academicJournals

Vol. 8(21), pp.1174-1178, 9 June, 2013
DOI: 10.5897/IJPS12.476
ISSN 1992-1950 © 2013 Academic Journals
http://www.academicjournals.org/IJPS

International Journal of Physical Sciences

*Full Length Research Paper*

# Structural properties of binary semiconductors

**D. S. Yadav[1] and Chakresh Kumar[2]***

[1]Department of Physics, Ch. Charan Singh P G College, Heonra, Etawah-206001 (U.P.) India.
[2]Department of Electronics and Communication Engineering Tezpur University, Napam-784001, India.

Accepted 30 May, 2013

**Using the plasma oscillations theory of solids, 2 empirical relations have been proposed for the calculation of the structural properties such as bond-stretching central force constant (*α*) and bond-bending non-central force constant (*β*) for II-VI and III-V group binary semiconductors. We find that α =D $(\hbar\omega_p)^2$ and β = S $(\hbar\omega_p)^2$, where D and S are constants. The numerical values of *D* and *S* are respectively, 0.151 and 0.016 for II-VI and 0.177 and 0.031 for III-V group binary semiconductors. The structural properties of binary semiconductors exhibit a linear relationship when plotted on a log-log scale against the plasmon energy $\hbar\omega_p$ (in eV), which lies on the straight lines. We have applied the proposed empirical relations on these binary semiconductors and found a better agreement with the experimental data as compared to the values evaluated by earlier researchers.**

**Key words:** Plasmon energy, structural properties, III-V and II-VI Semiconductors.

## INTRODUCTION

In recent years (Kamran et al., 2008; Kumar et al., 2010; Hasan et al., 2009, 2010; Breidi et al., 2010), II-VI and III-V group binary tetrahedral semiconductors have been extensively studied because of their technical and scientific importance and because they have zinc-blende and wurtzite structure. Using the valence-force-field model of Keating (Keating, 1966), the elastic properties of II-VI and III-V group semiconductors with a sphalerite-structure have been analyzed by Martin (Martin, 1970) and several other workers (Phillips, 1970; Yogurtcu et al., 1981).

A considerable amount of discrepancies have been obtained between theory and experiment in determining vibrational modes on the basis of the model parameters derived from elastic constant data. Nowadays more reliable elastic constant data are available which differ partially from those obtained by Martin (Martin, 1970). In the Martin analysis, the contribution of Coulomb force to the elastic constants has been described in terms of macroscopic effective charge which is responsible for the splitting of transverse and longitudinal optical modes. Lucovsky et al. (1971) has pointed out that the Martin approach (Martin, 1970) is incorrect. The ratio of β/α = 0.3 $(1-f_i)$ measures the importance of covalent bonds in determining the stability of the tetrahedral structures. The overall trend of (β/α) tends to zero for purely ionic crystal that is, for which ionicity $(f_i)$ is unity.

Neumann (1985, 1989) has extended the Keating model (Keating, 1966) considering localized effective charge to account for long range Coulomb force and dipole-dipole interaction in analysing the vibrational properties of binary and ternary compounds with a sphalerite-structure. Neumann (1985) has taken experimental values of bond length d (in nm) and spectroscopic bond iconicity $(f_i)$ (Phillips, 1970) to determine the constant associated with the above theory. Reddy et al. (2003) have reported a simple correlation between lattice energy, bond stretching and bond bending force constants, ionicity and micro-hardness for $A^{II}B^{VI}$ and $A^{III}B^{V}$ semiconductors.

*Corresponding author. chakreshk@gmail.com

**PACS Nos.** : 52.25.-b, 72.80.Ey.

Recently, Yadav and Singh (2012) have calculated the static and dynamical properties of II-VI and III-V group binary solids with the help of plasma oscillations theory. This is based on the fact that the plasmon energy, $\hbar\omega_p = \hbar (4\pi ne^2/m)$, is related to the effective number of valence electrons (n) in a compound. In many cases empirical relations do not give highly accurate results for each specific material, but they still can be very useful.

In particular, the simplicity of empirical relation allows a broader class of researchers to calculate useful properties and often trend become more evident. Therefore, we thought it would be of interest to give an alternative explanation for bond stretching central force constant (α in N/m) and bond-bending non-central force constant (β in N/m) of II-VI and III-V group binary semiconductors.

The purpose of this work is to obtain structural properties of the II-VI and III-V group binary semiconductors using the plasma oscillations theory of solids. The theoretical concept is given. We also presented and discussed the simulation results for structural properties of binary semiconductors. Finally, the conclusion is given.

## THEORETICAL CONCEPTS

The nearest-neighbour bond-stretching central forces have been characterized by the parameter *α,* and next neighbor bond-bending non-central forces by the parameter *β*. These parameters depend on inter-atomic distance obtained from lattice vibration data. The lattice vibration data have been further obtained from various types of two-body inter-atomic potential given in literature. Such potentials have the advantage of keeping the repulsive and attractive forces in the same mathematical form.

The simplest form of inter-atomic potential has been described by Neumann (1989), Harrison (1983) and Harrison and Freeman (1989) in which it has been assumed that both the repulsive and attractive parts of inter-atomic potential are described by the power law of inter-atomic distance (*d*). This form of potential for the total energy or cohesive energy per pair of atom can be written as (Neumann, 1989):

$$V_1(d) = C/d^m - D/d^n \quad (1)$$

Where *C*, *D, m* and *n* are numerical constants and *d* is the nearest neighbour distance.

These parameters have been estimated for equilibrium condition when the repulsion is half of the attraction that is m = 2n (Neumann,1989) and the following equation has been obtained:

$$\alpha = \alpha_0 d^{-x} \quad (2)$$

where $\alpha_0$ and *x* are the constants. The other form of potential is based on Morse potential. In this type of potential both the repulsive and attractive terms are described by exponential functions of inter-atomic distance.

The general form of Morse potential is given by Neumann (1989):

$$V_2(d) = A \exp(-ad) - B \exp(-bd) \quad (3)$$

Where *A, B, a* and *b* are constants. The above equation has been further used to describe the two-body interaction in total energy calculation of Si (Sobotta et al., 1986). Neumann (1985, 1989) has also extended it to ternary chalcopyrites. Solving above equation (3) for equilibrium condition a = 2b, the following relation has been obtained Neumann (1989).

$$\alpha = \alpha_1 \exp(-bd) \quad (4)$$

where $\alpha_1$ and *b* are the numerical constants. Presently, Reddy et al. (2003) has described the correlation between lattice energy, bond stretching force constant (*α*) and bond banding force constant (*β*) for $A^{II}B^{VI}$ and $A^{III}B^{V}$ compound semiconductors as follows:

$$\alpha = m_\alpha U - b_\alpha \quad (5)$$

$$\beta = m_\beta U - b_\beta \quad (6)$$

where $m_\alpha$, $m_\beta$, $b_\alpha$, and $b_\beta$ are constants.

Recently, Verma (2009) has derived an empirical relations for the bond-stretching and bond-bending force constants of $A^{II}B^{VI}$ and $A^{III}B^{V}$ group binary solids in term of the product of ionic charges of cation and anion with nearest-neighbor distance *d* (in $A^0$) by the following expressions as:

$$\alpha = A (Z_1 Z_2)^S d^{-3} \quad (7)$$

$$\beta = V (Z_1 Z_2)^B d^{-3} \quad (8)$$

Where *A*, *S*, *V* and *B* are the numerical constants depending upon the group of materials. In a previous work (Yadav and Singh, 2012) we proposed the simple expressions for static and dynamical properties such as bulk modulus B (in GPa) and cohesive energy $E_{coh}$ (in Kcal/mole) of II-VI and III-V group binary solids in term of the plasmon energy $\hbar\omega_p$ (in eV) by the following relations:

$$B = D (\hbar\omega_p)^S \quad (9)$$

$$E_{Coh} = D^* (\hbar\omega_p)^{S^*} \quad (10)$$

Where *D*, *S D** and *S** are numerical constants. Using this idea to get better agreement with experimental and theoretical data for the bond-stretching and bond-bending force constants of binary semiconductors, equations (7) and (8) may be extended as:

$$\alpha = D (\hbar\omega_p)^2 \quad (11)$$

$$\beta = S (\hbar\omega_p)^2 \quad (12)$$

Where D and S are numerical constants, depends upon the structure of the compounds, semiconductor and plasmon energy (ħωp) (Yadav and Singh, 2012; Kumar et al., 1996). The values of D and S turn out to be equal to 0.151 and 0.016 for II-VI group and 0.177 and 0.031 for III-V group binary solids, respectively. A detailed study of structural properties of these materials has been given elsewhere (Keating, 1966; Martin, 1970; Phillips, 1970; Yogurtcu et al., 1981; Lucovsky et al., 1971; Van-Vechten, 1969) and will not be presented here.

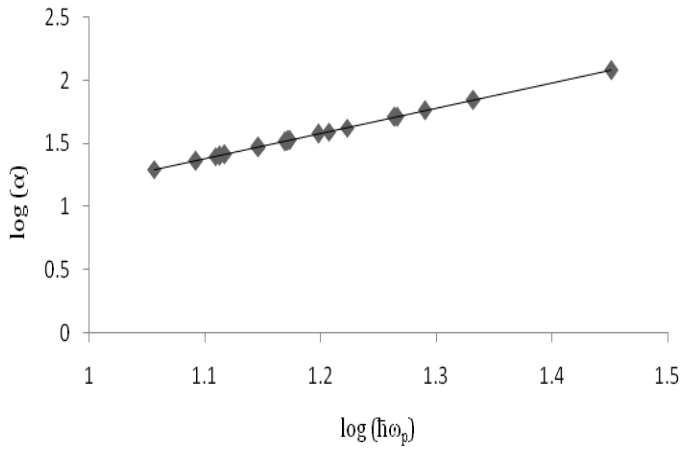


**Figure 1.** Plot of bond-stretching force constant versus plasmon energy of II-VI group binary semiconductors.

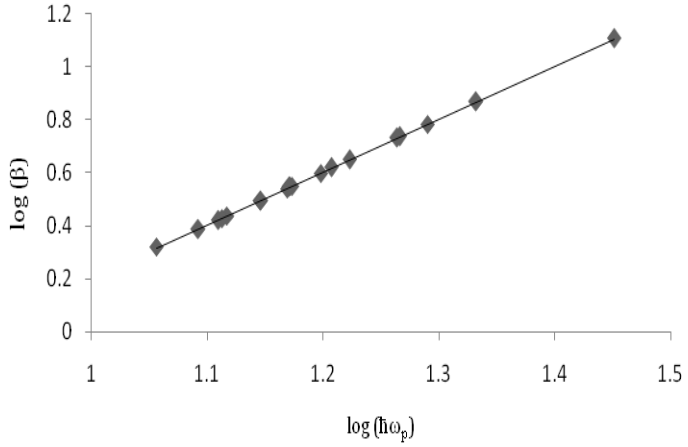


**Figure 2.** Plot of bond-bending force constant versus plasmon energy of II-VI group binary semiconductors.

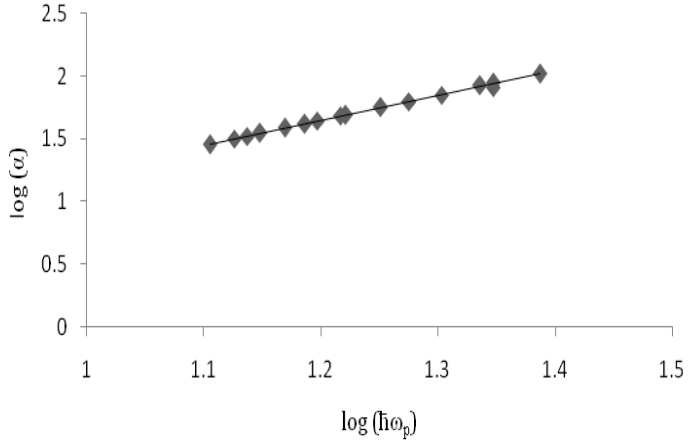


**Figure 3.** Plot of bond-stretching force constant versus plasmon energy of III-V group binary semiconductors.

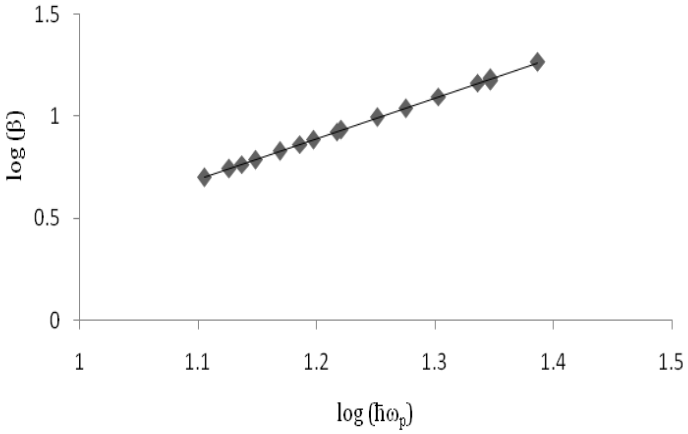


**Figure 4.** Plot of bond-bending force constant versus plasmon energy of III-V group binary semiconductors.

## RESULTS AND DISCUSSION

The present paper reports 2 expressions between the bond stretching force constant α (in N/m) and bond-bending force constant β (in N/m) with their plasmon energy of binary semiconductors. This can be successfully employed to estimate the bond stretching and bond-bending force constant from their plasmon energies. We have plotted log-log curve for II-VI and III-V group binary semiconductors, which are presented in Figures 1 to 4, we observed that in the plot of inter-atomic force constants and $\hbar\omega_p$ of these materials, the data points lies on the straight lines.

From this Figure 1 to 4, it is quite obvious that the bond stretching force constant ($\alpha$) and bond-bending force constant ($\beta$) trends in these compounds increase with increasing their plasmon energy and lies on the straight line. The proposed empirical relations (11) and (12) have been applied to calculate the structural properties of binary semiconductors. The calculated values are presented in Tables 1 and 2, respectively, along with their literature values. We note that the values of the bond stretching and bond-bending force constant calculated from our proposed empirical relations are in fairly good agreement with the values reported by earlier researchers (Neumann, 1985, 1989; Reddy, 2003; Verma, 2009).

These results shows that our current approach is quite reasonable and can give us a useful guide in calculating and predicting the inter-atomic force constants of these materials.

## Conclusion

From the above results and discussion obtained by using the proposed empirical relation based on plasma oscillations theory of solids, it is quite obvious that the

**Table 1.** Structural properties of II-VI group binary semiconductors.

| $A^{II}B^{VI}$ | $\hbar\omega_p$ (eV) | $\alpha$ (in N/m) | | | | $\beta$ (in N/m) | | | |
|---|---|---|---|---|---|---|---|---|---|
| | [16, 21] | Calc. | [20] | [12-14] | [15] | Calc. | [20] | [12-14] | [15] |
| ZnO | 21.48 | 69.67 | --- | --- | 71.31 | 7.38 | --- | --- | 6.973 |
| ZnS | 16.71 | 42.16 | 42.22 | 44.73 | 48.67 | 4.46 | 4.46 | 4.36 | 4.561 |
| ZnSe | 15.78 | 37.60 | 36.34 | 38.61 | 44.18 | 3.98 | 3.84 | 4.65 | 4.083 |
| ZnTe | 14.76 | 32.89 | 29.40 | 32.04 | 39.02 | 3.48 | 3.11 | 4.47 | 3.534 |
| ZnPo | 12.36 | 23.07 | --- | --- | --- | 2.44 | --- | --- | --- |
| CdO | 18.46 | 51.45 | --- | --- | --- | 5.45 | --- | --- | --- |
| CdS | 14.88 | 33.43 | 33.81 | --- | 39.70 | 3.54 | 3.57 | --- | 3.606 |
| CdSe | 14.01 | 29.64 | 30.08 | --- | 35.21 | 3.14 | 3.18 | --- | 3.128 |
| CdTe | 13.09 | 25.87 | 24.38 | 29.44 | 30.21 | 2.74 | 2.58 | 2.48 | 2.602 |
| CdPo | 11.43 | 19.73 | -- | --- | --- | 2.09 | --- | --- | --- |
| BeO | 28.25 | 120.50 | --- | --- | --- | 12.76 | --- | --- | -- |
| BeS | 19.52 | 57.53 | --- | --- | 62.64 | 6.08 | ---- | --- | 6.018 |
| BeSe | 18.39 | 51.06 | --- | --- | 56.96 | 5.41 | --- | --- | 5.445 |
| BeTe | 16.12 | 39.24 | --- | --- | 45.75 | 4.16 | -- | --- | 4.250 |
| BePo | 14.91 | 33.56 | --- | --- | --- | 3.55 | --- | --- | --- |
| HgS | 14.84 | 33.25 | 33.41 | --- | --- | 3.52 | 3.53 | --- | --- |
| HgSe | 13.99 | 29.55 | 29.74 | 37.43 | --- | 3.13 | 3.14 | 2.37 | --- |
| HgTe | 12.85 | 24.93 | 24.65 | 29.32 | --- | 2.64 | 2.61 | 2.54 | --- |
| MgTe | 12.97 | 25.40 | --- | --- | 29.83 | 2.69 | --- | --- | 2.555 |

**Table 2.** Structural properties of III-V group binary semiconductors.

| $A^{III}B^{V}$ | $\hbar\omega_p$ (eV) | $\alpha$ (in N/m) | | | | $\beta$ (in N/m) | | | |
|---|---|---|---|---|---|---|---|---|---|
| | [12, 30*] | Calc. | [15] | [20] | [12- 14] | Calc. | [15] | [20] | [12- 14] |
| BN | 22.75 | 91.60 | 88.357 | --- | --- | 16.04 | 17.179 | --- | --- |
| BP | 21.71 | 83.71 | 75.037 | 87.14 | --- | 14.61 | 14.447 | 15.60 | --- |
| BAs | 20.12 | 70.80 | 67.044 | 74.95 | --- | 12.54 | 12.855 | 13.42 | --- |
| BSb | 17.85 | 56.39 | --- | 56.61 | --- | 9.87 | --- | 10.14 | --- |
| AlN | 22.27 | 87.78 | 81.091 | 97.30 | --- | 15.37 | 15.705 | 17.42 | --- |
| AlP | 16.65 | 49.06 | 49.122 | 48.41 | --- | 8.59 | 9.219 | 8.67 | --- |
| AlAs | 15.75 | 43.90 | 44.278 | 44.34 | --- | 7.68 | 8.236 | 7.94 | --- |
| AlSb | 13.72 | 33.31 | 33.137 | 33.81 | 35.74 | 5.83 | 5.975 | 6.05 | 6.63 |
| GaN | 20.46 | 74.10 | 76.248 | 95.76 | --- | 14.97 | 14.722 | 17.15 | --- |
| GaP | 16.50 | 48.18 | 48.395 | 48.41 | 48.57 | 8.44 | 9.071 | 8.67 | 10.40 |
| GaAs | 15.35 | 41.70 | 42.098 | 43.27 | 43.34 | 7.30 | 7.794 | 7.75 | 8.88 |
| GaSb | 13.38 | 31.68 | 31.200 | 34.19 | 34.42 | 5.55 | 5.582 | 6.12 | 7.16 |
| InN | 18.82 | 62.69 | 60.505 | 70.70 | --- | 10.97 | 11.528 | 12.66 | --- |
| InP | 14.76 | 38.56 | 38.950 | 38.83 | 44.29 | 6.75 | 7.155 | 6.95 | 6.26 |
| InAs | 14.07 | 35.04 | 35.075 | 35.79 | 37.18 | 6.14 | 6.369 | 6.41 | 5.47 |
| InSb | 12.73 | 28.68 | 27.567 | 28.68 | 30.44 | 5.02 | 4.845 | 5.14 | 4.73 |

bond stretching and bond-bending force constant reflecting the structural properties can be expressed in term of plasmon energy of these materials; this is a surprising phenomenon. The calculated values of these parameters are presented in Table 1 and 2, respectively. We come to the conclusion that plasmon energy of any compound is the input parameter for calculating the structural properties. The inter-atomic force constants of

binary semiconductors exhibit a linear relationship when plotted on a log-log scale against the plasmon energy $\hbar\omega_p$ (in eV), which lies on the straight lines.

In the present study, we find that both the inter-atomic force constants $\alpha$ and $\beta$ directly depends upon the plasmon energy of these compounds semiconductor. Thus, this theory can be easily extended to binary semiconductors. A fairly good agreement between our calculated values of inter-atomic force constants with the values reported by earlier researchers has been found. It is also note worthy that the proposed empirical relations are simple and widely applicable.

**REFERENCES**


Breidi A, Hasan Haj El F, Nouet G, Drablia S, Meradji H, Pages O, Ghemid S (2010). Theoretical study **of** InAs, InSb and their alloys InAsxSb1-x. J. Alloys Compounds 49380.

Harrison WA (1983). A theory of force constant models is derived for tetrahedral semiconductors from Harrison's Phys. Rev. B 27:3592.

Harrison WA, Freeman WH (1989). Electronic Structure and the Properties of Solids (Dover, New York, 1989).

Hasan El Haj F, Annane F, Meradji H, Ghemid S (2010). First principle investigation of AlAs and AlP compounds and ordered $AlAs_{1-x}P_x$ alloys, Comput. Mater. Sci., 50: 274-278.

Hasan El Haj F, Drablia S, Meradji H, Ghemid S, Nouet G (2009). First principles investigation of barium chalcogenide ternary alloys Computational Mater. Sci. 46:376–382.

Kamran S, Chen K, Chen L (2008). Semi-empirical formulae for elastic moduli and brittleness of covalent crystals", Phys. Rev. B 77:094109.

Keating PN (1966). Effect of Invariance Requirements on the Elastic Strain Energy of Crystals with Application to the Diamond Structure, Phys. Rev. 145:637–645.

Kumar V, Prasad GM, Chetal AR, Chandra D (1996). Microhardness and bulk modulus of binary tetrahedral semiconductors, 57(4):503–506.

Kumar V, Shrivastava AK, Jha V (2010). Bulk modulus and microhardness of tetrahedral semiconductors, J. Phys. Chem. Solids, 71:1513.

Lucovsky G, Martin RM, Burstein E (1971). Localized Effective Charges in Diatomic Crystals Phys. Rev. B 4:1367–1374.

Martin RM (1970). Elastic Properties of ZnS Structure Semiconductors. Phys. Rev. B1:4005.

Neumann H (1985). Interatomic force constants and localized effective charges in sphalerite-structure compounds. Cryst. Res. Technol. 20(6):773-780.

Neumann H (1989). Interatomic force constants in AIIBIVCV2 chalcopyrite compounds. Cryst. Res. Technol. 24(6):619-624.

Phillips JC (1970). Bonds and Bands in Semiconductors ,Rev. Mod. Phys. 42:317.

Reddy RR, Nazeer Ahammed Y, Abdul Azeem P, Gopal KR, Sasikala D, Rao TVR, Behere SH (2003). Interatomic force constants, ionicity and microhardness of binary tetrahedral semiconductors. Ind. J. Phys. 77(3):237-241.

Sobotta H, Neumann H, Reide V, Kuhn G (1986). Lattice vibrations and interatomic forces in LiInS2. Cryst. Res. Technol. 21:1367-1371

Van Vechien JA (1969). Quantum dielectric theory of electronegativity in covalent systems. I. Electronic dielectric constant. Phys. Rev. 182:891-905.

Verma AS (2009). Electronic and Optical Properties of Rare-earth Chalcogenides and Pnictides, Afr. Phys. Rev. 3:0003.

Yadav DS, Singh DV (2012). Static and dynamical properties of II–VI and III–V group binary Solids,Phys.Scr. 85:015701.

Yogurtcu YK, Miller AJ, Saunders GA (1981). Pressure dependence of elastic behaviour and force constants of GaP. J. Phys. Chem. Solids 42(1):49-56.