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# Elastic properties of elemental, binary and ternary semiconductor materials

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Elastic properties of elemental (C, Si, Ge), binary (II-VI, III-V) and ternary (I-III-$VI_2$, II-IV-$V_2$) semiconductors have been studied. New relations, based on plasma oscillation theory of solids, have been proposed for the calculation of bulk modulus (*B*), microhardness (*H*) and shear modulus (*G*) of these materials. The values of *B, H, G* and *G*/*B* ratio have been calculated for 13 new compounds of II-IV-$V_2$ family. The calculated values are compared with the available experimental and reported values. Reasonably good agreement has been obtained between them. The average percentage deviation of proposed relations has also been estimated and found to be better than earlier correlations.

**Keywords:** Bulk modulus, Microhardness, Shear modulus, Elastic properties, Plasma energy, Elemental, Binary and ternary semiconductors

## 1 Introduction

In the recent past, the elastic properties of elemental (C, Si, Ge), binary (II-VI, III-V) and ternary (I-III-$VI_2$, II-IV-$V_2$) semiconductor materials, have been studied. Elemental semiconductors are the back bone for modern electronic industries and having potential applications in fabricating diodes, bi-polar junction transistors (BJTs), field effect transistors (FETs), logic gates, integrated circuits (ICs), nano-electronics and lasing devices[1]. The semiconductors of group II-VI are important for nuclear, industrial and medicinal applications. They are widely used in optoelectronic devices[2], quantum wells[3], quantum wires[4], quantum dots[5], lasing devices[6] and detectors for nuclear power plants[7]. Group III-V semiconductors are the most promising materials for cutting-edge classes of electronic and optoelectronic devices[8,9]. The nitrides of III-V group are used in designing short wavelength laser diodes (LDs), high efficient blue and white light emitting diodes (LEDs) and optical data storage systems[10]. The ternary chalcopyrites of I-III-$VI_2$ (I = Cu, Ag; III = Al, Ga, In, Tl, Fe; VI = S, Se, Te) and II-IV-$V_2$ (II = Zn, Cd; IV = Si, Ge, Sn; V = P, As) families are widely used in photovoltaic solar cells, LEDs, LDs, photo-detectors (PDs), frequency conversion applications, optical parametric oscillators (OPO) and nonlinear optical (NLO) devices[11-13]. Recently, new chalcopyrites of II-IV-$V_2$ family have been developed by replacing group II atom with Be, Mn and Mg atoms, which are also having potential applications in spintronics and magnetically controlled NLO devices[14-16]. In spite of their potential applications, elastic properties of group IV, II-VI, III-V, I-III-$VI_2$, II-IV-$V_2$ semiconductors are still not sufficiently studied. A large variation in the experimental values has been obtained in some of these semiconductors, e.g., experimental values of *H* of ZnS (1.7-3.5) vary more than 100%, CdSe (0.7 to 1.2) varies approximately 72%, C ranges from 57 to 104 and BN from 34.3 to 73. In the case of B, it varies from 35.7 to 76.6 for $AgGaTe_2$ semiconductor. Therefore, it has been thought of interest to further study the elastic properties of these materials.

The elastic properties such as bulk modulus (*B*), microhardness (*H*) and shear modulus (*G*) of these semiconductors have been studied experimentally and theoretically. A state of the art review[17] of earlier models for the calculation of *B* and *H* has been presented. Gilman[18] has proposed an expression for the calculation of *G* of metals based on quantum mechanical description. Kamran *et al*[19]. have correlated *G* with $f_i$ and *d* for II-VI and III-V diamond like and zinc-blende binary crystals and shown that the product of *G* and $d^{5.5}$ is linearly related to $f_i$. Abdellaoui *et al*[20]. have calculated the values of *G* for $CuAlX_2$ (X = S, Se, Te) compounds using elastic constant data $C_{ij}$. Other researchers[21, 22] have proposed empirical relations for the calculation of *B*, *H* and *G*

of I-III-$VI_2$ and II-IV-$V_2$ groups of chalcopyrites. Recently, Kumar *et al*[13]. have calculated the values of $B$, $G$ and $G/B$ ratio of various compounds of II-IV-$V_2$ family using first-principle calculations.

The models proposed by earlier researchers require experimental data of number of parameters such as bond ionicity $f_i$, bond length $d$, melting temperature $T_m$ and atomic volume $\Omega$ in their calculation. The values of these parameters are not known for some of these compounds specially the new magnetic materials of II-VI-$V_2$ family. Their calculations are also complex in nature and limited for particular group of materials. Therefore, simple models have been developed, which can be applicable for all groups of compounds and do not require any experimental data or less number of experimental data. Recently, simple models based on plasmon energy ($\hbar\omega_p$) data for the calculation of various elastic and thermal properties of these semiconductors[17,23] have been developed. In the present paper, the applicability of $\hbar\omega_p$ for the calculation of $B$, $H$ and $G$ have been explored, which give better results than the earlier models.

## 2 Calculation of Bulk Modulus, Microhardness and Shear Modulus

The bulk modulus $B$ is a measure of resistance to volume change by applied pressure. Based on empirical relations, a number of theoretical models have been proposed for the calculation of bulk modulus ($B$). In almost all earlier models, it has been found that $B$ is related to the bond length[17] ($d$). Kumar *et al.*[23] have shown that the bond length $d$ is related to the plasmon energy ($\hbar\omega_p$). This is because of the fact that $d$ and $\hbar\omega_p$ both are related to the effective number of valence electrons in a semiconductor. This shows that there must be a relation between $B$ and $\hbar\omega_p$. For tetrahedrally coordinated semiconductor materials, the bond length $d$ can be written as[17,23]:

$$d = 15.30\,(\hbar\omega_p)^{-2/3} \qquad \ldots(1)$$

where bond length $d$ and plasma energy $\hbar\omega_p$ are in Å and eV, respectively.

Further, Plendl *et al*[24]. have shown that $B$ is directly proportional to $H$, i.e., $B \alpha H$, which shows that $H$ is also related to the $\hbar\omega_p$. This shows that the elastic properties of material have fundamental relation among $B$, $H$ and $\hbar\omega_p$. Based on this, we have simulated the data taking the experimental values of $B$ and the calculated values of plasmon energy $\hbar\omega_p$ as well as the experimental data of $H$ and $\hbar\omega_p$ and proposed the following polynomial relation for the calculation of $B$ and $H$ for Gr. IV, II-VI, III-V, I-III-$VI_2$ and II-IV-$V_2$ semiconductors materials:

$$B \text{ and } H = K_1(\hbar\omega_p)^2 + K_2(\hbar\omega_p) + K_3 \qquad \ldots(2)$$

where $K_1$, $K_2$ and $K_3$ are the constants and having different values for $B$ and $H$ (in GPa) for different groups of semiconductors. The simulated values of $K_1$, $K_2$ and $K_3$ are listed in Table 1 and the calculated values of $B$ and $H$ from Eq. (2) are listed in Tables 2 and 3 along with the available experimental and reported values.

Shear modulus $G$ is another quantity for measuring the stiffness of materials, which measures the resistance of reversible deformations upon the shear stress. It is related to the Poison's ratio and bulk modulus[25]. Kamran *et al.*[19] have derived the following relation for the calculation of $G$ of diamond like and zincblende binary crystal:

$$G = \frac{C_1 - C_2 f_1}{d^{5.5}} \qquad \ldots(3)$$

where $f_i$ is the ionocity, $d$ is the bond length and $C_1$ and $C_2$ are the constants. The numerical values of $C_1$ and $C_2$ are, respectively, 5954.02 and 4538.40 for diamond like and 9058.22 and 6905.86 for zincblende crystals. Recently, Kumar *et al*[26,27]. have correlated $f_i$ with the plasmon energy $\hbar\omega_p$ by the relation:

$$f_1 = \kappa_1 + \kappa_2(\hbar\omega_p) \qquad \ldots(4)$$

where $\kappa_1$and $\kappa_2$ are the constants and their numerical values are given elsewhere[26,27]. Eqs. (1), (3) and (4) show that $G$ is related to $\hbar\omega_p$. Based on this, we have

Table 1 — Numerical values of the constants $K_1$ to $K_5$ used in proposed relations

| Constants | Elastic Moduli | Compound family | | | | |
|---|---|---|---|---|---|---|
| | | IV | II-VI | III-V | I-III-$VI_2$ | II-IV-$V_2$ |
| $K_1$ | $B$ | 0.172 | 0.718 | -0.171 | 1.365 | -0.021 |
| | $H$ | -0.047 | 0.016 | 0.189 | 0.161 | 0.549 |
| $K_2$ | $B$ | 15.44 | -12.56 | 15.2 | -25.38 | 8.865 |
| | $H$ | 5.579 | -0.094 | -3.852 | -4.107 | -14.32 |
| $K_3$ | $B$ | -205.6 | 84.71 | -117.9 | 127.5 | -65.86 |
| | $H$ | -67.35 | -1.139 | 20.46 | 27.22 | 96.71 |
| $K_4$ | $G$ | 6.426 | 0.236 | 1.532 | 0.7589 | 0.640 |
| $K_5$ | $G$ | 0.142 | 0.300 | 0.220 | 0.244 | 0.267 |

Table 2 — Bulk modulus, microhardness and shear modulus of group IV, II-VI and III-V semiconductors

| Group IV | $\hbar\omega_p$ [Ref.17] (eV) | Bulk modulus ($B$) (GPa) Expt.[+] [Ref.17] | This work Eq.(2) | Reported [Ref. 17] | [Ref. 30] | [Ref. 31] | [Ref. 31] | Microhardness ($H$) (GPa) Expt. | This work Eq.(2) | Reported [Ref.17] | [Ref.34] | Shear modulus ($G$) (GPa) Expt[#,+] [Ref.19] | This work Eq.( 5) | Reported [Ref.19] | $G/B$ Ratio This work | Expt.[$] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 |
| C | 31.14 | 442 | 441.99 | 430 | 435 | | | 10(M)[a] (57-104)[b,+] | 60.80 | 96.92 | 80.0 | 535.7 | 534.98 | 534.5 | 1.2093 | 1.2119 |
| Si | 16.58 | 98 | 97.68 | 98.82 | 98 | 92 | 100.7 | 11.27[b], 11.50[b] 12.35[c,+] | 12.23 | 12.33 | 13.3 | 70.8 | 67.67 | 82.4 | 0.8435 | 0.7224 |
| Ge | 15.59 | 77.2 | 76.91 | 85.60 | 76 | 79 | 79.1 | 7.644[a], 8[b,+] | 8.20 | 8.96 | 9.85 | 56.6 | 58.79 | 65.5 | 0.8516 | 0.7331 |
| **Average % deviation** | | | **0.13** | **4.78** | **1.01** | **4.22** | **2.6** | | **1.13** | **4.05** | **10.27** | | **2.81** | **10.77** | | |
| $A^{II}B^{VI}$ | | | | | | | | [Ref.35] | | | [Ref.35] | | | | | |
| BeO | 28.26 | | 303.17 | 265.12 | | | | 9.1[+]- 12.7 | 8.98 | 8.21 | 11.6 | | 1134.64 | | 3.7425 | |
| BeS | 19.52 | | 113.11 | 111.81 | | | | | 3.12 | 3.01 | | | 92.44 | 76.7 | 0.8172 | |
| BeSe | 18.39 | | 96.55 | 97.29 | | | | | 2.54 | 2.52 | | | 58.73 | 60.1 | 0.6082 | |
| BeTe | 16.12 | | 68.81 | 71.54 | | | | | 1.50 | 1.64 | | | 29.72 | 42 | 0.4319 | |
| ZnO | 21.48 | | 146.19 | 139.78 | 90 | 61 | 75.21 | 3.9, 4.8, 4[+](M) | 4.22 | 3.96 | 4.6 | | 148.42 | | 1.0152 | |
| ZnS | 16.71 | 77 | 75.31 | 77.80 | 75 | 58 | 65.7 | 1.7[+], 2.8, 3.5 | 1.75 | 1.86 | 3.3 | 31.9 | 35.48 | 29.1 | 0.4711 | 0.4142 |
| ZnSe | 15.78 | 62 | 65.30 | 68.07 | 59 | 54 | 61.46 | 1.3 - 1.8 | 1.36 | 1.52 | 1.7 | 32.9 | 26.84 | 31.7 | 0.4110 | 0.5306 |
| ZnTe | 14.76 | 51 | 55.74 | 58.24 | 69 | 66 | 61.6 | 0.8 - 1.1 | 0.96 | 1.19 | 1.0 | 24.8 | 19.76 | 25.4 | 0.3545 | 0.4862 |
| CdS | 14.88 | 62 | 56.79 | 59.35 | 60 | 60 | 58.9 | 1.2[+], 1.22[b] | 1.00 | 1.23 | 1.1 | 16.9 | 20.49 | 17.6 | 0.3608 | 0.2725 |
| CdSe | 14.01 | 53 | 49.67 | 51.57 | 47 | 56 | 41.6 | 0.7[+]- 1.2 | 0.68 | 0.96 | 0.8 | 13.6 | 15.78 | 13.9 | 0.3176 | 0.2566 |
| CdTe | 13.09 | 42 | 43.32 | 44.01 | | | | 0.4[+]- 0.64 | 0.37 | 0.71 | 0.5 | 10.5 | 11.97 | 9.8 | 0.2763 | 0.2500 |
| MgTe | 12.97 | | 42.58 | 43.07 | | | | | 0.33 | 0.68 | | | 11.55 | | 0.2712 | |
| HgS | 14.85 | | 56.52 | 59.07 | | | | | 0.99 | 1.22 | | | 20.30 | 15 | 0.3591 | |
| HgSe | 13.99 | | 49.52 | 51.39 | | | | | 0.68 | 0.96 | | 16.5 | 15.69 | 15.4 | 0.3168 | |
| HgTe | 12.85 | | 41.87 | 42.15 | | | | | 0.29 | 0.65 | | 12.9 | 11.14 | 12.2 | 0.2660 | |
| **Average % deviation** | | | **5.77** | **6.0** | **14.98** | **14.38** | **6.91** | | **4.58** | **5.01** | **2.35** | | **12.75** | **3.86** | | |
| $A^{III}B^{V}$ | | | | | | | | | | | | | | | | |
| BN | 24.53 | | 152.06 | 218.52 | | | | 34.3 - 73.0 | 39.70 | 29.57 | 45.8 | 414 | 338.04 | 400.9 | 2.2152 | |
| BP | 21.71 | | 131.49 | 164.33 | | | | 31.4[+]- 40 | 25.91 | 20.81 | 32.3 | 139 | 181.77 | 142.3 | 1.3823 | |
| BAS | 20.12 | | 118.70 | 137.61 | | | | 19.0 | 19.46 | 16.50 | 10.9 | | 128.12 | 165.4 | 1.0793 | |
| AlP | 16.65 | 86 | 87.77 | 88.47 | 87 | 79 | 86.7 | | 8.71 | 8.55 | 6.30 | | 59.71 | 61.7 | 0.6803 | |
| AlAS | 15.75 | 77 | 79.08 | 77.71 | 79 | 66 | 75.3 | | 6.67 | 6.81 | | | 48.98 | 54.2 | 0.6193 | |
| AlSb | 13.72 | 58 | 58.45 | 56.32 | 57 | 61 | 55.4 | 4.0[c,+] | 3.18 | 3.36 | 10.90 | 31.1 | 31.34 | 28.2 | 0.5361 | 0.5362 |
| GaN | 21.98 | | 133.58 | 169.14 | | | | | 27.10 | 21.60 | | | 192.90 | 144 | 1.4440 | |
| GaP | 16.50 | 89 | 86.34 | 86.63 | 87 | 74 | 89.79 | 9.45[a] | 8.55 | 8.25 | | 58 | 57.77 | 57.6 | 0.6690 | 0.6516 |
| GaAs | 15.35 | 75 | 75.12 | 73.20 | 77 | 65 | 70.6 | 7.50[a], 7.21[b,+] | 5.86 | 6.08 | | 48.8 | 44.86 | 50.1 | 0.5971 | 0.6506 |
| GaSb | 13.38 | 57 | 54.86 | 53.12 | 58 | 59 | 55.5 | 4.48[a] | 2.75 | 2.84 | | 35.4 | 29.08 | 34.1 | 0.5300 | 0.6210 |
| InN | 18.82 | | 107.59 | 117.75 | | | | | 14.90 | 13.28 | | | 96.25 | 73.3 | 0.8946 | |
| InP | 14.76 | 71 | 69.19 | 66.80 | 67 | 63 | 68.75 | 4.10[a], 4.30[b,+] | 4.78 | 5.05 | 5.30 | 36.5 | 39.40 | 36.5 | 0.5694 | 0.5140 |
| InAs | 14.07 | 60 | 62.11 | 59.73 | 61 | 61 | 58.19 | 3.30[a], 3.84[b,+] | 3.68 | 3.91 | | 31.4 | 33.85 | 33.7 | 0.5450 | 0.5233 |
| InSb | 12.73 | 47 | 47.88 | 47.30 | 47 | 55 | 45.05 | 2.20[+] | 2.05 | 1.90 | | 24.2 | 25.20 | 23.3 | 0.5263 | 0.5148 |
| **Average % deviation** | | | **2.37** | **2.84** | **2.15** | **10.13** | **3.02** | | **10.08** | **22.18** | **30.30** | | **5.21** | **3.65** | | |

[+]These values have been used for regression of Eqs (2) and (5) and calculating average % deviation, where more than one experimental values are available

[#]References of individual experimental values of G are given in [Ref. 19]

[$]G/B Ratio have been calculated from the experimental values of B and G listed in column 3 and 13

[a][Ref. 32], [b][Ref. 33], [c][Ref. 34]

Table 3 — Bulk modulus, microhardness and shear modulus of group I-III-$VI_2$ and II-IV-$V_2$ semiconductors

| Compds | $\hbar\omega_p$ | Bulk modulus ($B$) (GPa) | | | | | | | Microhardness ($H$) ( GPa) | | | | | Shear modulus ($G$) (GPa) | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | (eV) | This | | Reported | | | | | This | Expt*. | Reported | | | This | Reported | | G/B Ratio | |
| | [Ref.17] | Work Eq.(2) | Expt*. [Ref.17] | [Ref.36] | [Ref.17] | [Ref.37] | [Ref.38] | [Ref.39] | Work Eq.(2) | [Ref.17] | [Ref.40] | [Ref.17] | [Ref.41] | Work Eq.(5) | | | This Work | reported [Ref.13] |
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
| **$A^IB^{III}C_2^{VI}$** | | | | | | | | | | | | | | | | | | |
| $CuAlS_2$ | 17.25 | 95.86 | $94^+$, 99 | | 84.02 | 96.8 | 96 | 85.3 | 4.28 | $4.33^+$ | 2.45 | 3.84 | 2.56 | 51.06 | 51.56[a] | 40.443[b] | 0.5326 | |
| $CuAlSe_2$ | 15.86 | 68.32 | $84^+$ | | 69.06 | 77.3 | 80 | 72.9 | 2.58 | $3.19^+$, 2.06 | 2.21 | 2.95 | 2.23 | 36.37 | 35.89[a] | 32.917[b] | 0.5323 | |
| $CuAlTe_2$ | 14.35 | 44.38 | | | 54.68 | 57.2 | 64 | 53.5 | 1.44 | $1.78^+$, 1.82 | 2.50 | 2.09 | 2.06 | 25.16 | 26.81[a] | 28.964[b] | 0.5669 | |
| $CuGaS_2$ | 17.10 | 92.64 | $94^+$, 96, 97 | | 82.32 | 95.8 | 94 | 98.0 | 4.07 | $4.22^+$, 4.81-7.10 | 2.25 | 3.74 | 2.40 | 49.23 | 50.06[a] | | 0.5314 | |
| $CuGaSe_2$ | 15.92 | 69.40 | $71^+$, 94 | | 69.67 | 76.6 | 79 | 69.3 | 2.64 | $3.23^+$,1.93 , 4.2 | 1.93 | 2.98 | 2.06 | 36.91 | 37.29[a] | | 0.5318 | |
| $CuGaTe_2$ | 14.30 | 43.69 | $44^+$ | | 54.24 | 55.4 | 38 | 48.5 | 1.41 | $1.77^+$, 2.11, 3.14, 3.5 | 2.35 | 2.07 | 1.81 | 24.86 | 25.78[a] | | 0.5690 | |
| $CuInS_2$ | 16.12 | 73.07 | $75^+$ | | 71.73 | 84.4 | 81 | 72.9 | 2.85 | $2.84^+$, 4.9-6.2, 2.26, 2.55 | 1.37 | 3.10 | 1.37 | 38.76 | 37.29[a] | | 0.5304 | |
| $CuInSe_2$ | 15.09 | 55.33 | $53^+$, 48, 62, 72 | | 61.49 | 68.4 | 69 | 64.0 | 1.91 | $1.81^+$ , 2.05 | 1.57 | 2.49 | 1.38 | 30.14 | 31.71[a] | | 0.5447 | |
| $CuInTe_2$ | 13.66 | 35.51 | $36^+$, 45.4 | | 48.74 | 50.6 | 51 | 45.0 | 1.60 | $1.49^+$, 1.87, 0.4 | 1.63 | 1.74 | 1.37 | 21.26 | 21.89[a] | | 0.5987 | |
| $CuTlS_2$ | 15.89 | 68.86 | | 71 | 69.36 | | | | 2.61 | $2.96^+$ | | 2.96 | | 36.64 | | | 0.5320 | |
| $CuTlSe_2$ | 14.88 | 52.07 | | 53 | 59.51 | | | | 1.76 | | | 2.37 | | 28.64 | | | 0.5500 | |
| $CuFeS_2$ | 17.19 | 94.57 | | 105 | 83.33 | | | | 4.20 | | | 3.79 | | 50.32 | | | 0.5320 | |
| $AgAlS_2$ | 16.26 | 75.71 | | | 73.19 | 79.9 | 82 | 75.2 | 3.01 | $3.19^+$ | | 3.19 | | 40.10 | | | 0.5296 | |
| $AgAlSe_2$ | 15.16 | 56.45 | | | 62.15 | 65 | 70 | 62.8 | 1.96 | $1.60^+$, 1.57 | 1.68 | 2.53 | | 30.66 | 30.97[a] | | 0.5431 | |
| $AgAlTe_2$ | 14.50 | 46.48 | | | 56.02 | 48.8 | 54 | 40.4 | 1.52 | $1.49^+$, 1.46 | 1.64 | 2.17 | | 26.10 | 20.64[a] | | 0.5615 | |
| $AgGaS_2$ | 16.10 | 72.70 | $72^+$, 60, 67, 90 | | 71.52 | 77.6 | 76 | 67.2 | 2.83 | | 1.71 | 3.09 | | 38.57 | 37.46[a] | | 0.5305 | |
| $AgGaSe_2$ | 14.76 | 50.26 | $59.8^+$, 65 | | 58.39 | 63.8 | 63 | 59.9 | 1.67 | $1.43^+$, 1.40 , 4.4 | 1.55 | 2.32 | | 27.81 | 27.94[a] | | 0.5533 | |
| $AgGaTe_2$ | 13.63 | 35.15 | $35.7^+$, 71.5, 76.6 | | 48.49 | 48.6 | 21 | 38.9 | 1.15 | $1.32^+$, 1.76, 1.8 | 1.63 | 1.73 | | 21.11 | 20.49[a] | | 0.6005 | |
| $AgInS_2$ | 15.21 | 57.25 | | | 62.63 | 71.6 | 66 | 55.0 | 2.00 | $2.2^+$ | | 2.56 | | 31.04 | 29.26[a] | | 0.5421 | |
| $AgInSe_2$ | 14.23 | 42.74 | $42^+$ | | 53.62 | 58.3 | 50 | 48.7 | 1.38 | $1.24^+$, 1.85 | 1.00 | 2.02 | | 24.44 | 23.50[a] | | 0.5718 | |
| $AgInTe_2$ | 13.04 | 28.65 | | | 43.73 | 44.1 | 29 | 24.5 | 1.04 | $1.15^+$ , 1.18 | 1.14 | 1.44 | | 18.28 | 18.06[a] | | 0.6380 | |
| $AgFeS_2$ | 16.24 | 75.33 | | | 72.98 | | | | 2.98 | | | 3.18 | | 39.91 | | | 0.5298 | |
| **Average %** | **Devi.** | **05.35** | | | **11.77** | **13.14** | **10.42** | **5.69** | **11.72** | | **17.27** | **18.28** | **20.62** | | | | | |
| **$A^{II}B^{IV}C_2^V$** | | | [Ref.13] | [Ref.42] | [Ref.17] | [Ref.43] | [Ref.44] | [Ref.45] | | | [Ref.40] | [Ref.17] | [Ref.41] | | | | | [Ref.13] |
| $ZnSiP_2$ | 17.02 | 78.93 | $79^+$ | 73.2 | 93.13 | 120.3 | 79.0 | 66.9 | 12.01 | $12.20^+$ , 10.79 , 11 | 8.83 | 11.43 | 10.45 | 60.22 | 48.59[a] | 59.31[c] 55.45[d] | 0.7629 | 0.77 |
| $ZnGeP_2$ | 16.64 | 75.83 | $86^+$ | 86.0 | 88.35 | 107.6 | 73.6 | 71.2 | 10.43 | $9.80^+$, 9.61 , 8.1 | 6.23 | 10.06 | 7.60 | 54.41 | 39.19[a] | 54.87[c] | 0.7175 | 0.82 |
| $ZnSnP_2$ | 15.55 | 66.91 | $68.4^+$ | | 75.44 | 84.2 | 67.5 | 57.7 | 6.78 | $6.5^+$ , 7.00 , 6.37 | 5.20 | 6.35 | 4.90 | 40.67 | | 46.05[c] 40.97[e] | 0.6078 | 0.74 |
| $CdSiP_2$ | 16.19 | 72.15 | $97^+$ | 71.9 | 82.88 | 97.0 | 48.0 | 60.9 | 8.77 | $9.30^+$, 10.5 | 7.16 | 8.50 | 7.49 | 48.25 | 40.24[a] | 45.28[c] | 0.6687 | 0.60 |
| $CdGeP_2$ | 15.52 | 66.66 | $68.1^+$ | 67.4 | 75.10 | 86.4 | 47.0 | 60.4 | 6.70 | $6.70^+$, 5.54 , 4.02, 5.65 | 4.61 | 6.26 | 5.10 | 40.34 | 29.35[a] | 42.30[c] | 0.6051 | 0.65 |

*Contd —*

Table 3 — Bulk modulus, microhardness and shear modulus of group I-III-$VI_2$ and II-IV-$V_2$ semiconductors — *Contd*

| Compds | $\hbar\omega_p$ | Bulk modulus ($B$) (GPa) | | | | | | | Microhardness ($H$) ( GPa) | | | | | Shear modulus ($G$) (GPa) | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | (eV) | This Work Eq.(2) | Expt*. | Reported | | | | | This Work Eq.(2) | Expt*. | Reported | | | This Work Eq.(5) | Reported | | G/B Ratio | |
| | | | | | | | | | | | | | | | | | This Work | reported [Ref.13] |
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
| $CdSnP_2$ | 14.82 | 60.90 | | 55.9 | 67.43 | 67.2 | 52.5 | 50.2 | 5.06 | $5^+$, 5.29 | 2.50 | 4.10 | 2.69 | 33.47 | 20.42[a] | 34.02[c] | 0.5495 | 0.57 |
| $ZnSiAs_2$ | 16.05 | 71.01 | 69.6[+] | 69.6 | 81.22 | 93.4 | 68.0 | 53.2 | 8.29 | 9.02[+], 8.80 , 9.2 | 8.04 | 8.02 | 8.07 | 46.48 | 37.16[a] | 48.85[c] | 0.6545 | 0.76 |
| $ZnGeAs_2$ | 15.66 | 67.81 | 67[+] | 53.8 | 76.68 | 85.7 | 67.0 | | 7.09 | 6.8[+] , 6.60 , 6.67 | 6.18 | 6.714 | 6.70 | 41.88 | 31.08[a] | 44.20[c] | 0.6176 | 0.78 |
| $ZnSnAs_2$ | 14.82 | 60.90 | 56.6[+] | 56.6 | 67.43 | 67.0 | 55.8 | | 5.06 | 5.40[+] , 4.46, 4.55 | 4.22 | 4.10 | 4.39 | 33.47 | 25.40[a] | 31.98[c] | 0.5495 | 0.62 |
| $CdSiAs_2$ | 15.35 | 65.26 | | | 73.19 | 77.0 | 54.0 | | 6.25 | 6.10[+] , 6.85 | 6.03 | 5.71 | 6.29 | 38.55 | 28.88[a] | 36.60[c] | 0.5907 | 0.59 |
| $CdGeAs_2$ | 14.90 | 61.56 | 69.7[+] | 47.7 | 68.28 | 69.7 | 41.3 | | 5.22 | 5.20[+] , 4.61, 4.70 | 4.61 | 4.30 | 4.79 | 34.19 | 23.00[a] | 30.12[c]<br>30.54[f]<br>27.95[f] | 0.5553 | 0.54 |
| $CdSnAs_2$ | 14.12 | 55.12 | 54.8[+] | 49.9 | 60.23 | 54.8 | 37.1 | | 3.96 | 4.00[+] , 3.43, 3.28, 3.45 | 3.04 | 2.00 | 3.09 | 27.76 | 19.11[a] | 29.52[c] | 0.5036 | 0.57 |
| **Average %** | **Dev.** | **06.48** | | **10.49** | **11.79** | **20.78** | **17.39** | **18.49** | **2.68** | | **14.81** | **9.13** | **10.72** | | | | | |
| $BeSiP_2$ | 18.13 | 87.95 | | | | | | | 17.54 | | | | | 80.99 | | | 0.9208 | |
| $BeSiAs_2$ | 16.91 | 78.04 | | | | | | | 11.54 | | | | | 58.47 | | | 0.7492 | |
| $BeGeP_2$ | 17.61 | 83.74 | | | | | | | 14.78 | | | | | 70.49 | | | 0.8417 | |
| $BeGeAs_2$ | 16.46 | 74.36 | | | | | | | 9.74 | | | | | 51.85 | | | 0.6972 | |
| $BeSnp_2$ | 16.45 | 74.28 | | | | | | | 9.70 | | | | | 51.72 | | | 0.6962 | |
| $BeSnAs_2$ | 15.48 | 66.33 | | | | | | | 6.59 | | | | | 39.91 | | | 0.6016 | |
| $MgSiP_2$ | 16.04 | 70.93 | | | | | | | 8.26 | | | | | 46.35 | | | 0.6534 | |
| $MgSiAs_2$ | 15.08 | 63.04 | | | | | | | 5.61 | | | | | 35.87 | | | 0.5690 | |
| $MgGeP_2$ | 15.67 | 67.89 | | | | | | | 7.12 | | | | | 41.99 | | | 0.6185 | |
| $MgGeA_2$ | 14.68 | 59.75 | | | | | | | 4.80 | | | | | 32.24 | | | 0.5395 | |
| $MgSnP_2$ | 14.73 | 60.16 | | | | | | | 4.89 | | | | | 32.67 | | | 0.5430 | |
| $MgSnA_2$ | 13.93 | 53.55 | | | | | | | 3.76 | | | | | 26.39 | | | 0.4928 | |
| $MnGeP_2$ | 15.64 | 67.65 | | | | | | | 7.03 | | | | | 41.66 | | | 0.6158 | |

*References of individual experimental data of B are given in [Ref. 17]

+These values have been taken for regression of Eqs. (2) and (5) and calculating average percentage deviation, where more than one experimental values are available.

[a][Ref.21], [b][Ref.20], [c][Ref.13] , [d][Ref.46], [e][Ref.27], [f][Ref.47]

simulated the known values of $G$ and $\hbar\omega_p$ and proposed a simple relation for the calculation of $G$ (in GPa) for IV, II-VI, III-V, I-III-$VI_2$ and II-IV-$V_2$ semiconductor materials:

$$G = K_4 \exp|K_5 \hbar\omega_p)| \quad \ldots(5)$$

where $K_4$ and $K_5$ are the constants and their numerical values are given in Table 1. The calculated values of shear modulus $G$ from Eq. (5) are listed in Tables 2 and 3 along with the available experimental and reported values. The ratio of $G/B$ gives the information about covalent and ionic behaviour of materials on the basis of their brittle and ductile character in solids[28,29], are also calculated and presented in Tables 2 and 3. The upper limits of $G/B$ are 1.1 for brittle and 0.6 for ductile character, i.e., if $G/B \leq 0.60$, the materials are ductile (ionic), otherwise brittle (covalent) in nature.

## 3 Results and Discussion

Using Eqs (2) and (5), the values of $B$, $H$ and $G$ of group IV, II-VI and III-V semiconductor materials have been calculated and listed in Table 2 and I-III-$VI_2$, and II-IV-$V_2$ materials in Table 3 along with the available experimental and reported values. The values of these parameters for 13 new compounds of II-IV-$V_2$ family have been calculated for the first time and listed in bottom rows of Table 3. The calculated values are in good agreement with the available experimental and reported values. We have also calculated the average percentage deviation of proposed Eqs. (2) and (5) using the relation: Percentage deviation = [|Experimental value– Calculated Valuel/Experimental value] × 100. In the case of Eq. (2), the average percentage deviation of $B$ for IV, II-VI and III-V materials has been estimated between 0.13% to 5.77% against the earlier estimations between 1.01 to 14.98%. However, in the case of I-III-$VI_2$ and II-IV-$V_2$ chalcopyrites, it has been estimated between 5.35 to 6.48% against the earlier estimations between 5.69-20.78%. The average percentage deviation of Eq. (2) for $H$ has been found between 1.13 to 10.08% against the earlier estimations between 2.35 to 30.30% for group IV, II-VI and III-V, and 2.68 to 11.72% against the earlier estimations between 9.13 and 20.62% for I-III-$VI_2$ and II-IV-$V_2$ semiconductors. In the case of Eq. (5), the average percentage deviation of $G$ for group IV, II-VI and III-V semiconductors has been found in the range 2.81-12.75% against earlier values between 3.65-10.77%. The average percentage deviation of $G$ for ternary chalcopyrite has not been calculated due to unavailability of experimental values. However, these data have been compared with the reported values. The calculated values of $G/B$ ratio, which show the ionic and covalent nature of the materials, are also listed in Table 2 for group IV, II-VI and III-V, and Table 3 for I-III-$VI_2$ and II-IV-$V_2$ materials along with available experimental values in few cases where the experiments have been performed and the reported values. A fairly good agreement has obtained between them. The calculated average percentage deviations of all groups of semiconductor materials are also listed in Tables 2 and 3. In almost all cases, the average percentage deviation of proposed relations is lower than the earlier correlations. The main advantage of the present models is the simplicity of the formulae, which do not require any experimental data except the plasmon energy of the materials while the earlier models require the experimental values of bond length, ionicity, melting temperature and atomic volume in their calculation.

## 4 Conclusions

Hence, it is possible to calculate the values of $B$, $H$ and $G$ of group IV, II-VI, III-V, I-III-$VI_2$ and II-IV-$V_2$ semiconductor materials from their plasmon energy data. The predictive nature of the proposed relations is of great importance in predicting the values of $B$, $H$, $G$ and $G/B$ ratio of new compounds of these group having the same crystal structure. The lower percentage deviation shows the significant improvement over the earlier models.

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