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Calculation of the elastic properties of semiconductors

San-Guo Shen†‡§

† China Centre of Advanced Science and Technology (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China

‡ Fundamental and Applied Science Research Institute of Henan, Henan, People's Republic of China

§ Department of Physics, Zhengzhou University, Zhengzhou 450052, Henan, People's Republic of China

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Abstract. For 30 diamond- and zincblende-structure semiconductors, the bond length d , bond polarity α_p , bulk modulus B , elastic shear constants $(c_{11} - c_{12})/2$ and c_{44} , bond-stretching force constant α , bond-bending force constant β , internal displacement parameter ζ , effective atomic charge Z^* , transfer parameter β^* , transverse charge e_T^* , and piezoelectric charge e_p^* are calculated from bond orbital calculations based on the tight-binding method. The results are compared with previous theoretical calculations and experiments.

1. Introduction

Theoretical studies for the elastic properties of semiconductors have been made by many researchers, using, for example, a bond-orbital model (BOM) [1, 2], band-structure calculations and the 'special-points' method [3], a first-principles linear-combination of atomic orbitals (LCAO) method [4], pseudopotential methods with the local-density approximation (LDA) [5–7], the linear muffin-tin orbitals (LMTO) method [8, 9], the universal tight-binding parameters (UTBP) method [10], and the extended Hückel tight-binding (XHTB) method [11].

The LDA has proven to be an effective and useful means for studying both structural and electronic properties in a few materials [5–7]. However, the inclusion of a total-energy calculation in the problem necessarily makes the LDA theory more complicated than the BOM theory; systematic study of the properties in many materials would need a powerful computer, and it will take much time; therefore, the cost will be expensive.

In order to obtain the structural trends, the simple BOM is used in this paper to study the elastic properties of semiconductors systematically. We calculate the bond length d , and bond polarity α_p , bulk modulus B , elastic shear constants $(c_{11} - c_{12})/2$ and c_{44} , bond-stretching force constant α , bond-bending force constant β , internal displacement parameter ζ , effective atomic charge Z^* , transfer parameter β^* , transverse charge e_T^* , the piezoelectric charge e_p^* , and the ratios c_{12}/c_{11} , $[(c_{11} - c_{12})/2]/B$ and β/α for 30 diamond- and zincblende-structure semiconductors and compare the values with others from theoretical calculations and experiments.

2. Theoretical formalism

2.1. Bond length and polarity

Tight-binding theory has been able to obtain approximate but meaningful predictions of the bonding properties of solids. In order to improve the description of the bond energy, Baranowski [2] made a very simple modification of the overlap interaction on the basis of the idea and method proposed by Harrison [1] and gave a formula for the bond length of semiconductors. For all tetrahedral compounds, the bond length d can be obtained from [2]

$$d = \frac{(-2\eta_\sigma \hbar^2/m)^{1/2}}{(k^2 \bar{\epsilon}_h^2 - 4V_3^2)^{1/4}} \quad (1)$$

where for sp^3 bonds $\eta_\sigma = \frac{1}{4}\eta_{ss\sigma} - (2\sqrt{3}/4)\eta_{sp\sigma} - \frac{3}{4}\eta_{pp\sigma}$, in which $\eta_{ss\sigma} = -1.4$, $\eta_{sp\sigma} = 1.84$ and $\eta_{pp\sigma} = 3.24$ are dimensionless Harrison [1] universal parameters and $\hbar^2/m = 7.62 \text{ eV \AA}^2$. The effective parameter k will be given by the following average:

$$k = (k_i k_j)^{1/2} \quad (2)$$

where k_i and k_j are connected with rows i and j , respectively, of the periodic table. The cation-anion average hybrid energy $\bar{\epsilon}_h$ is the weighted average given by

$$\bar{\epsilon}_h = \frac{1}{8}(n_c \epsilon_h^c + n_a \epsilon_h^a) \quad (3)$$

where n_c and n_a are the numbers of electrons associated with cations and anions, respectively, which participate in the bonds. ϵ_h^c and ϵ_h^a are the average values of the cation and anion hybrid energies, respectively:

$$\begin{aligned} \epsilon_h^c &= \frac{1}{4}(\epsilon_s^c + 3\epsilon_p^c) \\ \epsilon_h^a &= \frac{1}{4}(\epsilon_s^a + 3\epsilon_p^a) \end{aligned} \quad (4)$$

in which ϵ_s^c , ϵ_p^c , ϵ_s^a and ϵ_p^a are the free-atom energies for s and p states for the cations and anions, respectively [12]. V_3 is the hybrid polar energy, which can be approximated in the following way:

$$V_3 = \frac{1}{2}(\epsilon_h^c - \epsilon_h^a). \quad (5)$$

The bond polarity of the compound can be obtained from

$$\alpha_p = \frac{V_3}{(V_2^2 + V_3^2)^{1/2}} \quad (6)$$

where V_2 is the hybrid covalent energy, which can be approximated in the following way:

$$V_2 = -\eta_\sigma \frac{\hbar^2}{md^2}. \quad (7)$$

2.2. Bulk modulus and elastic shear constant

According to the BOM proposed by Baranowski [2], the bulk modulus is given by

$$B = \frac{2\sqrt{3}}{3} \left(V_2 \alpha_c^3 + \frac{7.8}{d^2} \right) \frac{1}{d^3} \quad (8)$$

where the hybrid covalency α_c is defined by $(1 - \alpha_p^2)^{1/2}$.

The elastic shear constant $(c_{11} - c_{12})/2$ is given by

$$\frac{(c_{11} - c_{12})}{2} = \frac{\sqrt{3}}{4} (V_2 \alpha_c^3 (1 + \lambda) - \frac{3}{4} |V_{pp\pi}|) \frac{1}{d^3} \quad (9)$$

where λ is a dimensionless parameter, which is defined as follows:

$$\lambda = \frac{\sqrt{3} V_{sp\sigma} - 3 V_{pp\sigma}}{V_{ss\sigma} - 2\sqrt{3} V_{sp\sigma} - 3 V_{pp\sigma}} \quad (10)$$

where $V_{ss\sigma}$, $V_{sp\sigma}$, $V_{pp\sigma}$ and $V_{pp\pi}$ in equation (9) are the matrix elements [1]. Combining equations (8), (9) and $B = \frac{1}{3}(c_{11} + 2c_{12})$, one can obtain the elastic constants

$$c_{11} = \frac{\sqrt{3}}{3} \left(V_2 \alpha_c^3 (3 + \lambda) - \frac{3}{4} |V_{pp\pi}| + 2 \frac{7.8}{d^2} \right) \frac{1}{d^3} \quad (11)$$

and

$$c_{12} = \frac{\sqrt{3}}{6} \left(V_2 \alpha_c^3 (3 - \lambda) + \frac{3}{4} |V_{pp\pi}| + 4 \frac{7.8}{d^2} \right) \frac{1}{d^3}. \quad (12)$$

Within the framework of the valence force field model [1], the elastic stiffness constant c_{44} and Kleinman's internal displacement parameter ζ of diamond- and zincblende-structure semiconductors are given by

$$c_{44} = 3(c_{11} + 2c_{12})(c_{11} - c_{12})/(7c_{11} + 2c_{12}) \quad (13)$$

$$\zeta = (c_{11} + 8c_{12})/(7c_{11} + 2c_{12}). \quad (14)$$

The macroscopic elastic constants B and $(c_{11} - c_{12})/2$ are related to force constants α and β by the equations [13]

$$3B = \frac{\sqrt{3}}{4d} (3\alpha + \beta) - 0.355SC_0 \quad (15)$$

and

$$\frac{(c_{11} - c_{12})}{2} = \frac{\sqrt{3}}{2d} \beta - 0.053SC_0 \quad (16)$$

where SC_0 is the Coulomb contribution (rather small for all III-V zincblende-structure semiconductors). If we neglect the Coulomb contribution, the bond-stretching force constant α and bond-bending force constant β can be obtained from

$$\beta = \frac{2d}{\sqrt{3}} \frac{(c_{11} - c_{12})}{2} \quad (17)$$

$$\alpha = \frac{4d}{\sqrt{3}} B - \frac{1}{3} \beta. \quad (18)$$

Table 1. Predicted bond length of semiconductors. The experimental bond lengths are taken from [14].

Material	d (Å)		Material	d (Å)	
	BOM	Experiment		BOM	Experiment
C	1.615	1.54	InAs	2.618	2.61
Si	2.357	2.35	InSb	2.820	2.81
Ge	2.448	2.44	BeS	1.900	2.10
Sn	2.802	2.81	BeSe	1.988	2.20
SiC	1.953	1.88	BeTe	2.190	2.40
BN	1.573	1.57	ZnS	2.302	2.34
BP	1.957	1.97	ZnSe	2.413	2.45
BAs	2.016	2.07	ZnTe	2.658	2.64
AlP	2.343	2.36	CdS	2.478	2.53
AlAs	2.417	2.43	CdTe	2.865	2.80
AlSb	2.610	2.66	CuF	1.534	1.84
GaP	2.370	2.36	CuCl	2.122	2.34
GaAs	2.443	2.45	CuBr	2.268	2.49
GaSb	2.635	2.65	CuI	2.576	2.62
InP	2.538	2.54	AgI	2.799	2.80

2.3. Transverse and piezoelectric charges

An effective charge Z^* for a cation can be obtained in tight-binding theory as the column number Z (it is less than four for a cation) for that element minus the sum over occupied states of the squared amplitudes of the orbitals of that atom. The bond orbital approximation gives an approximate value of [1]

$$Z^* = Z - 4 + 4\alpha_p. \quad (19)$$

The transverse charge e_T^* is given by

$$e_T^* = Z^* + \frac{4}{3}\beta^* \quad (20)$$

where β^* is the transfer parameter, which is defined by

$$\beta^* = (d/4)\partial Z^*/\partial d = 2\alpha_p(1 - \alpha_p^2). \quad (21)$$

Similarly, the piezoelectric charge e_p^* is given by

$$e_p^* = Z^* - (4\beta^*/3)(1 - \zeta)/\zeta. \quad (22)$$

All effective charges for the anion are the negative charges of the corresponding charges for the cations given here.

3. Results and discussion

In this section we present the results of the BOM calculation for the bond length d , bond polarity α_p , bulk modulus B , elastic shear constants $(c_{11} - c_{12})/2$ and c_{44} , bond-stretching force constant α , bond-bending force constant β , internal displacement parameter ζ , effective atomic charge Z^* , transfer parameter β^* , transverse charge e_T^* and piezoelectric charge e_p^* for 30 diamond- and zincblende-structure semiconductors and compare their values with other values from theoretical calculations and experiments.

(i) Predictions of the bond length for semiconductors are given in table 1 together with the experimental values [14]. It is remarkable that the simple equation (1), which has been given by Baranowski [2], can reproduce the bond length with an accuracy of the order of a few per cent for most cases.

(ii) Results for the polarity α_p obtained from BOM are listed in table 2, together with those for the UTBP, Hückel tight-binding (HTB), the XHTB methods [11], the cluster (Cl) method, and Brillouin-zone (BZ) integration of the LCAO Hamiltonian [15]. For comparison, the values of polarity α_p ($\equiv f_i^{1/2}$) given by Phillips (Ph) [11] and obtained by experiment (from the experiment-deduced ionicity scale (the definition is the same as Harrison's polarity) of Falter *et al* [16]), are also given in table 2. From a comparison of these values, we see that results obtained from BOM are in good agreement with the experiments.

Table 2. Comparison of polarities from various calculations. Results for polarity α_p obtained from the BOM, the band-structure calculations based on the UTBP, HTB and XHTB methods, Cl method, BZ integration of LCAO Hamiltonian. For comparison, the values of polarity α_p obtained by Ph and in experiment are also given.

Material	α_p							Experiment
	Cl	BZ	UTBP	HTB	XHTB	Ph	BOM	
SiC							0.16	0.10
AlP	0.42	0.44					0.34	0.33
AlAs	0.39	0.41					0.34	0.31
AlSb	0.32	0.34					0.29	0.30
GaP	0.38	0.40	0.35	0.42	0.59	0.57	0.32	0.31
GaAs	0.35	0.37	0.33	0.37	0.53	0.56	0.32	0.30
GaSb	0.28	0.30	0.27	0.26	0.38	0.51	0.26	0.29
InP	0.46	0.48	0.43	0.46	0.66	0.65	0.40	0.32
InAs	0.42	0.44	0.40	0.42	0.61	0.60	0.40	0.30
InSb	0.35	0.37	0.35	0.33	0.49	0.57	0.34	0.29
ZnS	0.55	0.56	0.61	0.62	0.86	0.79	0.55	0.60
ZnSe	0.55	0.56	0.60	0.58	0.82	0.79	0.55	0.59
ZnTe	0.54	0.55	0.57	0.51	0.73	0.77	0.54	0.57
CdTe	0.58	0.59	0.63	0.54	0.77	0.82	0.61	0.58

(iii) The values of the transverse and piezoelectric charges obtained from equations (20) and (22) with a β -value obtained from equation (21), are listed together with the corresponding Z^* in table 3. The experimental values [16] are also listed for comparison. It is clear from table 3 that the effective atomic charges are in good agreement with the experiments in most cases; the transverse charges are about one electron less than in the experiments. When the experimental value of α_p is used in equation (20), one cannot obtain the transverse charges, which are comparable with experiments. So the difference is not only from α_p ; this suggests a significant error in equation (20). The piezoelectric charges are in good agreement with the experiments for III-V compound semiconductors.

(iv) The results for the covalency α_c , the values of the bulk modulus B together with the elastic stiffness constants $(c_{11} - c_{12})/2$ and c_{44} , bond-stretching force constant α , bond-bending force constant β and Kleinman's internal displacement parameters ζ are shown in table 4. The reliable values for ζ are those obtained recently by Molinas-Mata and Cardona [17] by the fitting of the phonon dispersion curves along the [100] and [111] axes with planar force constants. The values that they obtained are 0.564 ± 0.030 and 0.577 ± 0.027 for Si and Ge, respectively, to be compared with our values of 0.548 and 0.548. The LDA [5] results of ζ for Si and Ge are 0.56 and 0.57, respectively; they are in excellent agreement with the results of [17].

The ratios c_{12}/c_{11} , $[(c_{11} - c_{12})/2]/B$ ($\equiv \kappa$) and β/α are also given in table 4. It is clear from the table that, according to our calculations, the ζ and the ratio c_{12}/c_{11} monotonically

Table 3. Results calculated for diamond- and zincblende-structure semiconductors of effective atomic charge Z^* , transfer parameter β^* , transverse charge e_T^* and the piezoelectric charge e_p^* . For comparison, the values of experiment are also given.

Material	Z^*		β^*	e_T^*		e_p^*	
	BOM	Experiment		BOM	Experiment	BOM	Experiment
SiC	0.640	0.38	0.312	1.06	2.57	0.300	
BN	-0.096	0.55	0.429	0.476	2.47	-0.577	
BP	-0.452		0.269	-0.093		-0.745	
BAs	-0.480		0.256	-0.139		-0.759	
AlP	0.350	0.30	0.598	1.15	2.28	-0.270	
AlAs	0.350	0.26	0.598	1.15	2.30	-0.270	-0.22
AlSb	0.157	0.19	0.530	0.864	1.93	-0.402	
GaP	0.279	0.24	0.574	1.04	2.04	-0.320	-0.28
GaAs	0.272	0.20	0.572	1.03	2.16	-0.325	-0.47
GaSb	0.051	0.15	0.498	0.703	2.15	-0.470	-0.42
InP	0.588	0.27	0.669	1.48	2.55	-0.086	
InAs	0.592	0.21	0.670	1.49	2.53	-0.083	-0.13
InSb	0.381	0.16	0.608	1.19	2.42	-0.248	-0.24
BeS	-0.451		0.658	0.427		-1.12	
BeSe	-0.452		0.658	0.426		-1.12	
BeTe	-0.511		0.641	0.344		-1.17	
ZnS	0.198	0.42	0.767	1.22	2.15	-0.490	0.33
ZnSe	0.211	0.34	0.768	1.23	2.03	-0.475	0.13
ZnTe	0.168	0.28	0.766	1.19	2.00	-0.524	0.08
CdS	0.456		0.765	1.48	2.77	-0.176	
CdTe	0.442	0.32	0.766	1.46	2.35	-0.194	0.09
CuF	-0.805		0.767	0.218		-1.49	
CuCl	-0.445	0.30	0.756	0.563	1.12	-1.05	0.35
CuBr	-0.393	0.29	0.750	0.607	1.49	-0.974	
CuI	-0.294	0.21	0.734	0.684	2.40	-0.835	
AgI	-0.064	0.29	0.677	0.839	1.40	-0.495	

decrease, while the ratios $[(c_{11} - c_{12})/2]/B$ and β/α monotonically increase with increase in covalency. The results versus covalency are shown in figures 1-4. The trend of ζ as a function of α_c is shown in figure 1; it is similar to that given by Martin [13], Harrison [1] and Kitamura and Harrison [10]. The trends of $[(c_{11} - c_{12})/2]/B$ and c_{12}/c_{11} versus covalency α_c are shown in figures 2 and 3, which are similar to that given by Kitamura *et al* [11]. Falter *et al* [16] have given the ratio of the non-central (bond-bending) force constant β to the central (bond-stretching) force constant α as a function of polarity. This ratio is a measure of the importance of the covalent bond in stabilizing the tetrahedral structure. In figure 4, we give a plot of β/α as a function of covalency α_c . The trend is similar to that given by Falter *et al* [16].

(v) It is worth noting that there are several differences between the BOM and XHTB methods. One is the basis state chosen. In the BOM, sp^3 orbitals for cations and anions are selected as the basis states while, in the XHTB method, atomic orbitals are used as the basis states. A second is that the BOM method includes only the first-nearest-neighbour interaction for which universal parameters are optimized whereas, in the XHTB method, interactions are taken into account up to a sufficiently large distance that the interactions became negligibly small. The third is that the value of λ in the BOM method is a constant value of 0.738 for all the diamond- and zincblende-structure semiconductors, while its value in the XHTB method varies from 0.615 to 0.815. In addition, the bond length used in the BOM method is the theoretical value, while in the XHTB method it is the experimental value.

Table 4. Results for covalency α_c defined by $(1 - \alpha_p^2)^{1/2}$, values of the bulk modulus B together with elastic stiffness constants $(c_{11} - c_{12})/2$ and c_{44} , bond-stretching force constant α and bond-bending force constant β , Kleinman's internal displacement parameters ζ , the ratios c_{12}/c_{11} , κ ($\equiv [(c_{11} - c_{12})/2]/B$) and β/α are also given.

	α_c	B (10^{11} erg cm $^{-3}$)	$(c_{11} - c_{12})/2$ (10^{11} erg cm $^{-3}$)	c_{44} (10^{11} erg cm $^{-3}$)	α (10^3 erg cm $^{-2}$)	β (10^3 erg cm $^{-2}$)	ζ	c_{12}/c_{11}	κ	β/α
C	1.00	69.1	33.6	46.9	236	62.6	0.548	0.410	0.486	0.264
Si	1.00	10.5	5.08	7.10	52.3	13.8	0.548	0.410	0.486	0.264
Ge	1.00	8.65	4.20	5.87	44.9	11.9	0.548	0.410	0.486	0.264
Sn	1.00	4.40	2.14	2.99	26.2	6.92	0.548	0.410	0.486	0.264
SiC	0.987	25.9	12.5	17.5	107	28.1	0.551	0.414	0.481	0.262
BN	0.974	74.0	35.3	49.5	247	64.0	0.554	0.417	0.476	0.259
BP	0.991	25.9	12.5	17.5	107	28.2	0.550	0.413	0.482	0.262
BAAs	0.992	22.4	10.8	15.1	95.7	25.1	0.550	0.413	0.483	0.263
AlP	0.942	9.31	4.31	6.11	46.5	11.6	0.563	0.427	0.463	0.251
AlAs	0.941	7.98	3.69	5.23	41.1	10.3	0.563	0.427	0.463	0.251
AlSb	0.957	5.65	2.65	3.74	31.4	7.99	0.558	0.422	0.470	0.255
GaP	0.947	8.94	4.14	5.89	45.2	11.3	0.561	0.425	0.466	0.251
GaAs	0.948	7.69	3.58	5.07	40.0	10.1	0.561	0.425	0.466	0.252
GaSb	0.965	5.49	2.59	3.65	30.8	7.88	0.556	0.420	0.474	0.256
InP	0.918	5.89	2.67	3.80	31.9	7.82	0.570	0.435	0.453	0.245
InAs	0.917	5.04	2.28	3.25	28.2	6.89	0.570	0.435	0.453	0.245
InSb	0.937	3.66	1.69	2.40	22.0	5.50	0.563	0.428	0.462	0.250
BeS	0.922	25.3	11.5	16.4	102	25.2	0.568	0.434	0.455	0.246
BeSe	0.922	20.2	9.18	13.1	85.6	21.1	0.568	0.434	0.455	0.246
BeTe	0.928	12.6	5.77	8.21	59.0	14.6	0.566	0.432	0.457	0.247
ZnS	0.836	7.78	3.20	4.69	38.5	8.51	0.598	0.468	0.412	0.221
ZnSe	0.833	6.12	2.51	3.68	31.8	6.99	0.599	0.469	0.411	0.220
ZnTe	0.840	3.84	1.59	2.33	21.9	4.88	0.596	0.466	0.415	0.222
CdS	0.789	4.79	1.84	2.75	25.7	5.26	0.618	0.491	0.385	0.205
CdTe	0.792	2.33	0.90	1.34	14.4	2.98	0.616	0.490	0.387	0.207
CuF	0.836	59.3	24.4	35.8	195	43.3	0.598	0.468	0.412	0.221
CuCl	0.769	9.87	3.68	5.53	45.4	9.02	0.627	0.502	0.372	0.199
CuBr	0.758	6.88	2.51	3.79	33.8	6.57	0.632	0.509	0.365	0.194
CuI	0.736	3.44	1.21	1.84	19.3	3.60	0.644	0.522	0.350	0.187
AgI	0.679	1.96	0.61	0.95	12.0	1.97	0.677	0.563	0.308	0.164

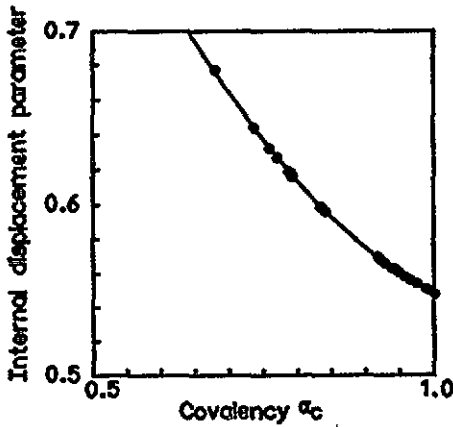


Figure 1. Kleinman's internal displacement parameters ζ versus covalency α_c .

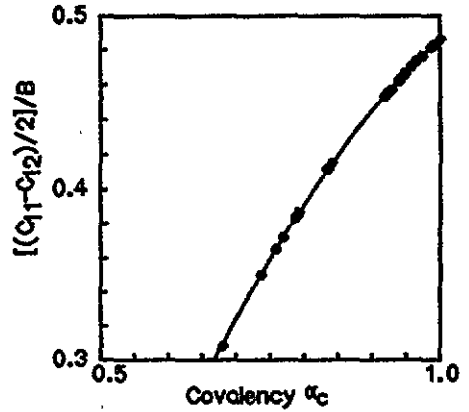


Figure 2. Plot of $\kappa (\equiv [(c_{11} - c_{12})/2]/B)$ versus covalency α_c listed in table 4.

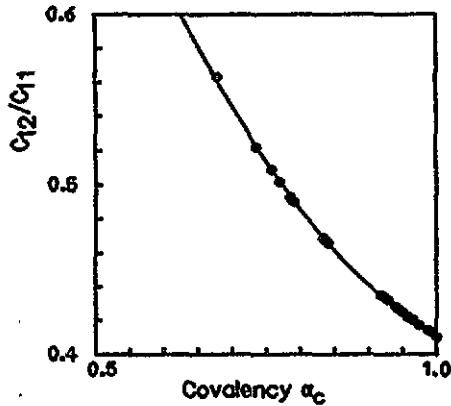


Figure 3. Curve for the ratio c_{12}/c_{11} as a function of covalency α_c .

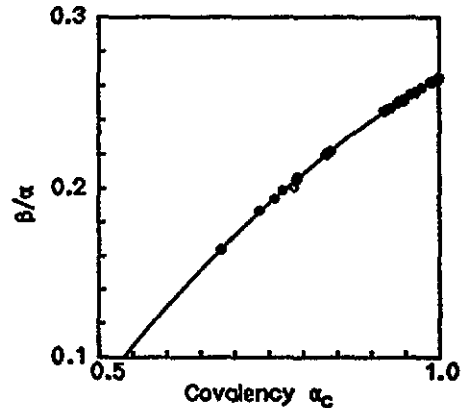


Figure 4. Ratio β/α of bond-bending constant β to central-force constant α as a function of the covalency α_c .

Comparison of bulk modulus B and elastic stiffness constants $(c_{11} - c_{12})/2$, and c_{44} , obtained from BOM calculations with the experimental values and XHTB calculation results [11] are shown in table 5. The bond-stretching force constant α and bond-bending force constant β obtained from BOM calculations (neglecting the Coulomb contribution) with the theoretical quantities α and β derived from the experimental values of B and $(c_{11} - c_{12})/2$ (the Coulomb contribution is included) are also given in the table. Table 5 indicates that the results obtained by using the BOM are in good agreement with the experimental and other theoretical results.

(vi) Table 6 shows the LDA results together with the experiment and our calculations for bulk Si, Ge, AlP, AIAs, GaP and GaAs. Comparing the LDA results with experiment, we can see that the LDA results agree very well. The excellent agreement between LDA results and experimental data prove that the LDA method is accurate. Although the BOM results are not as accurate as the LDA, the BOM results are reasonable. Because the BOM is very

Table 5. Comparison of bulk moduli B , elastic stiffness constants $(c_{11} - c_{12})/2$ and c_{44} , bond-stretching force constants α and bond-bending force constants β obtained from BOM calculations and experimental and xHTB calculational results. The theoretical quantities α and β were derived from the experimental values of B and $(c_{11} - c_{12})/2$.

	B ($\times 10^{11}$ erg cm^{-3})		$(c_{11} - c_{12})/2$ ($\times 10^{11}$ erg cm^{-3})		c_{44} ($\times 10^{11}$ erg cm^{-3})		α ($\times 10^3$ erg cm^{-2})		β ($\times 10^3$ erg cm^{-2})	
	BOM	Experiment [18]	xHTB	BOM	Experiment [18]	xHTB	BOM	Theory [13]	BOM	Theory [13]
C	69.1	56.7 44.2	39.3	33.6	26.5 47.6	35.0	46.9	236	129.33	62.6
Si	10.46	9.78	8.70	5.08	5.09	7.14	7.10	52.3	48.50	13.8
Ge	8.65	7.52	7.63	4.20	4.03	5.49	5.87	6.87	38.67	11.9
Sn	4.40	5.31	4.60	2.14		3.43	2.99	4.14	25.45 [19]	6.92
SiC	25.9	22.8	18.5	12.5	10.5	9.60	17.5	13.6	88.00 [19]	28.1
BPc	25.9	17.2	16.5	12.5	10.8	14.2	17.5	14.4	107	28.2
AlP	9.31	8.60	8.05	4.31		3.55	6.11	5.20	46.5	11.7
AlAs	7.98	7.73	7.40	3.69		3.77	5.23	5.14	41.1	10.3
AlSb	5.65	5.93	5.41	2.65	2.26	3.36	3.74	4.30	31.4	7.99
GaP	8.94	8.87	8.15	4.14	3.94	3.55	5.89	5.56	45.2	11.3
GaAs	7.69	7.48	7.24	3.58	3.25	3.25	5.07	5.29	40.0	10.1
GaSb	5.49	5.63	5.54	2.59	2.41	3.28	3.65	4.52	30.8	7.88
InP	5.89	7.25	6.08	2.67	2.23	2.01	3.80	3.75	31.9	7.82
InAs	5.04	5.80	5.63	2.28	1.90	2.16	3.25	3.73	28.2	6.89
InSb	3.66	4.66	4.40	1.69	1.51	1.41	2.40	3.35	22.0	5.50
ZnS	7.78	7.80	7.33	3.20	1.95	1.41	4.69	2.49	38.5	8.51
ZnSe	6.12	5.95	6.51	2.51	1.61	1.56	3.68	2.64	31.8	6.99
ZnTe	3.84	5.09	5.19	1.59	1.53	1.80	2.33	2.75	21.9	4.88
CdS	4.79	6.44	5.32	1.84		0.71	2.75	1.64	25.7	5.26
CdTe	2.33	4.24	4.02	0.90	0.84	1.12	1.34	1.92	14.4	2.98

Table 6. Comparison of bulk moduli B and elastic stiffness constants $(c_{11} - c_{12})/2$ and c_{44} obtained from LDA calculations and experimental and BOM calculational results.

	B ($\times 10^{11}$ erg cm^{-3})				$(c_{11} - c_{12})/2$ ($\times 10^{11}$ erg cm^{-3})				c_{44} ($\times 10^{11}$ erg cm^{-3})			
	BOM	Experiment [18]	LDA [5]	LDA [7]	BOM	Experiment [18]	LDA [5]	LDA [7]	BOM	Experiment [18]	LDA [5]	LDA [7]
Si	10.46	9.78	9.70	9.30	5.08	5.09	5.00	4.90	7.10	7.96	8.00	8.50
Ge	8.65	7.52	7.70	7.20	4.20	4.03	4.25	4.25	5.87	6.71	6.90	6.30
AlP	9.31	8.60	8.65 [6]		4.31				6.11			
AlAs	7.98	7.73	7.41 [6]		3.69				5.23			
GaP	8.94	8.87	8.97 [6]		4.14	3.94			5.89	7.05		
GaAs	7.69	7.48	7.25 [6]	7.30	3.58	3.25		3.50	5.07	5.92		6.20

simple, it can be used for the systematic study of structural properties in many materials and obtains the structural trends.

4. Summary

We have calculated the bond length d , bond polarity α_p , bulk modulus B , elastic shear constant $(c_{11} - c_{12})/2$ and c_{44} , bond-stretching force constant α , bond-bending force constant β , internal displacement parameter ζ , effective atomic charge Z^* , transfer parameter β^* , transverse charge e_T^* and piezoelectric charge e_p^* for 30 diamond- and zincblende-structure semiconductors using the BOM and compared these results with values obtained from other theoretical calculations and experiments. For most materials, we find the following.

(1) The bond length and polarity are in good agreement with the experiments.

(2) The transverse charges are about one electron less than the experiments, and the piezoelectric charges are in good agreement with the experiments (for III-V compound semiconductors).

(3) The values of bulk modulus and elastic stiffness constants obtained from BOM calculations are in good agreement with the experimental and the XHTB and LDA theoretical results.

(4) ζ and the ratio c_{12}/c_{11} monotonically decrease, while the ratios $[(c_{11} - c_{12})/2]/B$ and β/α monotonically increase with increasing covalency. Their trends are the same as experimental and other theoretical results.

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