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Dependency of second order elastic coefficients (SOEC) on Plasmon energy for Different Common Cation Series of Binary Semiconductor belonging to II – VI and III – V groups of semiconductors

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Abstract

Second order elastic coefficient (SOEC) of II-VI and III-V groups of semiconductors have been calculated using plasmon energy data. On the basis of best fit data, new relations have been proposed for the calculations of SOEC. The calculated values of SOEC from the new relations have been compared with the values reported by different researchers, an excellent agreement have been obtained between them.

Keywords: SOEC, Inter atomic force constants, plasmon energy, II-VI and III-V groups of binary semiconductors

INTRODUCTION:

SOEC of II-VI and III-V groups of semiconductors have been an important parameter to study these semiconductors because these semiconductors have potential applications in a variety of optoelectronic devices such as Nonlinear optics, light emitting diodes, Photovoltaic cells, photodetectors, lasers, modulators, Integrated circuits and filters [1-5]. All the method enumerated in literature [6-8] for the evaluation of SOEC involve many experimentally determined parameters and tedious mathematical calculations.

The SOEC [9] shows dependency on Interatomic force constant (α, β) Kumar [10]. In the present paper we have proposed new relations to evaluate SOEC for II-VI and III-V groups of semiconductors. The calculated values of SOEC are compared with the values reported by Martin [9]. Although they have reported the values of SOEC for few semi-conductors belonging to II-VI and III-V groups of semiconductors. But these values can be considered as experimental. In this paper, we developed relationship between SOEC and plasmon energy.

THEORY:

The study of the second order elastic coefficient (SOEC) i.e. C_{11}, C_{12} and C_{44} is quite important for understanding the nature of the interatomic forces in binary semiconductors, SOEC depends on bond-stretching (α) and bond bending (β) force constants. The inter-atomic force constants (α, β) directly depend on plasmon energy of binary semiconductors.

On the basis of linear plots from the relationship between α and $\hbar w_p$ can be approximated by the following equation Singh [11].

$$\alpha = K_1\left(\hbar w_p\right)^{K_2} \tag{1}$$

where α is in Nm^{-1} and $\hbar w_p$ in eV. K_1 and K_2 are constants for a particular group of semiconductors, such that $K_1 = 0.356, 0.306$ and $K_2 = 1.702, 1.819$ for II-VI and III-V semiconductors respectively.

The relationship between β and α can be approximated by the following equation Indolia [12].

$$\beta = K_3(\alpha)^{K_4} \tag{2}$$

Where K_3 and K_4 are constants for a common cation series within III-V semiconductors, such that $K_3 = 0.1654, 0.3693$; and $K_4 = 1.063, 0.746$, respectively, for Ga-series and In-series.

The relationship between β and α for Zn-series can be approximated by the following equation Indolia [12].

$$\beta = K_5(\alpha)^{-K_6} \tag{3}$$

where $K_5 = 5.628$ and $K_6 = 0.062$ are constants.

Thus, in the present section, we have attempted to obtain SOEC by using plasmon energy data as follows

The SOEC are given as [9]

$$C_{11} = \frac{\sqrt{3}}{4d}(\alpha + 3\beta) - 0.083SC_0 \tag{4}$$

$$C_{12} = \frac{\sqrt{3}}{4d}(\alpha - \beta) - 0.136SC_0 \tag{5}$$

And

$$C_{44} = \left(\frac{\sqrt{3}}{4d}\right)(\alpha + \beta) - 0.136SC_0 - C\xi^2 \qquad (6)$$

Where S, C_0 and ξ are coulombic force constant, normalization modulus and internal-strain parameter respectively.

Martin [9] has shown that to a first approximation

$$S = f_i. \qquad (7)$$

The value of β Kumar [10] used the following relation given by Neumann [13].

$$\beta = \beta_0 (1 - f_i)\,\alpha \qquad (7_0)$$

By using equation (7) and (7_0) we get,

$$S = 1 - \left(\frac{\beta}{\beta_0 \alpha}\right) \qquad (8)$$

Where $\beta_0 = 0.28$ is the proportionality constant [13].

Using equations (1), (2) and (3) together with the equation (8), we can write expression for S in terms of plasmon energy for common cation series of binary semiconductors belonging to II-VI and III-V groups as follows,

Zn-series (ZnS, ZnSe, ZnTe)

$$S = 1 - 60.194(\hbar w_p)^{-1.807} \qquad (9)$$

Ga-Series (GaP, GaAs, GaSb)

$$S = 1 - 0.547(\hbar w_p)^{0.114} \qquad (10)$$

In-Series (InP, InAs InSb)

$$S = 1 - 1.780(\hbar w_p)^{-0.462} \qquad (11)$$

The normalization modulus C_0 is given as [9]

$$C_0 = \frac{e^2}{d^4} \qquad (12)$$

Where d(cm) is the bond length and e(esu) is the electronic charge.

Combining with equation (12) we get,

$$C_0 = 4.205 \times 10^8 \times (\hbar w_p)^{2.667} \qquad (13)$$

The internal strain parameters ξ is given as [9]

$$\xi = C^{-1}\left[\left(\frac{\sqrt{3}}{4d}\right)(\alpha - \beta) - 0.294S \rightleftarrows C_0\right] \qquad (14)$$

where

$$C = \left(\frac{\sqrt{3}}{4d}\right)(\alpha + \beta) - 0.266SC_0 \qquad (15)$$

Using above equations together with equations (1), (2) and (3). We have obtained expressions for SOEC (C_{11}, C_{12} and C_{44}) in terms of plasmon energy for different common cation series of binary semiconductors belonging to II-VI and III-V groups as

Zn-series

$$C_{11} = 0.509 \times 10^{11}(\hbar w_p)^{0.561} \left[1 + 0.0197(\hbar w_p)^{1.807}\right]$$

$$-0.349 \times 10^{8}(\hbar w_p)^{2.667}\left[1 - 60.194(\hbar w_p)^{-1.807}\right] \quad (16)$$

$$C_{12} = 0.169 \times 10^{11}(\hbar w_p)^{0.562}\left[0.059(\hbar w_p)^{1.807} - 1\right]$$

$$-0.571 \times 10^{8}(\hbar w_p)^{2.667}\left[1 - 60.194(\hbar w_p)^{-1.807}\right]$$

(16)

$$C_{44} = X - Y - Z \qquad (17)$$

where

$$X = 10.074 \times 10^{8}(\hbar w_p)^{2.369}\left[1 + 16.854(\hbar w_p)^{-1.807}\right]$$

$$Y = 0.571 \times 10^{8}(\hbar w_p)^{2.667}\left[1 - 60.194(\hbar w_p)^{-1.807}\right]$$

$$Z = \left\{10.074 \times 10^{8}(\hbar w_p)^{2.369}\left[1 + 16.854(\hbar w_p)^{-1.807}\right]\right.$$

$$\left.-1.118 \times 10^{6}(\hbar w_p)^{2.667}\left[1 - 60.194(\hbar w_p)^{-1.807}\right]\right\}^{-1}$$

$$\times \left\{0.169 \times 10^{11}(\hbar w_p)^{0.562}\left[0.059(\hbar w_p)^{1.807} - 1\right]\right.$$

$$\left.-1.236 \times 10^{8}(\hbar w_p)^{2.667}\left[1 - 60.194(\hbar w_p)^{-1.807}\right]\right\}^{2}$$

Ga-Series

$$C_{11} = 3.962 \times (\hbar w_p)^{2.599}\left[1 + 2.172(\hbar w_p)^{-0.114}\right]$$

$$-0.349 \times 10^{8}(\hbar w_p)^{2.667}\left[1 - 0.547(\hbar w_p)^{0.114}\right] \qquad (18)$$

$$C_{12} = 1.329 \times 10^{8}(\hbar w_p)^{2.667}\left[6.514(\hbar w_p)^{-0.114} - 1\right]$$

$$-0.571 \times 10^8 (\hbar w_p)^{2.667} \left[1 - 0.547 (\hbar w_p)^{0.114}\right] \tag{19}$$

$$C_{44} = X - Y - Z \tag{20}$$

$$X = 8.659 \times 10^8 (\hbar w_p)^{2.486} \quad \left[1 + 0.153 (\hbar w_p)^{0.114}\right]$$

$$Y = 0.571 \times 10^8 (\hbar w_p)^{2.667} \left[1 - 0.547 (\hbar w_p)^{0.114}\right]$$

$$Z = \Big\{8.659 \times 10^8 (\hbar w_p)^{2.486} \left[1 + 0.153 (\hbar w_p)^{0.114}\right]$$

$$-1.118 \times 10^8 (\hbar w_p)^{2.667} \left[1 - 0.547 (\hbar w_p)^{0.114}\right]\Big\}^{-1}$$

$$\times \Big\{1.329 \times 10^8 (\hbar w_p)^{2.667} \left[9.514 (\hbar w_p)^{-0.115} - 1\right]$$

$$-1.236 \times 10^8 (\hbar w_p)^{2.667} \quad \left[1 - 0.547 (\hbar w_p)^{0.114}\right]\Big\}^2$$

In-Series

$$C_{11} = 12.930 \times 10^8 (\hbar w_p)^{2.023} \left[1 + 0.667 (\hbar w_p)^{0.462}\right] \tag{21}$$

$$C_{12} = 4.319 \times 10^8 (\hbar w_p)^{2.023} \left[2.0 (\hbar w_p)^{0.462} - 1\right]$$

$$+0.571 \times 10^8 (\hbar w_p)^{2.667} \left[1.780 (\hbar w_p)^{-0.462} - 1\right] \tag{22}$$

$$C_{44} = X - Y - Z \tag{23}$$

Where

$$X = 8.659 \times 10^8 (\hbar w_p)^{2.486} \quad \left[1 + 0.498 (\hbar w_p)^{-0.462}\right]$$

$$Y = 0.571 \times 10^8 (\hbar w_p)^{2.667} \left[1 - 1.780 (\hbar w_p)^{-0.462}\right]$$

$$Z = \quad \Big\{8.659 \times 10^8 (\hbar w_p)^{2.486} \left[1 + 0.498 (\hbar w_p)^{-0.462}\right]$$

$$-1.118 \times 10^8 (\hbar w_p)^{2.667} \left[1 - 1.780 (\hbar w_p)^{-0.462}\right]\Big\}^{-1}$$

$$\times \Big\{4.319 \times 10^8 (\hbar w_p)^{2.023} \left[2.0 (\hbar w_p)^{0.462} - 1\right]$$

$$-1.236 \times 10^8 (\hbar w_p)^{2.667} \left[1 - 1.780 (\hbar w_p)^{-0.462}\right]\Big\}^2$$

We have calculated SOEC for Zn, -Ga-and In-common cation series of binary semiconductors, and reported in table 1 together with the literature values [9]. Our calculated values are found in close agreement within 14 percent with the literature values. The equations obtained by us for SOEC are useful and unique in the sense that we can directly calculate SOEC for binary semiconductors by having only the knowledge of their plasmon energy.

Another advantage of this proposed model is that we can predict elastic coefficients of those semiconductors whose experimental study has not been yet made. It has been observed from table 1 that the values of SOEC decreases with the decrease in plasmon energy for each common cation series, when we move from lighter to heavier semiconductor. It might be due to increase in their bond length in this process.

Table 2: The values of plasmon energy $\hbar\omega_p(eV)$ and bond length d (A°) of binary semiconductors

S. No.	Compound (II-VI)	$\hbar\omega_p$ [14]
1	BeO (Zb)	28.26
2	BeS (Zb)	19.52
3	BeSe (Zb)	18.39
4	BeTe (Zb)	16.12
5	MgTe (W)	12.96
6	ZnO (W)	21.48
7	ZnS (Zb)	16.71
8	ZnSe (Zb)	15.78
9	ZnTe(Zb)	14.76
10	CdS (W)	14.88
11	CdSe (W)	14.01
12	CdTe (W)	13.09

Cont.…2

	Compound (III-V)	
13	BN (Zb)	24.53
14	BP (Zb)	21.71
15	BAs (Zb)	20.12
16	ACN (W) AlN (W)	22.97
17	ACP (Zb) AlP (Zb)	16.65
18	AlAs (Zb)	15.75
19	AlSb (Zb)	13.72
20	GaN (W)	21.98
21	GaP (Zb)	16.5
22	GaAs (Zb)	15.35
23	GaSb (Zb)	13.38
24	InN (W)	18.82
25	InP (Zb)	14.76
26	InAs (Zb)	14.07
27	InSb (Zb)	12.73

Table 1: The values of second order elastic constants (C_{11}, C_{12} and C_{44})$_{10}$^{11} dynes/cm^2 of binary semiconductors

Compound	C_{11}		C_{12}		C_{44}	
	Expt. [9]	**Cal.**	**Expt. [9]**	**Cal**	**Expt. [9]**	**Cal**
ZnS	10.40	10.51	6.50	6.40	4.62	3.90
ZnSe	8.10	8.98	4.88	5.54	4.41	3.62
ZnTe	7.13	7.9	4.07	4.70	3.12	3.26
GaP	14.12	14.75	6.25	8.51	7.05	6.29
GaAs	11.81	12.28	5.32	9.03	5.92	3.90
GaSb	8.84	8.70	4.03	5.01	4.32	2.75
InP	10.22	9.60	5.76	5.60	4.60	3.65
InAs	8.33	8.68	4.53	4.94	3.96	3.23
InSb	6.67	6.88	3.65	3.83	3.02	2.50

RESULTANT DISCUSSION:

The advantage of this proposed model is that we can predict elastic coefficients of those semiconductors whose experimental study has not been yet made. It has been observed from table 1 that the values of SOEC decreases with the decrease in plasmon energy for each common cation series, when we move from lighter to heavier semiconductor. It might be due to increase in their bond length in this process.

CONCLUSION:

In the analysis, we have investigated the dependence of elastic coefficients i.e. second order elastic constants (SOEC) on plasmon energy. Using the theories [9, 15], we have established that SOEC mainly depend on bond length, bond–stretching (α) and bond–bending (β) force constants. Further, using the relationships for bond–length and inter–atomic force constants (α, β) with the plasmon energy, obtained by us in the previous section, we have obtained expressions for SOEC (C_{11}, C_{12} and C_{44}) in terms of only plasmon energy, for different common cation series of binary semiconductors belonging to II–VI and III–V groups. We have taken three series i.e. Zn–series, Ga–series and In–series, for this purpose, because experimental data of SOEC are available for these series for direct comparison. Our calculated values of SOEC for these common cation series have been found in close agreement within fourteen percent (overage) with the experimental values [72]. Although our results deviate from experimental values but our developed model is very useful, as it can predict the values of SOEC for binary semiconductor by having only the knowledge of their plasmon energy. It has been observed for each common cation series that when we move from lighter to heavier semiconductor, the values of SOEC decreases with the decrease in plasmon energy. It might be due to increase in their bond length in this process.

REFERENCES:

[1] Lazmerski,L. L.Nuovo Cimento 20,2013(1983).

[2] Deab, S.K..Zunger, A... Ternary and Multinary Compound Materials Research Soc... Conf..Proc; P.37, (1987).

[3] Berrah, S, A. Boukortt,A. and Abid.H..Physica Scripta, 75,414 (2007).

[4] Gaikwad, S.A... Samuel, E. P. Patil. D.S & Gautam, D.K. Indian Journal of Pure & Applied Physics,45, 238 (2007).

[5] S.K. Deab, A. Zunges, Ternary and multinary compounds. Materials research Soc Conf. Proc., 37 (1987).

[6] P.N. Keating, Phys. Rev. **145**, 637 (1966).

[7] M. Blackman, Phil. Mag. **3**, 831 (1959).

[8] E. Burstein, Physical Review **B4**, 1367 (1971).

[9] R.M. Martin, Phys. Rev. B1, 4005 (1970).

[10] V. Kumar, Journal of Physics and Chemistry of Solids **61**, 91 (2000).

[11] Singh. V.K., Indolia. R.S., Acta Ciencia Indica XXXIX. P. No. 3,147 (2013).

[12] Indolia. R.S., Science Phenomenon 5. P. No. 1-8 (2015).

[13] H. Neumann, Cryst. Res. Technol. **20**, 773 (1985).

[14] V. Kumar, G.M. Prasad and D. Chandra, J. Phys. Chem. Solids **58**, 463 (1997).

[15] H. Neumann, Kristallund Technik **15**, 849 (1980).