EMPIRICAL FORMULA FOR BULK MODULUS OF ELEMENTAL AND BINARY SEMI CONDUCTORS

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\A semi-empirical formula has been proposed in this paper to calculate bulk modulus of Zinc blende structured Gr. IV, IV-IV, III -V and II-VI semiconductors. In this formula bond energy and bond length appear which have been evaluated using Universal Parameter Tight Binding (UPTB) approach. Aphysical basis of inclusion of bond energy has been given. Values obtained using the proposed formula are in excellent agreement with the experimental and reported bulk moduli. Effect of group number of constituent elements on bulk moduli has been given. The role of p-electrons on bulk moduli of compounds has also been discussed.

I. INTRODUCTION

Considerable effort has been made in recent years in the study of various properties of semiconductors and their alloys due to their important practical and technological applications.[1-9] Among these the bulk modulus of binary semiconductors and their alloys has been extensively investigated.[10-17] In the theoretical front, several ab-initio techniques have been proposed which demand detailed understanding of the nature of bonding and their effects in solids.[2,18] Moreover, these methods require sophisticated computational facilities and significant effort and time. Empirical and semiempirical methods are, therefore, widely used which also estimate/predict values in close agreement with experimental values and /or those of ab-initio calculations. In one of the earliest such attempts bulk modulus B(GPa) of binary semiconductors could be computed using the empirical formula,[13] $B = 1971/d^{3.5}$,which gave values for III-V semiconductors in good agreement with experimental

values, but deviation was appreciable in case of II-VI semiconductors. This formula was then modified[13] as given below

$$B = (1971-220\lambda)/d^{3.5} \qquad (1)$$

where d is the bond length (in Å) and λ an empirical ionicity parameter with its values 0, 1, 2 for group IV, III-V and II-VI semiconductors. It was further modified as [14]

$$B = N_c (1972-220\lambda)/4d^{3.5} \qquad (2)$$

where N_c is the bulk co-ordination number. These formulae produce reasonably good results both for II-VI and III-V semiconductors.

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Lam *et al*[15], deduced an analytical relation of bulk modulus with lattice parameters within the local density formalism and pseudo-potential approach as

$$B = 1971/d^{3.5} – 408(\Delta z)^2/d^4 \qquad (3)$$

where $\Delta z = 0,1,2,3$ for Group- IV, III-V, II-VI and I-VII systems respectively. The results were similar to those of Cohen.[29] Neumann[16], on the other hand, proposed the relation of bulk modulus in terms of lattice parameter and spectroscopically defined bond ionicity. A formula similar to that of Cohen was also proposed by Al- Douri *et al*[17], which is given by

$$B = (3000-100\lambda) [a/2]^{-3.5} \qquad (4)$$

where a is the lattice parameter. This relation also could not produce better results .It showed a deviation of 34.8% in case of ZnS. The theoretical basis of Cohen's relation was attempted[2] on consideration of the second derivative of the total energy E with respect to volume at the equilibrium state as

$$B = \Omega \frac{\partial^2 E}{\partial \Omega^2} I_{\Omega = \Omega_o} \qquad (5)$$

and the bond gap energy E_g defined by[19]

$$E^2_g = E_h^2 + C^2 \qquad (6)$$

where Ω is the volume. E_h and C refer to the homopolar and ionic contributions to the bonding respectively. Then using the relation[19]

$$E_h = 39.74/d^{2.5} \qquad (7)$$

it has been shown that

$$B \propto 1/d^{3.5} \qquad (8)$$

Accordingly, the following formula for B was proposed by Kamran *et al*[2],

$$B = (1938.72 - 506.702\, f_i)/d^{3.5} \qquad (9)$$

where f_i is the ionicity fraction given by $f_i = 1 - (E_h^2/E_g^2)$. Results obtained using this formula, in general, fall within 19% of the experimental values. In the bond orbital method[21] however, the Bulk modulus was proposed as

$$B = 2\sqrt{3}\ (V_2 \alpha_c^3 + 7.8 / d^2) /3d^3 \qquad (10)$$

where V_2, the covalent energy, is given by,

$$V_2 = -\bar{\eta} h^2/md^2 \qquad (11)$$

Here η is the overlap parameter, α_c the covalence of the bond and m is the mass of the electron. Eq. (10) could give somewhat better result. These formulae notonly differ in their mode of bond distance dependence of bulk modulus, but also the values predicted differ widely among themselves and with the experimental values. The results indicate that some factor other than bond length should also be included in the formula of bulk modulus. In this paper, we propose the inclusion of bond energy along with bond length and accordingly an empirical formula is proposed for bulk modulus.

II. THEORETICAL APPROACH

It is argued that the bond energy of a strong bond must be higher and therefore, the material consisting of atoms with stronger bonds between them must have greater resistance against deformation resulting in higher bulk modulus. To substantiate the fact, bond strength (hardness) and bond energy were calculated for Gr. IV, III-V and II-VI semiconductors.

Bond hardness (strength) was calculated by Li and Xue[20] in terms of the electron holding energy defined as the electrostatic potential of shielded nuclear charge of an atom i to the electron at the atomic boundary, i.e

$$\chi_i = Z_i / r_i \tag{12}$$

where Z_i is the number of valence electrons and r_i the atomic radius of the ith atom. Then the atomic stiffness was defined as the electron holding energy of an atom per unit volume, i.e

$$\eta_i = \chi_i / r_i^3 \tag{13}$$

But in a molecule of a compound the atoms do not remain neutral. The bond is partially ionic and partially covalent although in case of semiconductors, the bond is predominantly covalent. Therefore, it would be logical to utilise covalent radius and not the atomic radius. We, therefore, define the electron holding energy of an atom i as,

$$E_i = Z_i / R_i \tag{14}$$

where Z_i is the valence electron number and R_i is the covalent radius of the ith atom. Accordingly, the atomic stiffness is expressed as

$$S_i = E_i / R_i^3 \tag{15}$$

The hardness (strength) of the covalent bond of a compound 'AB' defined as the electron holding energy of the bond per unit volume, is given by the geometric mean of atomic stiffness per bond of atoms, i.e

$$H_{AB} = [(E_A.E_B/C_{NA}.\ C_{NB})/\ R_A^3.R_B^3]^{1/2} \tag{16}$$

where C_{Ni} (i = A, B) is the Co-ordination number of the ith atom.

Bond energy E_b was calculated using the Universal parameter tight binding (UPTB) approach[22] in which

$$E_b = E_p + E_\sigma + E_o + E_m \tag{17}$$

where E_p, E_σ, E_O and E_m are respectively the promotional energy, the σ- bond formation energy, the overlap energy and the metallization energy of the system. These energies are expressed in terms of orbital electron energies for the binary semiconductor AB and their alloys.

The overlap energy is expressed as

$$E_o = 2\eta_o V_2^2 / |\varepsilon_h^A + \varepsilon_h^B| \tag{18}$$

where $\varepsilon_h^{A(B)}$ is the hybrid energy of A(B) atom for sp^3 hybridization, V_2 is the covalent energy and η_o is the overlap parameter. It arises due to non- orthogonality of or bitals of the neighbouring atoms forming the bond. In the UPTB formalism, η_o of a compound AB made up of elements of a particular period is considered to be the same as that of the Gr. IV element of the period of the periodic table. However, for the skew compounds the overlap parameter is considered as the geometric mean.[21-23]

$$\eta_o = \sqrt{(\eta_A \eta_B)} \tag{19}$$

where η_A and η_B are the overlap parameters of group-IV elements corresponding to the periods which the atoms A and B belong to. This consideration, however, gives a good estimation of bond distance and bond energy of pure binary semiconductors. Then a graph was plotted for H_{AB} Versus E_b for Gr. IV and IV-IV, III-V and II-VI semiconductors. The graphs were found to be linear with high correlation coefficients of 0.943, 0.945, and 0.957 respectively which show that a compound with strongly bonded atoms has higher bond energy and hence bulk modulus.

From definition, bulk modulus, the property of a material showing its resistance to volume change on compression, is given by

$$B = - P/(dV/V) \tag{20}$$

where dV/V, the volume strain is dimensionless and the stress $P = F/A = E/V$. Here E is the energy, V, the volume, F the force (restoring) and A is the area. The volume of unit cell of a cubic crystal $V \alpha d^3$, where d is the bond length. Therefore, $B \alpha E / d^3$. As discussed above, bond energy is proposed to be used in place of E. Accordingly, a graph was plotted for B versus E_b / d^3 which was found to be linear for Gr. IV and IV-IV, III-V and II-VI semiconductors. Regression analysis gives high correlation of 0.996, 0.991 and 0.979 respectively for these systems.

With the help of these graphs, the following relation is proposed for the estimation of bulk modulus of semiconductors,

$$B = [48.23 - 7.39\lambda^{0.63547}] E_b / d^3 + [41.97 - 5.80\lambda^{2.19784}] \tag{21}$$

where $\lambda = | G_B - G_A |/2$ with G_A and G_B being the group numbers in the periodic tableof elements A and B respectively, λ takes care of the ionicity effect. This is because $\lambda = 0,1,2$ for Group – IV and IV-IV, III-V and II-VI semiconductors respectively and the average ionicity of bond also increases as one moves from IV-IV $\rightarrow$ III-V$\rightarrow$ II-VI. With increasing ionic character of a bond between atoms of a compound, the bond strength decreases and hence the bulk modulus.

III.   RESULTS AND DISCUSSION

Calculated values of bond strength and bond energy of the systems are presented in Table I. Bond length and bond energy of semiconductors belonging to Gr. IV, IV-IV, III-V and II-VI are given in Table II. For comparison experimental and the reported values are also given. Values of bond length obtained are in reasonable agreement with the experimental values. Bulk modulus has been calculated employing the proposed formula Eq. (21) and the values are given in Tables III and IV along with the experimental and reported values for comparison.

TABLE I. Bond strength, H_{ab} (in GPa) and bond energy, E_b (in eV)

Systems (IV,IV-IV)	H_{ab}	E_b	Systems (III-V)	H_{ab}	E_b	Systems (II-VI)	H_{ab}	E_b
C	2.79	30.877	BN	2.57	31.6305	BeO	1.98	35.7414
Si	0.53	13.306	BP	1.05	19.8801	Bes	0.72	23.4149
Ge	0.44	12.273	BAS	0.89	17.8877	BeSe	0.61	21.5279
Sn	0.26	9.322	BSb	0.67	15.305	BeTe	0.46	18.2959
SiC	1.21	21.215	AlN	1.24	23.7627	ZnO	1.26	28.812
GeC	1.11	19.215	AlP	0.50	15.2071	ZnS	0.45	21.2467
SnC	0.85	16.639	AlAs	0.43	14.3587	ZnSe	0.38	19.6425
SiGe	0.48	12.18	AlSb	0.32	10.6317	ZnTe	0.29	16.9544
SiSn	0.37	11.238	GaN	1.25	22.7124	CdO	0.95	28.7744
GeSn	0.34	10.571	GaP	0.51	15.4453	CdS	0.35	19.6228
			GaAs	0.43	14.4047	CdSe	0.29	18.318
			GaSb	0.33	12.2028	CdTe	0.22	16.0049
			InN	0.95	19.6486	HgS	0.31	20.0506
			InP	0.39	13.8136	HgSe	0.26	18.4493
			InAs	0.33	13.0275	HgTe	0.20	16.3306
			InSb	0.25	11.1402			

TABLE II. Bond length, d (in Å) and bond energy, E_b (in eV) of semiconductors belonging to Gr. IV, IV-IV, III-V and II-VI semiconductors

Systems		d(in Å)				
		This study	Exp.[21]	Reported		E_b(in eV)
				Ref.[21]	Ref.[23]	
IV and IV-IV	C	1.532	1.544	1.61	1.596	-30.8772
	Si	2.326	2.352	2.35	2.346	-13.3063
	Ge	2.428	2.449	2.45	2.455	-12.2731
	Sn	2.703	2.81	2.80	2.734	-9.32222
	SiC	1.826	1.877	1.95	1.942	-21.5057
III-V	BN	1.538	1.565	1.57	1.561	-31.6305
	BP	2.039	1.965	1.96	2.356	-19.8801
	BAS	2.161	2.068	2.02	2.008	-17.8877
	AlN	1.993	1.904	1.88	1.900	-23.7627
	AlP	2.346	2.367	2.34	2.356	-15.2071
	AlAs	2.420	2.442	2.42	2.435	-14.3587
	AlSb	2.673	2.805	2.61	2.581	-10.6317
	GaN	2.026	1.953	1.90	1.930	-22.7124
	GaP	2.386	2.358	2.37	2.395	-15.4453
	GaAs	2.451	2.448	2.11	2.474	-14.4047
	GaSb	2.649	2.639	2.63	2.620	-12.2028
	InN	2.225	2.163	2.04	2.043	-19.6486
	InP	2.568	2.541	2.54	2.537	-13.8136
	InAs	2.613	2.623	2.62	2.622	-13.0275
	InSb	2.812	2.805	2.82	2.768	-11.1402
II-VI	BeO	1.521	1.65	1.46	1.256	-35.7414
	BeS	2.18	2.1		1.898	-23.4149
	BeSe	2.213	2.2		1.990	-21.5279
	BeTe	2.342	2.4		2.150	-18.2959

ZnO	1.933	1.992	1.75	1.793	-28.812
ZnS	2.332	2.341	2.30	2.388	-21.2467
ZnSe	2.428	2.445	2.30	2.509	-19.6425
ZnTe	2.693	2.642	2.65	2.697	-16.9544
CdO	2.101	2.03			-28.7744
CdS	2.482	2.526	2.48	2.544	-19.6228
CdSe	2.556	2.62	2.60	2.676	-18.318
CdTe	2.794	2.805	2.86	2.870	-16.0049
HgS	2.342	2.513		2.556	-20.0506
HgSe	2.783	2.635	2.59	2.690	-18.4493
HgTe	2.902	2.797	2.85	2.886	-16.3306

TABLE III. Bulk Modulus, B (in GPa), of III-V semiconductors

System	Bulk Modulus (B In GPa)							
	This Work		Exp.	Reported values				
	Using exp. d	Using cal. d	Ref.15	Ref. 1	Ref. 2	Ref. 29	Ref. 30	Ref. 4
BN	373.9	391.25	367	346	373	367	351.2	152.06
BP	143.18	131.95	165	165	180.4	166	154.1	131.49
BAS	118.77	108.56		138	151.8	138		118.7
AlN	176.77	158.76			180.9			
AlP	83.00	84.27	86	80.5	88.3	86.7	86.3	87.77
AlAs	76.44	77.55	77	74	80.5	78.3	78.3	79.08
AlSb	55.84	58.90	58.2	54.1	56.1	57	59	58.45
GaN	160.69	147.71						133.58
GaP	84.28	82.61	88.7	81.5	86.6	86.7	86.3	86.34
GaAs	76.27	76.12	74.8	72.4	77.4	76.1	76.1	75.12
GaSb	63.29	69.98	57	55.4	59.6	57.8	59.6	54.86

InN	115.47	169.02			111.1			107.59
InP	70.56	69.48	71	60.8	66.1	67	68.7	69.19
InAs	65.65	65.99	60	56.3	61.2	61	62.8	62.11
InSb	56.78	56.63	47.4	44	47.7	47.1	49.4	47.88

TABLE IV. Bulk modulus, B (in GPa), of II-VI semiconductors

System	Bulk Modulus, B (in GPa)		Exp.	Reported values				
	This study							
	Using exp. d	Using cal. d	Ref. 15	Ref. 1	Ref. 2	Ref. 29	Ref. 26	Ref. 4
BeO	307.76	388.65						303.17
Bes	108.28	98.42		120	132.7			113.11
BeSe	89.66	88.36		105	113.2			96.55
BeTe	64.00	67.70		78	86.5			68.81
ZnO	149.32	161.96						146.19
ZnS	76.22	76.93	77.1	73.3	82.8	78.1	72	75.31
ZnSe	64.75	65.79	62.4	65.1	69.3	66.5	63.9	65.3
ZnTe	49.15	47.26	51	51.9	55.6	51.2	52.2	55.74
CdO	141.77	129.38						
CdS	60.10	62.52	62	53.2	62.6	60.3	59.5	56.79
CdSe	52.79	55.67	53		54.4	52.6	53.9	49.67
CdTe	42.01	42.33	42.4	40.2	42.9	41.2	44	43.32
HgS	61.79	72.72			60.1			56.52
HgSe	52.42	46.82	50		55.1	51.9	53	49.52
HgTe	42.79	39.92	42.3		46.1		45.7	41.87

The proposed relation Eq. (21) contains E_b/d^3 having the dimension of the bulk modulus. Such a   relation was also suggested by Kitamura et al,[1]

$$B = \lambda V_2^h / d^3 \qquad\qquad (22)$$

where V_2^h is the covalent energy, d the bond length and λ a constant. The value of λ is different for different compounds ranging from 0.6 to 0.8. In fact, in case of semiconductors the bond is predominantly covalent in character, but there are other factors too which play their roles in deciding equilibrium state properties of solids. Bulk modulus is an equilibrium state property and so the contributions of covalent energy, polar energy, overlap energy, metallization energy etc. have been included in the analysis of bulk modulus. These energies form part of the bond energy. It is, therefore thought worth to utilize the bond energy and not the covalent energy only so as to include various potential factors which contribute to the formation of the bond. However, we have not considered the spin-orbit coupling, which has a small effect on total energy[22]. The effect of non-orthogonality of orbitals might have added to the discrepancy of results[1] using Eq. (22), because only $V2^h$ may not be adequate to take care of this effect. On the other hand bond energy compensates this effect through inclusion of the overlap energy. In earlier studies[1,2,4,6,13-17] the dominance of bond length effect on bulk modulus has been shown. An empirical relation between bulk modulus and inverse of volume was also proposed by Wang and Ye.[10] A similar correlation was also used by Verma.[6] In the estimation of bulk modulus of compounds, Makino and Miyake[25] utilised the power functional form $B = cd^{-m}$, where c and m are constants, but different values of m ranging from 3.10 to 8.24 were suggested for compounds having different types of bonding.

Bulk modulus has also been considered as a measure of material hardness[26-28]. Accordingly, some novel hard materials like C_3N_4 were predicted[29]. These results motivated material scientists to explore various avenues of understanding the inter-relationship between material hardness and bulk modulus. Recently, it has been realised that hardness is a complex quantity and bulk modulus is not a direct measure of hardness. This is because there are materials, which exhibit high bulk modulus but have low hardness. Notable among them are pseudo-cubic and cubic C_3N_4 for which the estimated bulk moduli are 421 and 496 GPa respectively[27], but the hardness(strength) is 45.2 GPa which is found even lower than that (70.5 GPa) of c-BN. However, another study[28] has shown that c-C_3N_4 has hardness (92.0 GPa) comparable to that (97.3 GPa) of diamond. Thus the study of bulk modulus is still

considered an important parameter in search of novel superhard materials. In Kamran *et al*'s[2] formula for estimation of bulk modulus, ionicity is included which is not uniquely defined. Indeed there are a number of approaches used for calculating ionicity.[19,31-36] They[2] also used ionicity values from six different sources[19,31,37-40] which differ widely. Direct use of ionicity, therefore, is justifiable if the same scale is utilised for all the systems. In this regard Cohen's approach of dealing with ionicity effect is more plausible in which the parameter λ is used with its values 0, 1, 2 for group IV, III-V and II-VI semiconductors respectively. In this study, we have also used the parameter λ and defined it as one half of the difference of group numbers of the elements in the periodic table corresponding to the atoms forming the binary semiconductor compounds (AB).The parameter λ takes care of the ionicity effect and to some extent the periodic properties of the constituent elements. Calculated bulk moduli of Gr. IV, IV-IV, III-V and II-VI semiconductors using the proposed relation Eq. (21) are in reasonable agreement with the experimental values. For comparison, calculated values are given in Table III to V along with the experimental and reported values. Group properties are clearly reflected in the results. The magnitude of bulk moduli follows the order C > SiC> Si > Ge> Sn . Similar order is also observed in II-VI and III-V semiconductors, i.e BeO> BeS> BeSe> BeTe ; CdO> CdS> CdSe> CdTe and HgS> HgSe> HgTe in II-VI semiconductors; and BN > BP > BAs ; AlN> AlP> AlAs> AlSb ; GaN> GaP> GaAs> GaSb and InN> InP> InAs> InSb in III-V semiconductors. For any system containing element(s) going down a group, the bulk modulus decreases. This is due to increase in size of the atom and also due to increase in ionicity as the electronegativity decreases down a group of the periodic table.

It is also interesting to note that compounds involving the elements from the carbon row exhibit high bulk moduli. For example C(442), SiC (211 GPa), BN (425 GPa), AlN (208 GPa), GaN(200 GPa), InN(126 GPa), BeO (320 GPa), ZnO (154 GPa), CdO (146 GPa) etc. have higher values of bulk modulus. In case of BeO, BeS, ZnO, CdO, GeC, SnC, SiGe, SiGe, SiSn and GeSn the experimental values, to the best of our knowledge, are not available, so we have quoted the calculated values, which appear to be reasonable as they agree well with other reported values. For CdO too, reported value was not found.

p - electron Effect

The high values of bulk modulus of compounds made up of C-row element(s) might be due to non-availability of p-sub shells in the core of atoms of such elements which allows valence electron orbitals to penetrate deeper while forming bonds with atoms of other elements leading to formation of strong bonds, and hence higher bulk moduli. With the increase in number of p- sub shells, the bond between atoms of the systems weakens and the bulk modulus decreases. In order to quantify roughly the effect of p-electrons on bulk moduli of systems, the following empirical relation is proposed,

$$B = a + be^{-cn_p}$$

(23)

where a, b, c are constants and n_p is the number of p - subshells of the bonding atoms A and B of the system $A^N B^{8-N}$. Values of a, b, c are 73.0469, 5132.9532, 1.3123 for Gr. IV and IV-IV, 42.1389, 1329.1454, 0.7014 for III-V and 32.000, 227.8125, 0.4055 for II-VI semiconductors respectively. Estimated values of bulk moduli using this relation are given in Table Vand VI.

TABLE V. Bulk Modulus, B (in GPa) of II-VI semiconductors

System	n_P	This study	Exp.	Reported values				
			Ref. 15	Ref. 1	Ref. 2	Ref. 29	Ref. 30	Ref. 4
BeO	2	132.4						303.17
Bes	3	99.49		120	132.7			113.11
BeSe	4	76.99		105	113.2			96.55
BeTe	5	61.99		78	86.5			68.81
ZnO	3	99.49						146.19
ZnS	4	76.99	77.1	73.3	82.8	78.1	72	75.31
ZnSe	5	61.99	62.4	65.1	69.3	66.5	63.9	65.3
ZnTe	6	51.99	51	51.9	55.6	51.2	52.2	55.74
CdO	4	76.99						

CdS	5	61.99	62	53.2	62.6	60.3	59.5	56.79
CdSe	6	51.99	53		54.4	52.6	53.9	49.67
CdTe	7	45.33	42.4	40.2	42.9	41.2	44	43.32
HgS	6	51.99			60.1			56.52
HgSe	7	45.33	50		55.1	51.9	53	49.52
HgTe	8	40.89	42.3		46.1		45.7	41.87

TABLE VI. Bulk modulus, B (in GPa), of III-V semiconductors

| | | Bulk modulus, B (in GPa) | | | | | | |
| | | | Exp. | Reported values | | | | |
System	n_P	This study	Ref. 15	Ref.1	Ref. 2	Ref. 29	Ref. 30	Ref. 4
BN	2	369	367	346	373	367	351.2	152.06
BP	3	204.23	165	165	180.4	166	154.1	131.49
BAS	4	122.52		138	151.8	138		118.7
AlN	3	204.23			180.9			
AlP	4	122.52	86	80.5	88.3	86.7	86.3	87.77
AlAs	5	82.00	77	74	80.5	78.3	78.3	79.08
AlSb	6	61.91	58.2	54.1	56.1	57	59	58.45
GaN	4	122.52						133.58
GaP	5	82.00	88.7	81.5	86.6	86.7	86.3	86.34
GaAs	6	61.91	74.8	72.4	77.4	76.1	76.1	75.12
GaSb	7	51.94	57	55.4	59.6	57.8	59.6	54.86
InN	5	82.00			111.1			107.59
InP	6	61.91	71	60.8	66.1	67	68.7	69.19
InAs	7	51.94	60	56.3	61.2	61	62.8	62.11
InSb	8	47.00	47.4	44	47.7	47.1	49.4	47.88

Results clearly reflect the effect of p-electrons. The limitation of Eq. (23) is that it gives the same value of B for a given value of n_p. It does not involve other factors. However, the general trend of the effect of n_p on B is exhibited.

The ionicity and metallicity too appear to affect bulk modulus. Its magnitude decreases with the ionicity, the order, in general, moves Gr. IV $\rightarrow$ III-V $\rightarrow$ II-VI semiconductors. However, for a given cation the ionicity decreases as the anion goes down the group. The bulk modulus follows the same trend indicating that some other factors must play the role to balance the effect of ionicity. Metallization energy decreases[23] as one goes down a group and it causes decrease in bulk modulus.

In the universal parameter tight binding approach, which has been utilised in this study, optimization of universal parameters is made confining the effect to the nearest-neighbour interaction only. This is supported by the origin of the extended x- ray absorption fine structure (EXAFS) which shows a short-range order effect[45] and not the long- range periodicity of the potential in the crystals except in cases where focusing effect dominates.[46]

IV. SUMMARY

We have proposed a semi- empirical formula for estimation of bulk modulus of semiconductors using bond energy. The universal parameter tight binding approach has been utilized in evaluating bond energy. Ionicity effect is also discussed in terms of group number of bonding atoms in the periodic table. The role of p- electrons of the core shell in bulk modulus has also been discussed. Improved results have been obtained using the proposed formula. However the detailed analysis of the role of ionicity and metallicity of bulk modulus has not been made in the present paper. This aspect will be taken up in future.

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