11}, and c_{12} are elastic constants.

The value of Poisson ratio is given by

$$\sigma = \frac{3B-2G}{2(3B-G)} \quad (8)$$

where ,B be the bulk modulus, G be the average shear modulus and G be the arithmetic mean of Voigt G_v and Reuss G_R,

Those values are expressed in term of elastic constants (c_{11}, c_{12} and c_{44}) are given by

$$G_v = \frac{1}{5}(c_{11} - c_{12} + 3c_{44}) \quad (9)$$

$$G_R = \frac{5(c_{11}-c_{12})c_{44}}{3(c_{11}-c_{12})+4c_{44}} \quad (10)$$

The value of Young's modulus in term of bulk modulus and shear modulus is given by

$$Y = \frac{9\,BG}{3B+G} \quad (11)$$

The calculated values of Young's moduli (Y),bulk moduli(B),shear moduli(G) and Poisson ratio (σ) in lead chalcogenides (PbX, X= Se and Te) are listed in table 1. and table 2. Our calculated values are close agreement with the experimental results.

3. CONCLUSIONS

The objective of the study was to understand some of thermodynamic parameter and elastic constants with help of lattice constants. In this paper, we have studied and analyzed the mechanical properties such asYoung's modulus (Y),bulk modulus

DOI: 10.31695/IJASRE.2019.33208

(B),shear modulus (G) and Poisson ratio (σ) in lead chalcogenides [(PbX, X= Se and Te)] with help of lattice constants and Reuss-Voigt-Hill method.Our calculated values of lattice constants are predicted in table 1.and table 2.The graph plotted between bulk modulus versus PbSe and PbTe is shown in fig1.Another graph predicted Young's modulus versus PbSe and PbTe (chalcogenide Compound) in fig 2.Finally,our calculated values of elastic constants are close agreement with experimental result.

Table 1.The values of lattice constant and bulk modulus (B) for lead chalcogenide [(PbX, X= Se and Te)]

Compound	c_{11}	c_{12}	c_{44}	Bulk modulus(B) GPa Exp.[22-23]	Bulk modulus(B) GPa Calc.
PbSe	123.75	19.34	15.92	52.2	53.94
PbTe	105.32	7.02	13.22	38.39	39.79

Table 2. The values of Young's modulus (Y) , shear modulus (G) and Poisson ratio for lead chalcogenide [(PbX, X= Se and Te)]

compound	Young's modulus(Y) GPa Exp . [22-23]	Young's Modulus (Y) GPa Calc.	Shear modulus(G)GPa Exp. [22-23]	Shear Modulus(G) GPa Calc.	Poisson ratio (σ) Exp. [22-23]	Poisson ratio (σ) Calc.
PbSe	57.65	67.73	21.9	26.24	0.315	0.290
PbTe	58.05	48.83	22.95	18.85	0.264	0.296

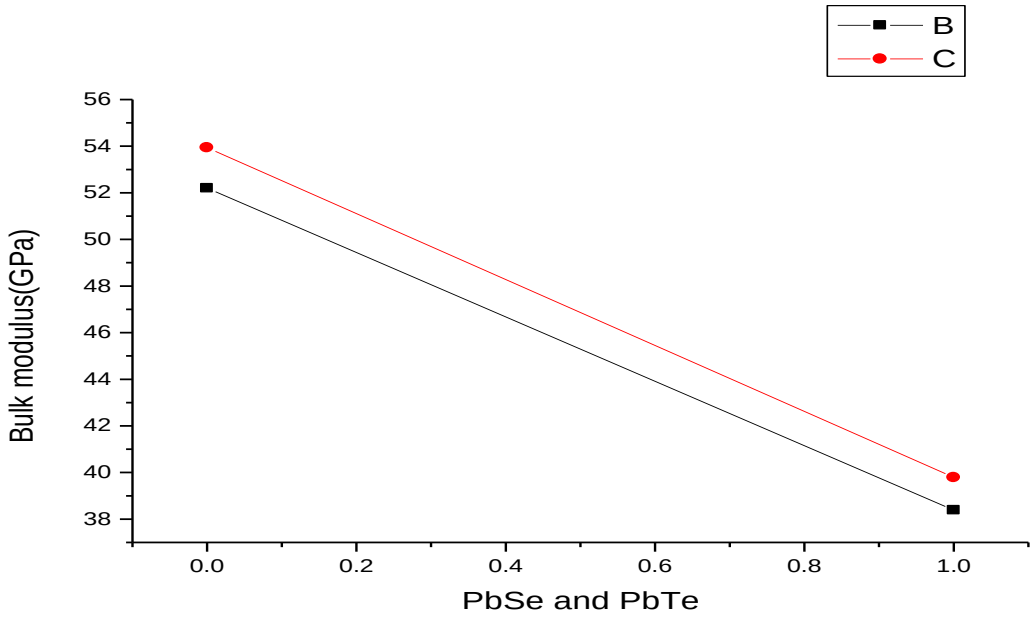

Fig.1. Bulk modulus for PbSe and PbTe

DOI: 10.31695/IJASRE.2019.33208

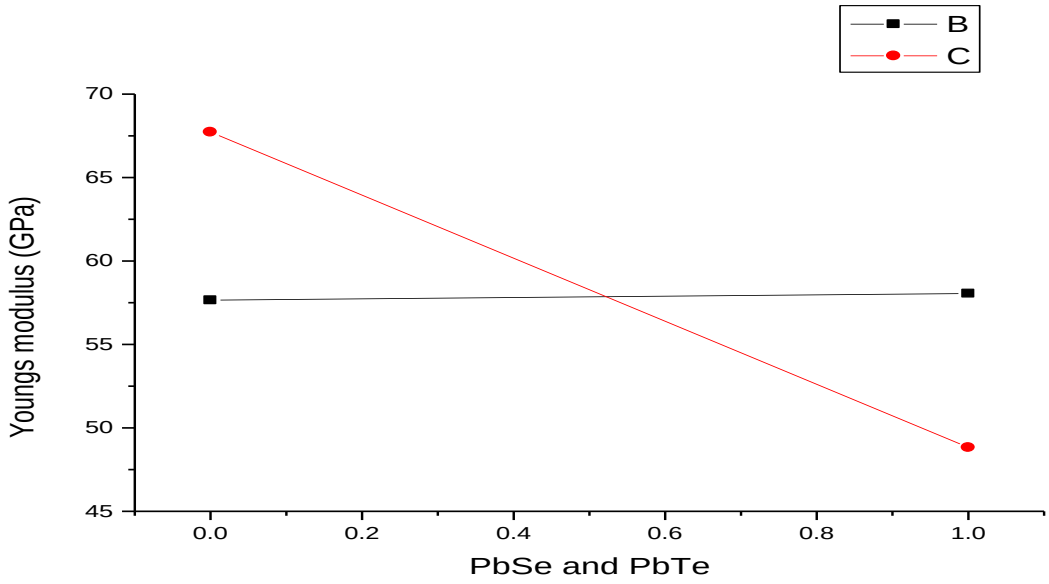

Fig.2.Young's modulus for PbSe and PbTe

REFERENCES

[1] V. I. Smelyansky and J. S. Tse, 1995, Physical Review B, vol. 52, no. 7, pp. 4658–4661

[2] A. Paul and G. Klimeck, 2011, Applied Physics Letters, vol. 98, no. 21, Article ID 212105

[3] E. A. Albanesi, C. M. I. Okoye, C. O. Rodriguez et al., 2000, Physical Review B: Condensed Matter and Materials Physics, vol. 61, no. 24, pp. 16589–16595

[4] A. Grzechnik and K. Friese, 2010, Journal of Physics Condensed Matter, vol. 22, no. 9, Article ID 095402

[5] G. Rousse, S. Klotz, A. M. Saitta et al.,2005, Physical Review B, vol. 71, no. 22, Article ID 224116

[6] S. V. Ovsyannikov, V. V. Shchennikov, A. Y. Manakov et al., 2007, Physica Status Solidi (B) Basic Research, vol. 244, no. 1, pp. 279–284

[7] B. K. Panda and H. C. Padhi, 1991,Physica Status Solidi B, vol. 166, no. 2, pp. 519– 523

[8] T. Chattopadhyay, A. Werner, H. G. von Schnering, and J. Pannetier, 1984,Revue de Physique Appliquee´ , vol. 19, no. 9, pp. 807–813

[9] T.Chattopadhyay,H.G.von Schnering,W.A.Grosshans,and W.B.Holzapfel,1986,Physica,vol.139-140,pp.356–360

[10] A. Svane, N. Christensen, M. Cardona, A. Chantis, M. Van Schilfgaarde, and T. Kotani, 2010, Physical Review B, vol. 81, no. 24, pp. 1–10

[11] L. Xu, H.-Q. Wang, and J.-C. Zheng, 2011, Journal of Electronic Materials, vol. 40, no. 5, pp. 641–647

[12] F. Kong,Y. Liu,B. Wang,Y.Wang, and L Wang, 2012, Computational Materials Science, vol. 56, pp. 18–24

[13] A. Crocker and M. Wilson, 1978,Journal of Materials Science, vol. 13, pp. 833–842

[14] Y. Gelbstein, G. Gotesman, Y. Lishzinker, Z. Dashevsky, and M. P. Dariel,2008,Scripta Materialia, vol. 58, no. 4, pp. 251–254

[15] J. E. Ni, E. D. Case, K. N. Khabir, R. C. Stewart, C.-I. Wu, T. P. Hogan, E. J. Timm, S. N. Girard, and M. G. Kanatzidis, 2010,Materials Science and Engineering: B, vol. 170, no. 1–3, pp. 58–66

[16] Y. Gelbstein,Z. Dashevsky and M.P.Dariel,2008,Journal of Applied Physics, vol. 104, no. 3, p. 033702

DOI: 10.31695/IJASRE.2019.33208

[17] Y. Gelbstein, Z. Dashevsky, and M. P. Dariel,2007,Physica B: Condensed Matter, vol. 396, no. 1–2, pp. 16–21

[18] R. Hill,1952,Proceedings of the Physical Society. Section A, vol. 65, p. 349

[19] S. Pugh, 1954, Philosophical Magazine, vol. 45, no. 367, pp. 823– 843

[20] F. Nye, 1964 Physical properties of crystals, 2nd ed. Oxford: Oxford University Press

[21] E. S. Bozin, C. D. Malliakas, P. Souvatzis, T. Proffen, N. A. Spaldin, M. G. Kanatzidis, and S. J. L. Science ,2010, 330, 1660

[22] O. Madelung, 2004, Semiconductors: Data Handbook, 3rd Edn., Springer, Berlin, Heidelberg

[23] J. E. Ni, et al. 2010, Materials Science and Engineering B 170 ,58–66

DOI: 10.31695/IJASRE.2019.33208