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Bond Hardness and Mechanical Properties of A^NB^{8-N} Semiconductors and their Alloys

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ABSTRACT

In this paper a linear relation $H= (0.199 – 0.037\lambda^{1.940}) B – (7.754 – 1.706\lambda^{1.746})$ where B is the bulk modulus and λ is a parameter which is the average difference of group numbers of the constituent atoms (in the periodic table) of the compounds is proposed for microhardness of A^NB^{8-N} (N = 2, 3, 4) semiconductors. This equation has been obtained through the linear relations proposed for microhardness and bulk modulus in terms of bond hardness. Estimated values of B for group- IV, IV-IV, II-VI and III-V semiconductors are in closer agreement with the experimental and reported values. Microhardness of Sn, SiC, GeC, SnC, SiGe, SiSn, GeSn, BSb and CdO has been reported for the first time.

Key words: (semiconductors; structural properties; microhardness; bulk modulus.)

1.Introduction

In recent years attention has been renewed to the theoretical and experimental study of various properties of tetrahedral semiconductors because of their potential applications in the fields of laser diode, light emitting diode, opto – electronic devices, quantum well, quantum dot, quantum wire, infrared detector, solar cell, spintronics etc.[1-35]. In addition to electronic properties of semiconducting materials, structural properties also need to be addressed in order to understand their mechanical behaviour. Microhardness and bulk modulus are important in understanding the mechanical behaviour of materials. But the experimental values of microhardness of quite a few of these materials vary in a wide range, for example, values of microhardness of C, BN, BP and BeO are 57-104, 34.3-73.0, 31-40 and 9.1 - 12.7 GPa respectively [36]. Besides, experimental values of microhardness of

several materials are not known. On the theoretical front, values of microhardness calculated by different researchers [20,23,35-39] vary widely among themselves and also from experimental values. For example, reported values of microhardness in case of AlP are 8.71 GPa[20], 8.55 GPa[23], 9.816 GPa[37], 10.9 GPa[39] and 9.84 GPa[40], whereas the experimental value is 5.5 GPa[36].

Similarly, in case of GaSb the calculated values of microhardness are 2.75GPa[20], 2.84 GPa[23], 3.091 GPa[37] and 2.42 GPa[40], but the experimental value is 4.48 GPa[36]. For the estimation of microhardness empirical relations have also been proposed by several researchers.[20,23,37,38] Plendl *et al* [38], kumar *et al*[20, 23] and Gorai[37] have proposed the linear relationship between microhardness and bulk modulus empirically. In this paper, we have made an attempt to substantiate the linear relation between microhardness and bulk modulus of binary semiconductors through bond hardness, which play an important role in deciding mechanical properties of materials.

2.Calculation

Earlier studies [20,23,37, 38,40] showed that microhardness may be regarded as a measure of bulk modulus of materials. Accordingly, Plendl *et al* [38] proposed that bulk modulus (B) and microhardness (H) are related by,

$$B = KH \quad (1)$$

where K is a constant.

Kumar *et al* [20,23,40] and Gorai [37] suggested the empirical relation

$$B = KH + Y \quad (2)$$

where K and Y are constants. These relations used different sets of constants for II-VI and III-V semiconductors and they were not applied for group IV semiconductors. It is argued that the nature of bonding and its strength must appear in the picture. This is because bond covalency, bond ionicity and electronic behaviour which change with the change of group number of elements (in the periodic table) taking part in forming the bond is expected to

affect bond strength and hence microhardness and bulk modulus. If the strength of a bond between constituent atoms of a system is higher, its microhardness is expected to be higher. With stronger bond between atoms the resistance against deformation may also be larger leading to higher value of bulk modulus. We have, therefore, attempted to compute bond hardness and tried to correlate it with microhardness and bulk modulus. Li and Xue [34] calculated the bond hardness using 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.

$$\chi_i = Z_i/r_i \qquad (3)$$

where Z_i is the number of valance electrons and r_i is the atomic radius of the i^{th} atom. The atomic stiffness is then defined as the electron – holding energy of an atom per unit volume, i.e.

$$\eta_i = \chi_i /r_i^3 \qquad (4)$$

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 in primarily covalent. Therefore, it is logical to utilise the covalent radius and not the atomic radius. We, therefore, define the electron holding energy of an atom i as

$$E_i = Z_i/R_i \qquad (5)$$

where Z_i is the number of valence electrons and R_i is the covalent radius of the i^{th} atom. Accordingly, the atomic stiffness is expressed as

$$S_i = E_i/R_i^3 \qquad (6)$$

The hardness of the covalent bond a-b 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

$$H_{ab}=(S_a*S_b/C_{Na}*C_{Nb}) = (Z_a*Z_b/C_{Na}*C_{Nb})^{0.5}/R_a^2*R_b^2 \qquad (7)$$

where C_{Ni} (i = a, b) is the co-ordination number of the i^{th} atom. Bond hardness of elemental and binary semiconductors was calculated using Eq. (7).

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The available experimental values of microhardness (H in GPa) of Gr. IV, III-V and II-VI semiconductors were then plotted against the computed bond hardness, H_{ab} (in GPa). Plots are linear (Fig. 1-3) with correlation of 0.999, 0.991 and 0.961 for Gr. IV, III-V and II-VI semiconductors indicating linear dependence of microhardness on bond hardness.

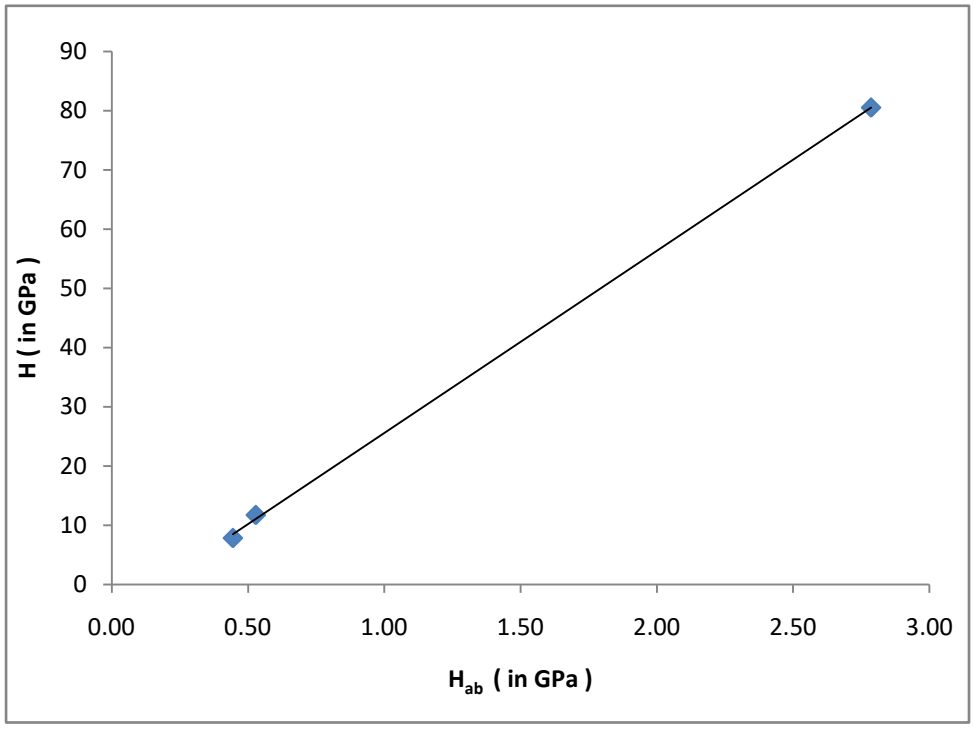

Figure 1. Plot of microhardness, H versus bond hardness, H_{ab} for Gr. IV semiconductors

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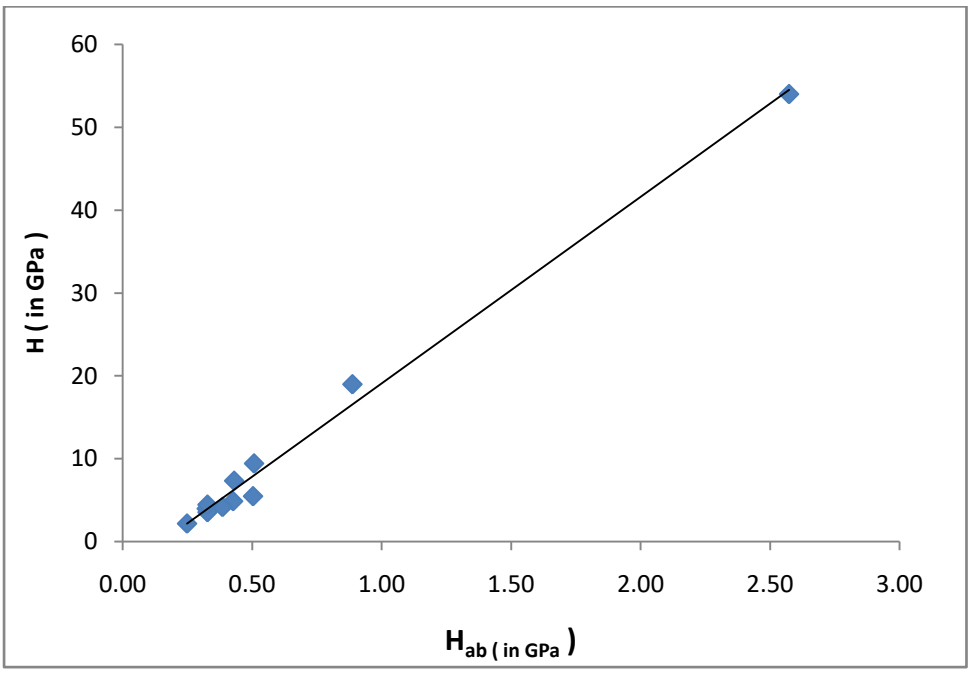

Figure 2. Plot of microhardness, H versus bond hardness, H_{ab} for III-V semiconductors

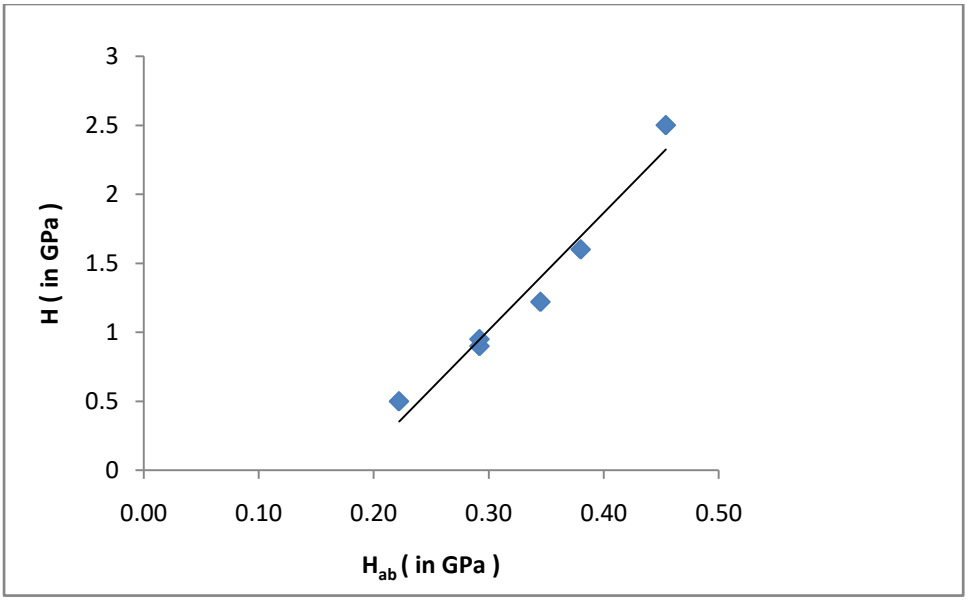

Figure 3. Plot of microhardness, H versus bond hardness, H_{ab} for II-VI semiconductors

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Accordingly, the following relation is proposed for microhardness

$$H = (30.76 - 8.27\ \lambda^{1.428})\ H_{ab} - (5.199 - 1.798\ \lambda^{1.027}) \quad (8)$$

where $$\lambda = (G_a - G_b)/\ 2 \quad (9)$$

Here $G_{a(b)}$ is the group number of the atom a(b) in the periodic table, i.e λ = 0,1 and 2 for Gr. IV and IV-IV, III-V and II-VI semiconductors respectively.

In case of C, BN, BP ZnSe, ZnTe, CdSe and CdTe for which the experimental values fall in a range, the intermediate values have been taken.

Secondly, bulk modulus (experimental) B (in GPa) of these compounds were plotted against the bond hardness H_{ab} (in GPa). As expected, straight lines were obtained with high correlation of 0.999, 0.998 and 0.973 for Gr. IV, III-V and II-VI semiconductors respectively (Fig. 4-6).

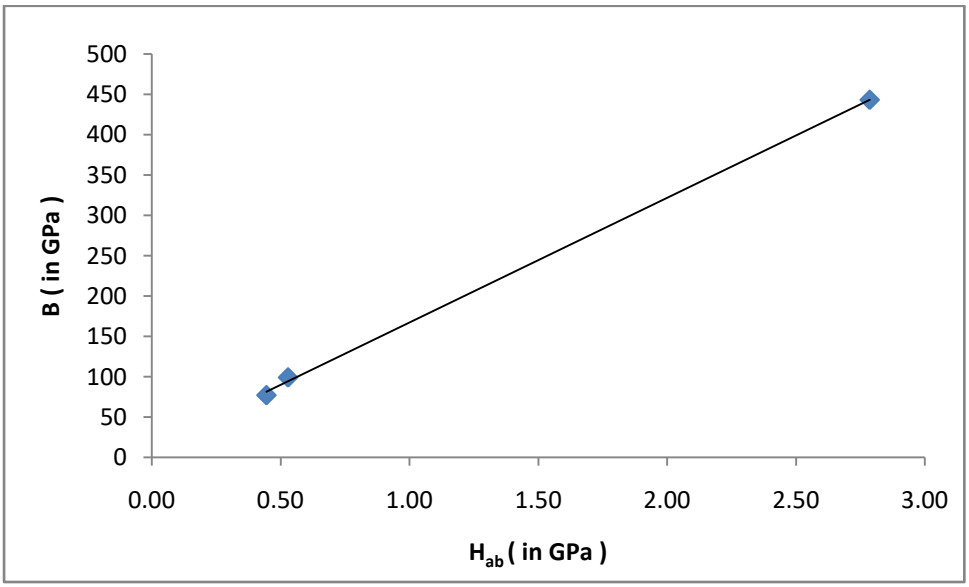

Figure 4. Plot of bulk modulus, B versus bond hardness, H_{ab} for Gr. IV semiconductors

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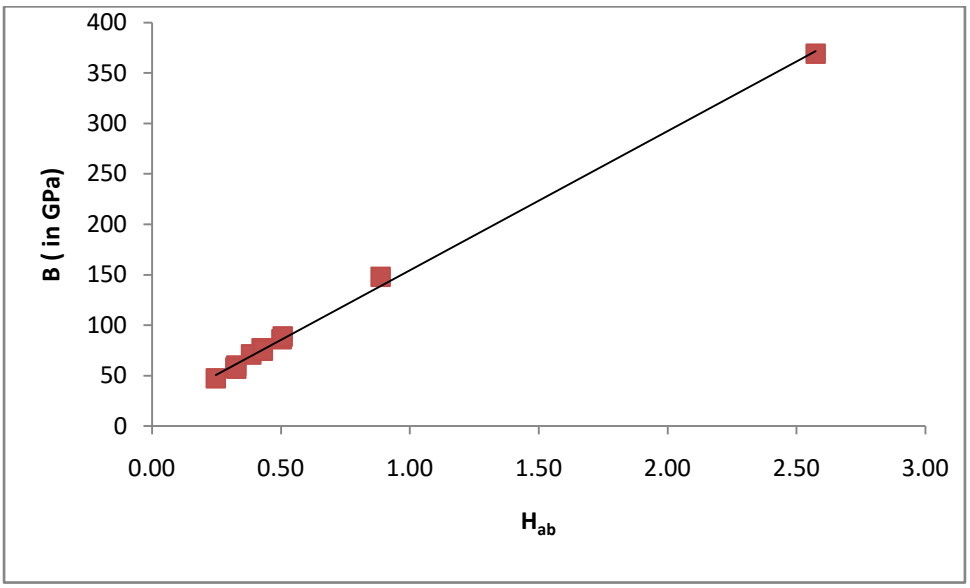

Figure 5. Plot of bulk modulus, B versus bond hardness, H_{ab} for III-V semiconductors

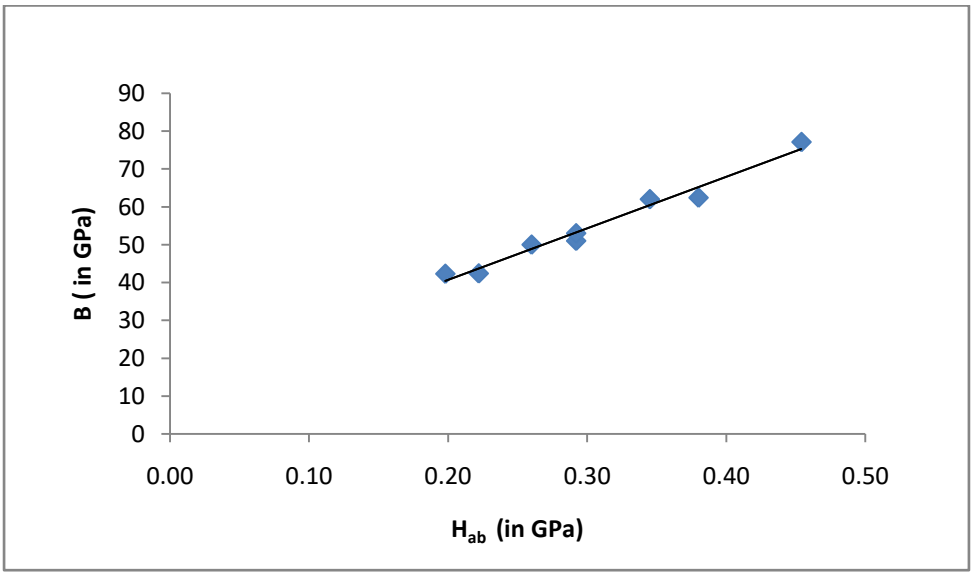

Figure 6. Plot of bulk modulus, B verses bond hardness, H_{ab} for II-VI semiconductors

Using these plots, the following relation is proposed for bulk modulus in terms of bond hardness,

$$B = (154.4 - 16.4\,\lambda^{0.142})\,H_{ab} + (12.85 + 3.42\,\lambda^{-2.690}) \qquad (10)$$

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Since both microhardness and bulk modulus of the materials are linearly related to the bond hardness, they must bear a linear relationship between them. To find the relation, if any, graphs were plotted for microhardness versus bulk modulus using their experimental values. As expected linear graphs were obtained for all the three sets of compounds with high correlations of 1, 0.992 and 0.951 respectively (Fig. 7-9).

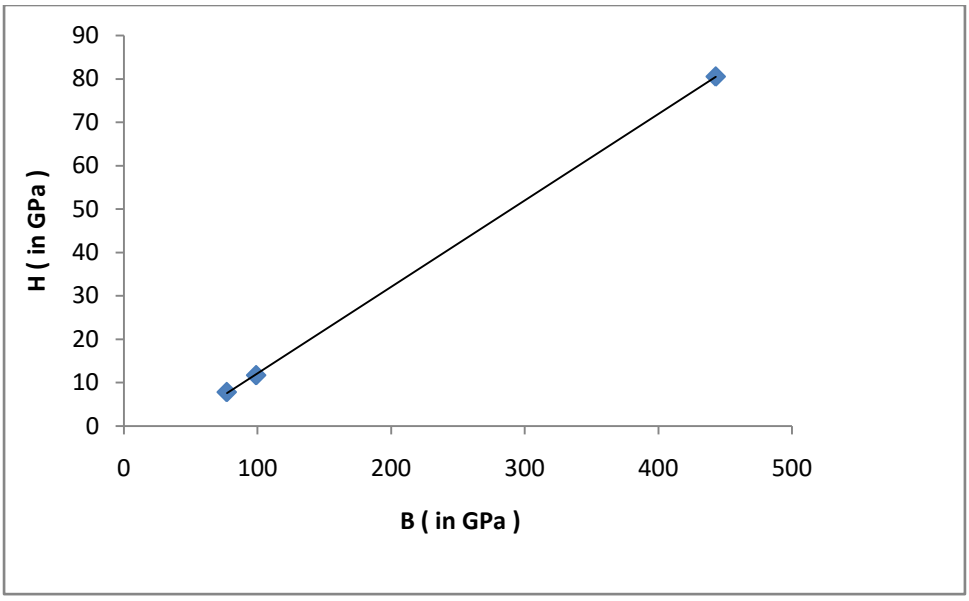

Figure 7. Plot of microhardness, H versus bulk modulus, B of Gr. IV semiconductors

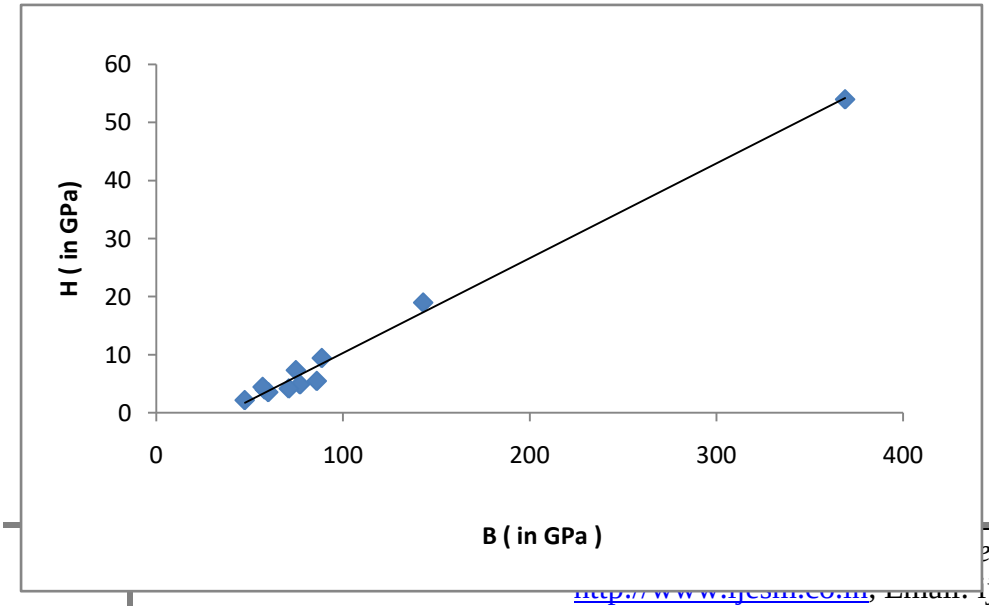

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Figure 8. Plot of microhardness, H versus bulk modulus, B of III-V semiconductors

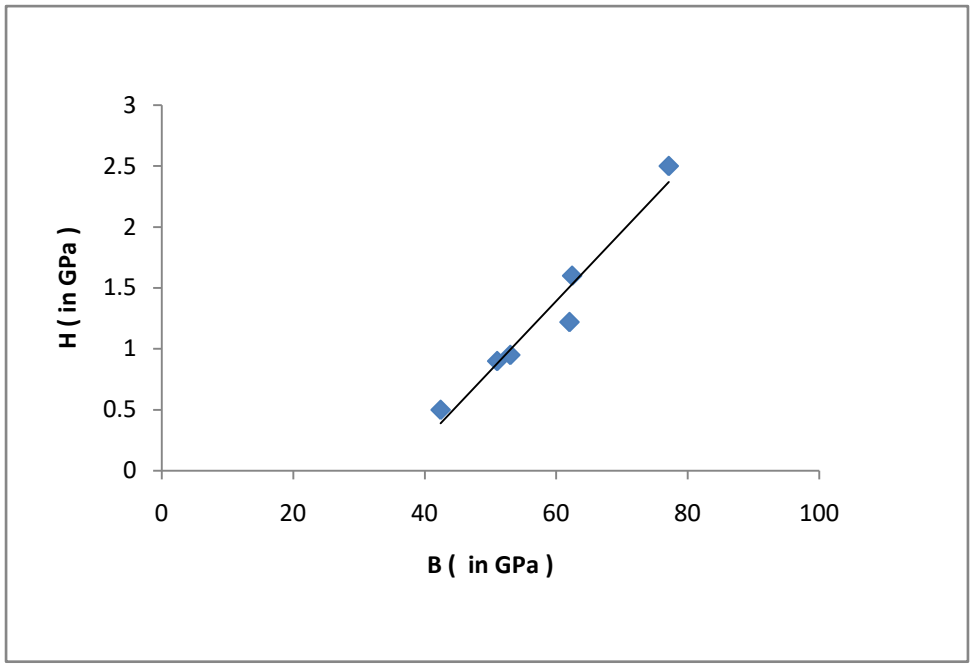

Figure 9. Plot of microhardness, H versus bulk modulus, B of II-VI semiconductors

Using these plots, the following formula is proposed for microhardness in terms of bulk modulus

$$H= (0.199 - 0.037\ \lambda^{1.940})\ B - (7.754 - 1.706\lambda^{1.746}) \qquad (11)$$

3.Results and Discussion

Bond hardness of group IV, III-V and II-VI semiconductors have been calculated using Eq. (7) and the results are given in Table. 1 along with bond ionicity[41].

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Table1. Calculated Bond Strength (H_{ab} in GPa) and bond ionicity for Gr. IV, III-V and II-VI semiconductors

Systems		H_{ab}	f_i
IV	C	2.79	0
	Si	0.53	0
	Ge	0.44	0
	Sn	0.26	0
III-V	BN	2.57	0.264
	BP	1.05	0.058
	BAS	0.89	0.026
	BSb	0.67	
	AlN	1.24	0.445
	AlP	0.50	0.388
	AlAs	0.43	0.432
	AlSb	0.32	0.433
	GaN	1.25	0.452
	GaP	0.51	0.328
	GaAs	0.43	0.315
	GaSb	0.33	0.265
	InN	0.95	0.496
	InP	0.39	0.421
	InAs	0.33	0.359
	InSb	0.25	0.329
II-VI	BeO	1.98	0.620
	Bes	0.72	0.611
	BeSe	0.61	0.610
	BeTe	0.46	0.592
	ZnO	1.26	0.653
	ZnS	0.45	0.621
	ZnSe	0.38	0.623
	ZnTe	0.29	0.599
	CdO	0.95	
	CdS	0.35	0.679
	CdSe	0.29	0.684
	CdTe	0.22	0.675
	HgS	0.31	
	HgSe	0.26	
	HgTe	0.20	

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Microhardness and bulk modulus of these materials were computed with the help of proposed Eqs. (8) and (10) respectively. Values obtained are given in Table 2 and 3 respectively along with experimental and reported values for comparison.

Table 2. Microhardness, H (in GPa) of Gr. IV, III-V and II-VI semiconductors obtained from bond hardness {Eq. (8)} along with experimental and reported values

System		Microhardness, H (in GPa)						
		This study	Exp. (Ref. 36)	Reported				
				Ref. 20	Ref. 23	Ref. 37	Ref. 39	Ref. 40
IV	C	80.50	57-104	60.80	96.92		80.0	
	Si	11.04	11.27,11.5,12.35	12.23	12.33		13.3	
	Ge	8.46	7.644,8	8.20	8.96		9.85	
	Sn	2.71						
III-V	BN	54.49	34.3-73.0	39.70	29.57	30.02	45.8	26.90
	BP	20.12	31.4-40	25.91	20.81	16.89	32.3	20.73
	BAS	16.55	19	19.46	16.50	12.33	24.2	17.24
	BSb	11.67						
	AlN	24.44				18		23.48
	AlP	7.91	5.5	8.71	8.55	9.816	10.9	9.64
	AlAs	6.18	4.8,5	6.67	6.81	6.914	6.3	7.67
	AlSb	3.89	4	3.18	3.36	4.351		3.23
	GaN	24.67		27.10	21.60	13.95		21.32
	GaP	8.00	9.45	8.55	8.25	7.41		9.32
	GaAs	6.27	7.5,7.21	5.86	6.08	5.172		6.79
	GaSb	3.95	4.48	2.75	2.84	3.091		2.42
	InN	17.94		14.90	13.28	9.816		14.40
	InP	5.26	4.10,4.30	4.78	5.05	4.813		5.50
	InAs	3.95	3.30,3.84	3.68	3.91	3.123		3.99
	InSb	2.18	2.20	2.05	1.90	1.464		1.06
II-VI	BeO	15.34	9.1-12.7	8.98	8.21	6.94		6.89
	BeS	4.56		3.12	3.01	3.72		3.23
	BeSe	3.63		2.54	2.52	2.59		2.75
	BeTe	2.39		1.50	1.64	1.74		1.80
	ZnO	9.18	3.9,4.8	4.22	3.96	3.39	4.6	4.05
	ZnS	2.33	1.7,2.8,3.5	1.75	1.86	1.78	3.3	2.05
	ZnSe	1.70	1.3-1.8	1.36	1.52	1.23	1.7	1.66
	ZnTe	0.95	0.8-1.1	0.96	1.19	0.75	1.0	1.23
	CdO	6.58						
	CdS	1.40	1.1,1.22	1.00	1.23	1.19	1.1	1.28
	CdSe	0.95	0.7-1.2	0.68	0.96	0.78	0.8	0.91
	CdTe	0.35	0.4-0.64	0.37	0.71	0.41	0.5	0.53
	HgS	1.08		0.99	1.22	0.89		
	HgSe	0.68		0.68	0.96	0.55		
	HgTe	0.15		0.29	0.65	0.24		

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Table 3. Bulk modulus, B (in GPa) of Gr. IV, III-V and II-VI semiconductors obtained from bond hardness [Eq. (10)] along with experimental and reported values.

System		Bulk modulus, B (in GPa)							
			Exp.		Reported values				
		This study	Ref.30	others	Ref.39	Ref. 33	Ref. 50	Ref. 20	others
IV	C	443.01	442		393	435	444.3	441.99	
	Si	94.37	98		87	99	100.1	97.68	
	Ge	81.40	77.2		76.3	85	87.4	76.91	
	Sn	52.53	53		46	57	55.8		
III-V	BN	371.48	367		346	367	351.2	152.06	
	BP	160.62	165		165	166	154.1	131.49	
	BAS	138.68		148[a]	138	138		118.7	
	BSb	108.73							114.3[31]
	AlN	187.11		201[b]					180.9[31]
	AlP	85.68	86		80.5	86.7	86.3	87.77	
	AlAs	75.06	77		74	78.3	78.3	79.08	
	AlSb	60.98	58.2		54.1	57	59	58.45	
	GaN	188.49		190[c]				133.58	164[31]
	GaP	86.24	88.7		81.5	86.7	86.3	86.34	
	GaAs	75.61	74.8		72.4	76.1	76.1	75.12	
	GaSb	61.40	57		55.4	57.8	59.6	54.86	
	InN	147.23		137[d]				107.59	
	InP	69.40	71		60.8	67	68.7	69.19	
	InAs	61.40	60		56.3	61	62.8	62.11	
	InSb	50.40	47.4		44	47.1	49.4	47.88	
II-VI	BeO	283.53						303.17	265.12[23]
	BeS	111.11			120			113.11	
	BeSe	96.11			105			96.55	
	BeTe	76.21			78			68.81	
	ZnO	185.12						146.19	
	ZnS	75.21	77.1		73.3	78.1	72	75.31	
	ZnSe	65.17	62.4		65.1	66.5	63.9	65.3	
	ZnTe	53.18	51		51.9	51.2	52.2	55.74	
	CdO	143.41							
	CdS	60.40	62		53.2	60.3	59.5	56.79	
	CdSe	53.18	53			52.6	53.9	49.67	
	CdTe	43.64	42.4		40.2	41.2	44	43.32	
	HgS	55.22						56.52	60.1[31]
	HgSe	48.82	50			51.9	53	49.52	
	HgTe	40.37	42.3				45.7	41.87	

a→ Ref. 48, b→ Ref. 54, c→ Ref. 55, d→ Ref. 53

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Microhardness has also been evaluated using the proposed relation Eq. (11) and the values are given in Table 4. Closer agreement is observed between the calculated and the experimental values.

Table 4. Calculated, experimental and reported values of microhardness (in GPa) using Bulk modulus [Eq. (11)] for Gr. IV, IV-IV, III-V and II-VI semiconductors.

System		Bulk modulus, B (in GPa)		Microhardness, H(in GPa)						
		Exp. (Ref. 31	Others	Exp. (Ref.36)	This work	Reported				
						Ref. 20	Ref. 23	Ref. 37	Ref. 39	Ref. 40
IV	C	442	443[a]	57-104	80.403	60.80	96.92		80.0	
	Si	98	99[a]	11.27,11.5, 12.35	11.947	12.23	12.33		13.3	
	Ge	77.2	77[a]	7.644,8	7.569	8.20	8.96		9.85	
	Sn	53	53[a]		2.793					
IV-IV	SiC	211	224[a]		34.235					
	GeC		157.498[b]		23.588					
	SnC		120.726[b]		16.270					
	SiGe		88.130[b]		9.784					
	SiSn		77.226[b]		7.614					
	GeSn		73.672[b]		6.907					
III-V	BN	367		34.3-73	53.73	39.70	29.57	30.02	45.8	26.90
	BP	165		31-40	20.844	25.91	20.81	16.89	32.3	20.73
	BAs		148[c]	19	17.118	19.46	16.50	12.33	24.2	17.24
	BSb		108.73**		11.566					
	AlN		201[d]		28.620			18		23.48
	AlP	86		5.5	7.814	8.71	8.55	9.816	10.9	9.64
	AlAs	77		4.8,5	6.426	6.67	6.81	6.914	6.3	7.67
	AlSb	58.2		4	3.380	3.18	3.36	4.351		3.23
	GaN		190[e]		24.732	27.10	21.60	13.95		21.32
	GaP	88.7		9.45	8.321	8.55	8.25	7.41		9.32
	GaAs	74.8		7.5,7.21	6.070	5.86	6.08	5.172		6.79
	GaSb	57		4.48	3.186	2.75	2.84	3.091		2.42
	InN		137[f]		14.364	14.90	13.28	9.816		14.40
	InP	71		4.1,4.3	5.454	4.78	5.05	4.813		5.50
	InAs	60		3.3,3.84	3.672	3.68	3.91	3.123		3.99
	InSb	47.4		2.2	1.631	2.05	1.90	1.464		1.06
II-VI	BeO		283.53**	9.1-12.7	14.131	8.98	8.21	6.94		6.89
	BeS		111.11**		4.303	3.12	3.01	3.72		3.23
	BeSe		96.11**		3.448	2.54	2.52	2.59		2.75
	BeTe		76.21**		2.314	1.50	1.64	1.74		1.80
	ZnO		185.2**	3.94,4.8	8.522	4.22	3.96	3.39	4.6	4.05
	ZnS	77.1		1.7,2.8,3.5	2.365	1.75	1.86	1.78	3.3	2.05
	ZnSe	62.4		1.3-1.8	1.527	1.36	1.52	1.23	1.7	1.66
	ZnTe	51		0.8-1.1	0.877	0.96	1.19	0.75	1.0	1.23
	CdO		143.41**		6.144					
	CdS	62		1.2,1.22	1.504	1.00	1.23	1.19	1.1	1.28
	CdSe	53		0.7-1.2	0.991	0.68	0.96	0.78	0.8	0.91
	CdTe	42.4		0.4-0.64	0.489	0.37	0.71	0.41	0.5	0.53
	HgS		55.22**		1.12	0.99	1.22	0.89		
	HgSe	50			0.82	0.68	0.96	0.55		
	HgTe	42.3			0.381	0.29	0.65	0.24		

* experimental, **fromTable III a→ Ref. 32, b→ Ref. 17, c→ Ref. 48, d→ Ref. 54, e → Ref. 55, f→ Ref. 53

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With reasonable values of microhardness and bulk modulus for the pure systems, the proposed model was extended to their binary and ternary alloys. In case of binary alloys (IV-IV systems) also the proposed formula Eq. (7) was utilised to obtain bond hardness. Results are shown in Table 5 along with those obtained from Vegard's law.

Table 5. Bond hardness, H_{ab} (in GPa) of semiconductor alloys (group. IV-IV)

System	SiC	GeC	SnC	SiGe	SiSn	GeSn
H_{ab}	1.21	1.11	0.85	0.48	0.37	0.34
H_{ab}(using Vegard's law)	1.66	1.62	1.53	0.48	0.39	0.35

Closer agreement of the two sets of values shows applicability of Vegard's law for bond hardness. Eqs. (8) and (10) were utilised to estimate the values of bulk modulus and microhardness of these solid solutions. Values have been shown in Tables 6 and 7.

Table 6. Bond hardness, H_{ab} (in GPa) and bulk modulus, B (in GPa) of semiconductor alloys (Gr. IV- IV) along with reported values and those obtained from Vegard's law

System	H_{ab}	Bulk Modulus, B (in GPa)				
		This Work	Reported			
			Ref. 51	Ref.52	Ref. 17	B(using Vegard's law)
SiC	1.21	200.14		229	187.87	271
GeC	1.11	184.54		188	157.49	260
SnC	0.85	143.47		133	120.73	248
SiGe	0.48	87.58	87.62		88.13	88
SiSn	0.37	69.67	68.55		77.22	76
GeSn	0.34	65.04	53.8		73.67	65

Table 7. Bond hardness, H_{ab} (in GPa) and microhardness (H in GPa) of semiconductor alloys (Gr. IV-IV) along with reported values and those obtained from Vegard's law

System	H_{ab}	Microhardness, H (in GPa)	
		This Work	Using Vegard's law
SiC	1.21	32.11	46.17
GeC	1.11	29.01	43.99
SnC	0.85	20.82	41.60
SiGe	0.48	9.69	9.76
SiSn	0.37	6.12	7.37
GeSn	0.34	5.20	5.18

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It is found that the calculated values of H_{ab}, B and H agree reasonably with those obtained from Vegard's law. But the deviation is more case of alloys containing C. This might be due to the absence of core p- orbitals in the C- atom which may allow valence orbitals to penetrate more making the bond harder. The remaining alloys obey Vegard's law for these properties.

Microhardness is also obtained from bulk modulus using the proposed relation [Eq. (11)] and the results are given in Table IV. Microhardness of Gr. IV- IV semiconductors has also been calculated for which experimental or reported values are, to the best of our knowledge, not available for comparison.

In case of ternary alloys of III-V and II-IV semiconductors, the covalent radius is modified in the estimation of bond hardness using Eq. (7). Two categories of ternary alloys were considered. First, the anionic substituted alloys of type $AB_{1-x}C_x$ in which $InP_{1-x}As_x$ and $ZnS_{1-x}Se_x$ were considered. In this case, R_b was calculated using the relation

$$R_b = (1-x)R_B + xR_C$$

where R_b, R_B and R_C are the covalent radii of $B_{1-x}C_x$, B and C respectively. Second, the cationic substituted alloys of the type $A_{1-x}B_xC$, in which R_a is replaced by

$$R_a = (1-x)R_A + xR_B$$

where R_a, R_A and R_B are the covalent radii of $A_{1-x}B_x$, A and B cations respectively. In this category, the alloys $In_{1-x}Ga_xP$ and $Cd_{1-x}Zn_xS$ were taken into consideration. The computed values of bond hardness were utilised for estimating microhardness and bulk modulus of the alloys. The corresponding graphs for bond hardness, microhardness and bulk modulus versus composition of alloys have been shown in Fig. 10-21.

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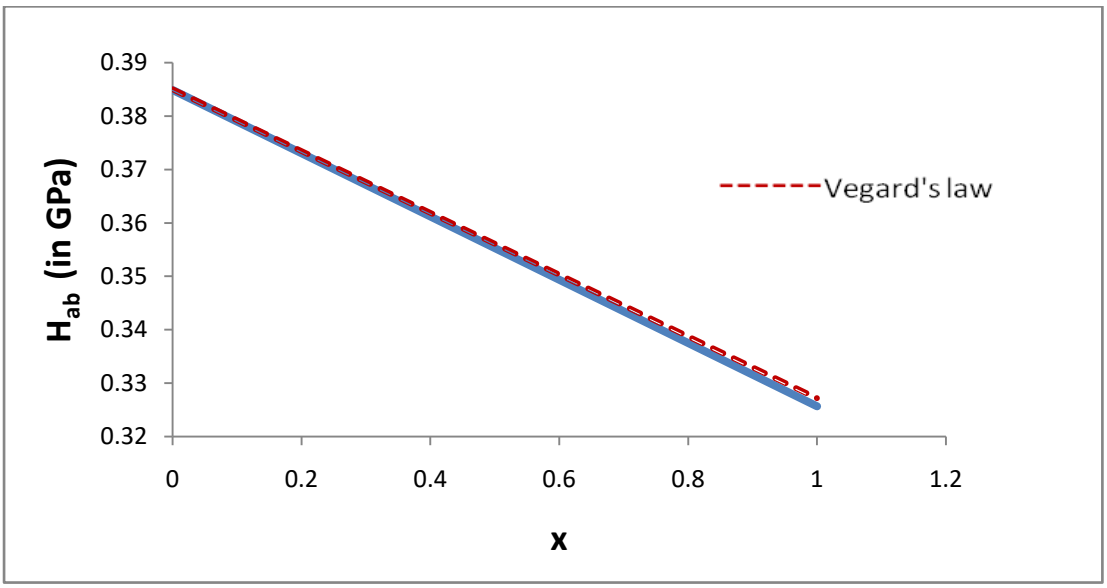

Figure 10. Plot showing variation of bond hardness, H_{ab} with composition (x) in $InP_{1-x}As_x$

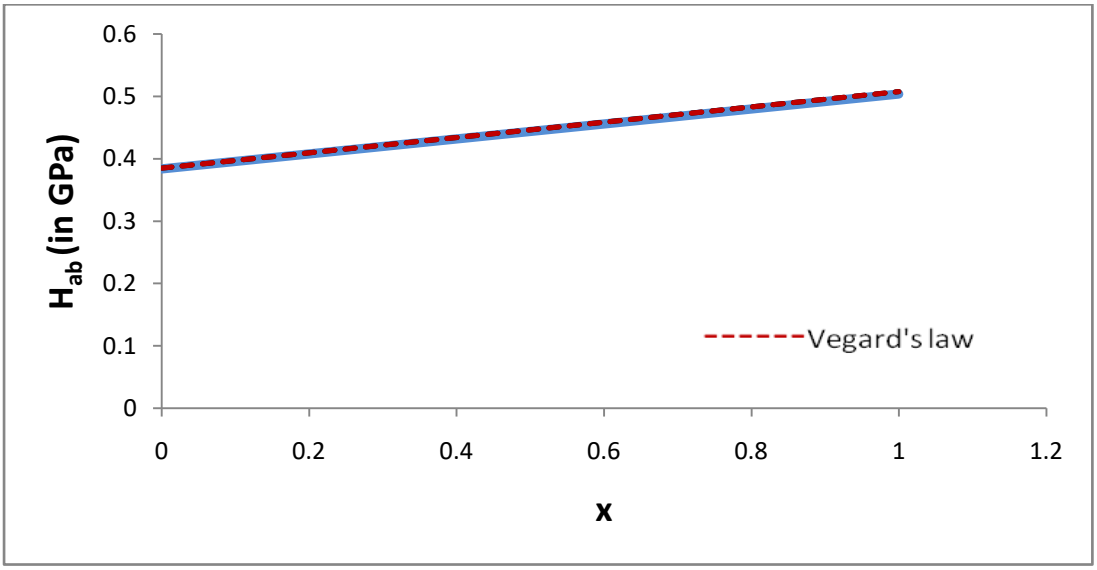

Figure 11. Plot showing variation of bond hardness, H_{ab} with composition(x) in $In_{1-x}Ga_xP$

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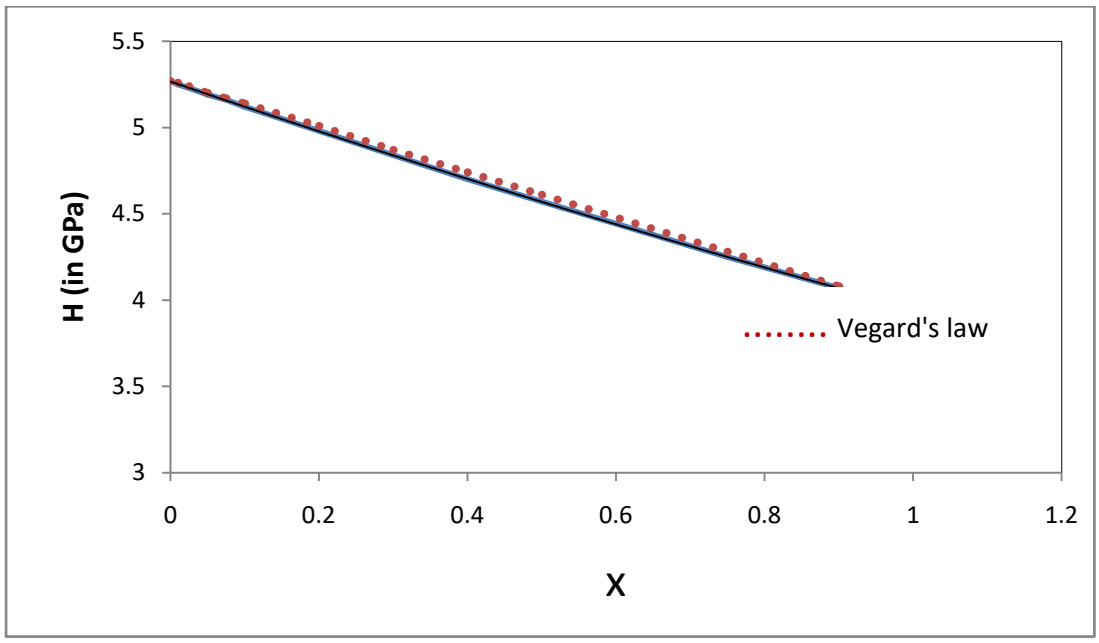

Figure 12. Plot showing variation of microhardness, H with composition (x) in $InP_{1-x}As_x$

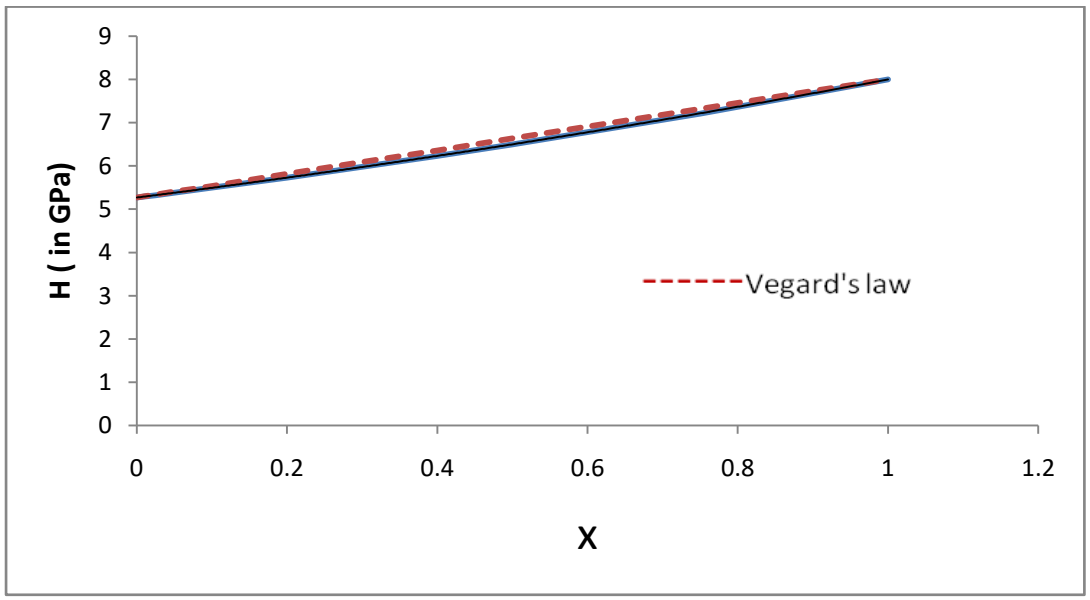

Figure 13. Plot showing variation of microhardness, H with composition(x) in $In_{1-x}Ga_xP$

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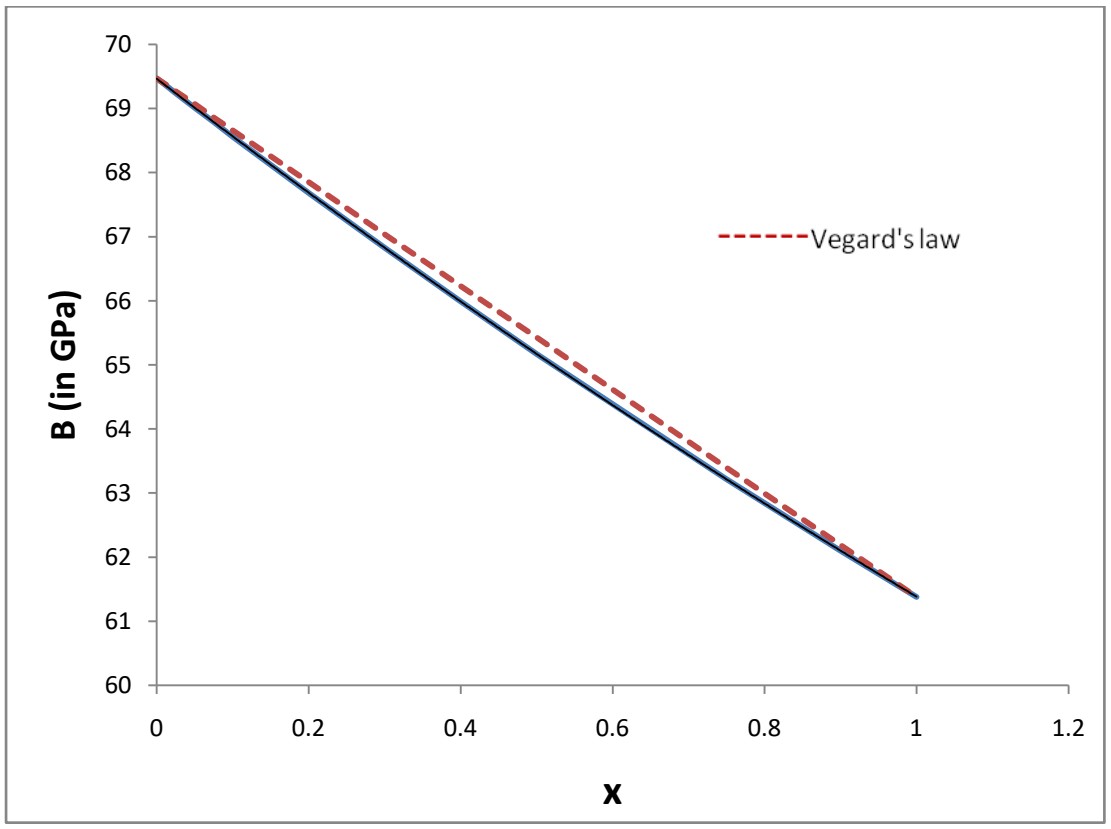

Figure 14. Plot showing variation of Bulk modulus, B with composition(x) in $InP_{1-x}As_x$

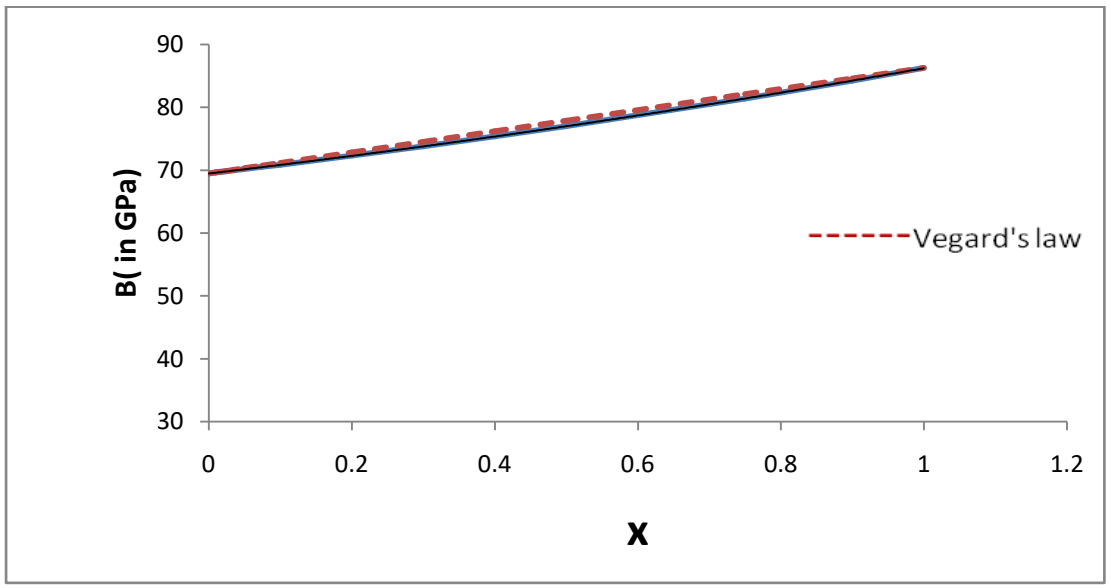

Figure 15. Plot showing variation of Bulk modulus, B with composition(x) in $In_{1-x}Ga_xP$

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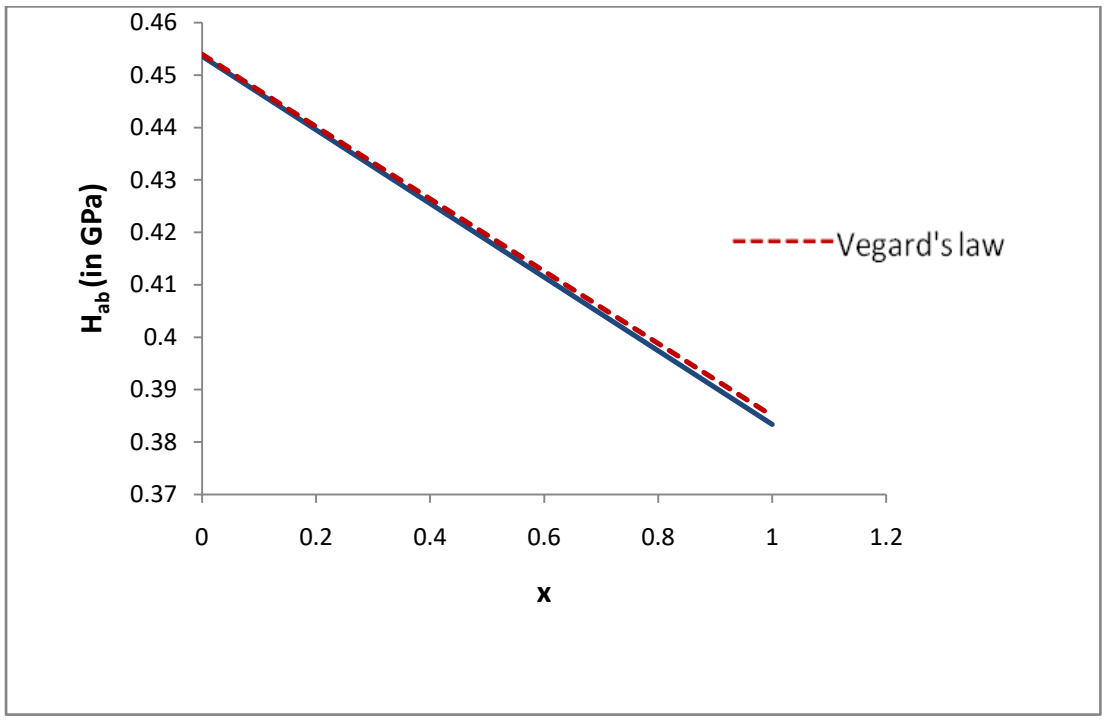

Figure 16. Plot showing variation of bond hardness, H_{ab} with composition(x) in $ZnS_{1-x}Se_x$

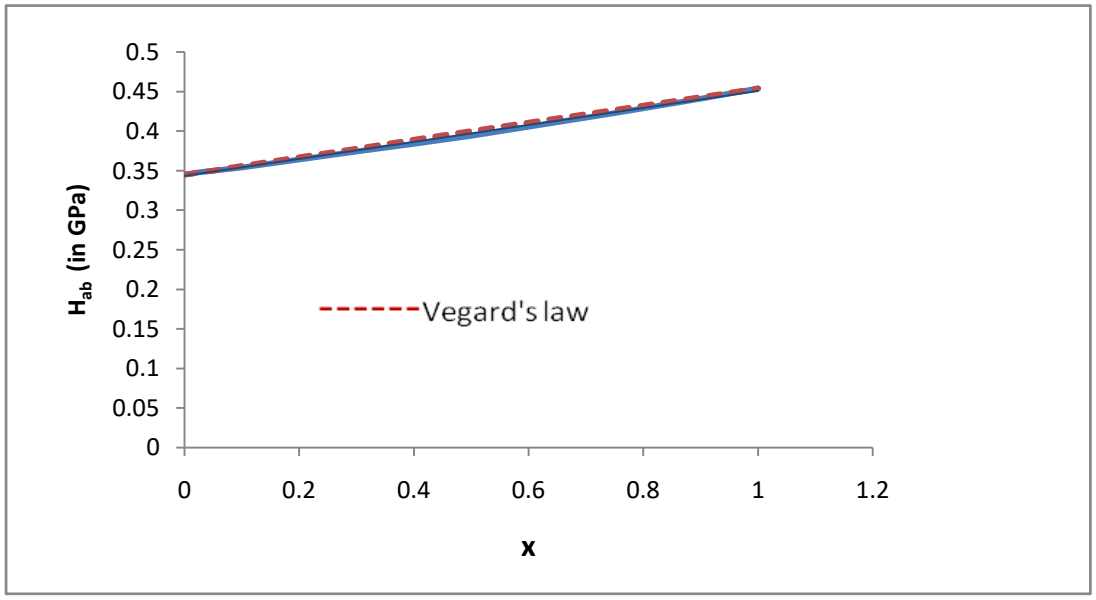

Figure 17. Plot showing variation of bond hardness, H_{ab} with composition(x) in $Cd_{1-x}Zn_xS$

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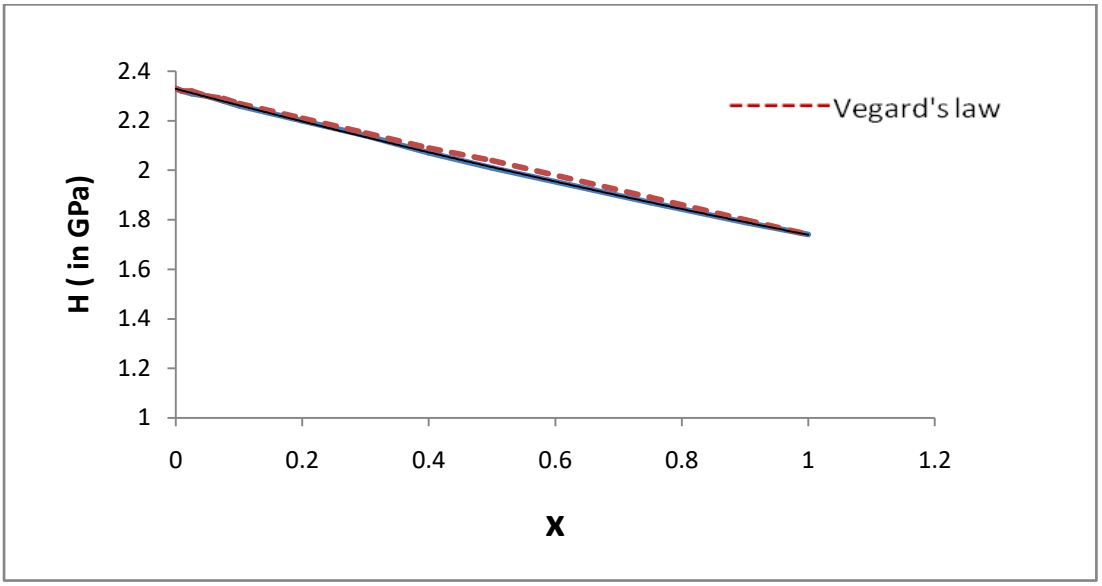

Figure 18. Plot showing variation of microhardness, H with composition(x) in $ZnS_{1-x}Se_x$

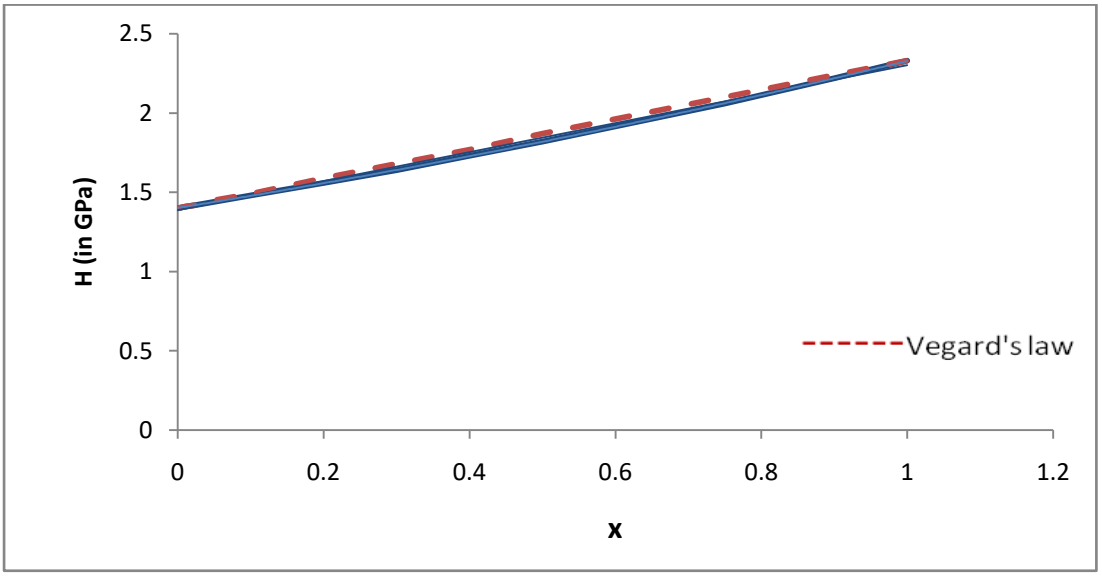

Figure 19. Plot showing variation of microhardness, H with composition(x) in $Cd_{1-x}Zn_xS$

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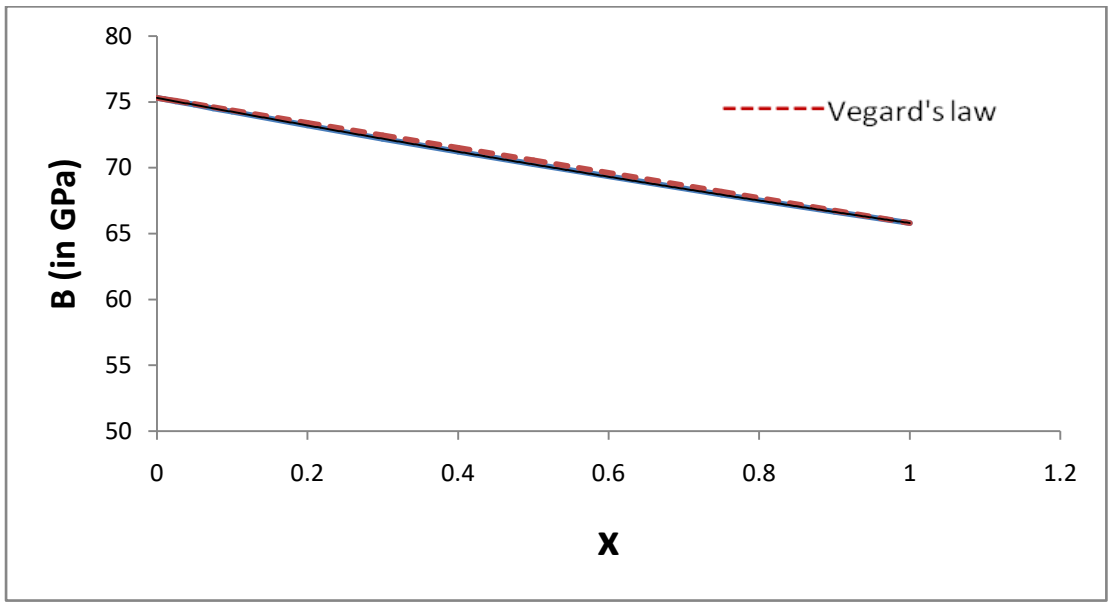

Figure 20. Plot showing variation of bulk modulus, B with composition(x) in $ZnS_{1-x}Se_x$

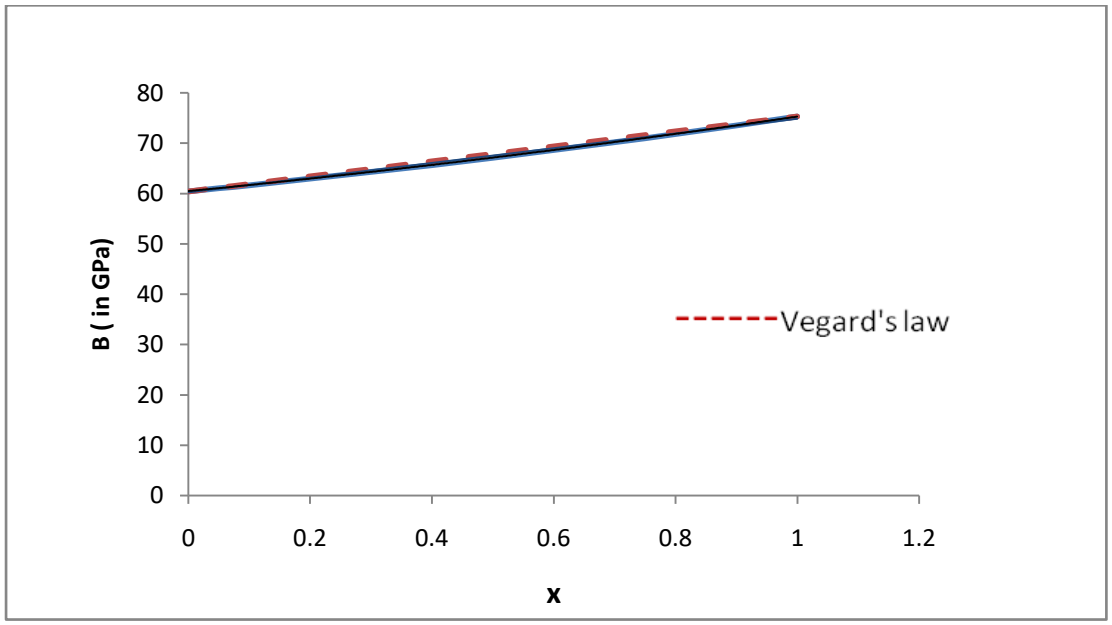

Figure 21. Plot showing variation of bulk modulus, B with composition(x) in $Cd_{1-x}Zn_xS$

The effect of size of constituent ions in the alloys is clearly reflected in these plots. The bond hardness in $InP_{1-x}As_x$ decreases with increasing value of As-content, but there is a gradual rise of bond hardness with x in $In_{1-x}Ga_xP$. A similar trend is observed for bond hardness in

$ZnS_{1-x}Se_x$ and $Cd_{1-x}Zn_xS$. Change of microhardness and bulk modulus of these systems with x are also found in these alloys. In case the size of the impurity ion is larger than the host ion, as in $InP_{1-x}As_x$ (P^{-3}= 21.2 nm, As^{-3}= 22.2 nm) and $ZnS_{1-x}Se_x$ (S^{-2}= 18.4 nm ,Se^{-2} = 19.1 nm)[56], the mechanical properties tend to decrease. On the contrary, these properties exhibit rising trend when impurity - ion size is smaller than the host - ion size. The effect appears reasonable, because doping of a larger ion will tend to increase the bond length of the system which in turn, will weaken the bond strength and hence microhardness and bulk modulus. Indeed, materials with shorter bonds have been identified as harder materials [43 – 45].

Ionicity has been another factor, which affects the bond strength and the mechanical properties. With increasing size of doped ion, as in case of $InP_{1-x}As_x$ and $ZnS_{1-x}Se_x$, the ionicity also increases and weakens the bond, whereas in case of cationic substitution like $In_{1-x}Ga_xP$ and $Cd_{1-x}Zn_xS$, the covalency increases giving rise to stronger bond and hence higher values of microhardness and bulk modulus. It is interesting to note how Vegard's law applies in these cases. Bond hardness obeys Vegard's law perfectly (Fig. 10, 11, 16, 17) but microhardness (Fig.12, 13, 18, 19) and bulk modulus (Fig. 14, 15, 20, 21) exhibit slight deviation from Vegard's law. These deviations are expressed as follows:

$$H(InP_{1-x}As_x) = 5.226 - 1.474\ x + 0.158\ x^2$$

$$H\ (In_{1-x}Ga_xP) = 5.27 + 2.190\ x + 0.538\ x^2$$

$$H(ZnS_{1-x}Se_x) = 2.329 – 0.676\ x + 0.085\ x^2$$

$$H(Cd_{1-x}Zn_xS) = 1.402 + 0.742\ x + 0.183\ x^2$$

$$B(InP_{1-x}As_x) = 69.46 – 9.097\ x + 1.015\ x^2$$

$$B(In_{1-x}Ga_xP) = 69.48 + 13.35\ x + 3.389\ x^2$$

$$B(ZnS_{1-x}Se_x) = 75.30 – 10.69\ x + 1.195\ x^2$$

$$B(Cd_{1-x}Zn_xS) = 60.47 + 11.81\ x + 3.006\ x^2$$

Such deviations from Vegard's law have also been reported for lattice constant, bulk modulus and energy gap in $B_xIn_{1-x}N$ alloys [25]; for band gap in $B_xGa_{1-x}N$ alloys[45]; for lattice

constant and bulk modulus in ZnS_xSe_{1-x}[46], and for lattice constant and band gap in $A_xZn_{1-x}O$ alloys (A = Ca, Cd, Mg)[47].

For bond hardness, perfect linearity is observed governed by the following relations

$H_{ab}(InP_{1-x}As_x) = 0.384 – 0.059\ x$

$H_{ab}\ (In_{1-x}Ga_xP) = 0.383 + 0.120\ x$

$H_{ab}\ (ZnS_{1-x}Se_x) = 0.453 – 0.070\ x$

$H_{ab}\ (Cd_{1-x}Zn_xS) = 0.343 + 0.107\ x$

In case of IV-IV alloys there is a gradual decrease in magnitude of bond hardness, microhardness and bulk modulus for alloys containing atoms of elements going down the group in order C → Si → Ge → Sn. However, bowing is observed in bulk modulus in case of SiC, GeC and SnC in which the mismatch of size of covalent radii is large (C = 7.74 nm, Si = 11.73 nm, Ge = 12.25 nm, Sn = 14.05 nm). The deviation is given by

$B_{PQ} = (1-x)P + xQ – b(1-x)x$

where the bowing parameter b = 1.8, 2.0 and 3.2 for SiC, GeC and SnC respectively. PQ denotes the alloy made up of elements P and Q and x=0.5 in this case. It is interesting to note that such deviations are not observed i.e. b = 0 in the case of SiGe, SiSn and GeSn. However, experimental values, to the best of our knowledge, are not available for comparison for these systems. Effect of atomic size and ionicity on bond hardness, microhardness and bulk modulus in case of IV-IV alloys are similar as in case of III-V and II-VI ternary alloys.

In some of the earlier studies[20,23,39] most of the nitride and oxide semiconductors have not been included for estimation of bulk modulus and microhardness of group III-V and II-VI systems respectively. BSb and CdO also do not figure in these studies. Even the experimental values of microhardness of BSb, AlN, GaN, InN, BeS, BeSe, BeTe and CdO are not available. Also, experimental results are not available for HgS, HgSe and HgTe. However, we have estimated the microhardness of these systems using Eqs. (8) and (11). Our estimated values are in reasonable agreement with reported values. In case of Sn, BSb and CdO, neither

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the experimental nor the theoretical values of microhardness have, to the best of our knowledge, been reported so far. Values have been reported for the first time. The two sets of values computed in this study (Table-II and IV) agree well and may be considered reasonable, because the values exhibit the decreasing trend as C→Si→Ge→Sn, BN→BP→BAs→BSb, CdO→CdS→CdSe→CdTe and also BeO→ZnO→CdO. The values of mechanical properties of these nitride and oxide systems are much higher than other semiconductors. This is primarily because of the smaller atomic size of N and O compared to other anions from group V and VI respectively. At the same time, the presence of N and O in the system from III-V and II-VI compounds strengthens the bonds more, because of absence of p- orbitals in their cores which allow them to penetrate deeper while forming bonds by overlap of valance orbitals. The bonds, therefore, become shorter and stronger giving rise to higher values of bond hardness, microhardness and bulk modulus. In case of BeO, the experimental value of microhardness ranges from 9.1 to 12.7 GPa, but the bulk modulus is not available. We, therefore, utilised the proposed relation Eq. (11) for estimating bulk modulus using the value (12.7 GPa) of experimental microhardness. The computed value 258 GPa is in reasonable agreement with the reported values of 265.12 GPa[23]. These results support the proposed relation between microhardness and bulk modulus. At the same time, our formula derived from bond hardness gives theoretical support to the empirical relations [20,23,37,38,40] proposed by earlier workers. Application of this relation can be extended to other ternary and quaternary semiconductor alloys too and will be taken up in future.

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Table 8. Bond hardness, H_{ab} (in GPa) and bulk modulus, B (in GPa) of $InP_{1-x}As_x$ and $In_{1-x}Ga_xP$ along with reported values and those obtained from Vegard's law

Sytems	X	Bond hardness, H_{ab} (in GPa)		Bulk Modulus, B (inGPa)			
		This Work	Using Vegards law	This Work	Using Vegard's law	Exp.	Reported
$InP_{1-x}As_x$	0	0.385	0.385	69.47	69.47	71[30]	60.8[39],67[33]
	0.01	0.385	0.384	69.38	69.39		
	0.025	0.384	0.384	69.24	69.27		
	0.05	0.382	0.382	69.01	69.07		
	0.075	0.381	0.381	68.79	68.86		
	0.1	0.379	0.379	68.56	68.66		
	0.2	0.373	0.373	67.68	67.85		
	0.3	0.366	0.368	66.83	67.04		
	0.4	0.360	0.362	65.99	66.23		
	0.5	0.354	0.356	65.17	65.43		
	0.75	0.340	0.342	63.22	63.40		
	0.9	0.332	0.333	62.10	62.19		
	1	0.327	0.327	61.38	61.38	60[30]	61[33],62.8[50]
$In_{1-x}Ga_xP$	0	0.385	0.385	69.47	69.47	71[30]	60.8[39],67[33]
	0.01	0.386	0.386	69.60	69.64		
	0.025	0.388	0.388	69.81	69.89		
	0.05	0.390	0.391	70.16	70.31		
	0.075	0.393	0.394	70.51	70.73		
	0.1	0.396	0.397	70.86	71.15		
	0.2	0.406	0.409	72.30	72.83		
	0.3	0.417	0.422	73.81	74.50		
	0.4	0.428	0.434	75.37	76.18		
	0.5	0.440	0.446	77.00	77.86		
	0.75	0.472	0.477	81.38	82.06		
	0.9	0.493	0.495	84.24	84.57		
	1	0.507	0.507	86.25	86.25	88.7[30]	81.5[39],86.7[33]

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Table 9. Bond hardness and bulk modulus of InP_{1-x} As_x and $In_{1-x}Ga_xP$ along with reported values and those obtained from Vegard's law

Sytems	X	Bond hardness, H_{ab} (in GPa)		Microhardness, H (inGPa)			
		This Work	Using Vegard's law	This Work	Using Vegard's law	Exp.(Ref.36)	Reported
InP_{1-x} As_x	0	0.385	0.385	5.27	5.27	4.10,3.30	4.78[20],5.05[23],4.813[37],5.50[40]
	0.01	0.385	0.384	5.25	5.26		
	0.025	0.384	0.384	5.23	5.24		
	0.05	0.382	0.382	5.19	5.20		
	0.075	0.381	0.381	5.16	5.17		
	0.1	0.379	0.379	5.12	5.14		
	0.2	0.373	0.373	4.98	5.01		
	0.3	0.366	0.368	4.84	4.87		
	0.4	0.360	0.362	4.70	4.74		
	0.5	0.354	0.356	4.57	4.61		
	0.75	0.340	0.342	4.25	4.28		
	0.9	0.332	0.333	4.07	4.08		
	1	0.327	0.327	3.95	3.95	3.30,3.84	3.68[20],3.91[23],3.123[37],3.99[40]
$In_{1-x}Ga_xP$	0	0.385	0.385	5.27	5.27	4.10,4.30	4.78[29],5.05[23],4.813[37],5.50[40]
	0.01	0.386	0.386	5.29	5.30		
	0.025	0.388	0.388	5.32	5.34		
	0.05	0.390	0.391	5.38	5.41		
	0.075	0.393	0.394	5.44	5.47		
	0.1	0.396	0.397	5.50	5.54		
	0.2	0.406	0.409	5.73	5.82		
	0.3	0.417	0.422	5.98	6.09		
	0.4	0.428	0.434	6.23	6.36		
	0.5	0.440	0.446	6.50	6.64		
	0.75	0.472	0.477	7.21	7.32		
	0.9	0.493	0.495	7.68	7.73		
	1	0.507	0.507	8.00	8.00	9.45	8.55[20],8.25[23],7.41[37],19.32[40]

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Table 10. Bond hardness, H_{ab} (in GPa) and bulk modulus, B (in GPa) of $ZnS_{1-x}Se_x$ and $Zn_{1-x}Cd_xS$ along with reported values and those obtained from Vegard's law

		Bond hardness, H_{ab} (in GPa)		Bulk Modulus, B (inGPa)			
Systems	X	This work	Using Vegard's law	This work	Using Vegard's law	Exp.(Ref. 30)	Reported
ZnS_{1-x} Se_x	0	0.454	0.454	75.31	75.31	77.1	73.3[31],72[32]
	0.01	0.454	0.453	75.20	75.21		
	0.025	0.452	0.452	75.04	75.07		
	0.05	0.450	0.451	74.78	74.83		
	0.075	0.449	0.449	74.51	74.60		
	0.1	0.447	0.447	74.25	74.36		
	0.2	0.439	0.440	73.21	73.41		
	0.3	0.432	0.433	72.20	72.46		
	0.4	0.424	0.426	71.22	71.51		
	0.5	0.417	0.420	70.26	70.56		
	0.75	0.400	0.402	67.96	68.18		
	0.9	0.391	0.392	66.65	66.75		
	1	0.385	0.385	65.80	65.80	62.4	65.1[39], 66.5[33]
$Cd_{1-x}Zn_xS$	0	0.345	0.345	60.46	60.46	62	53.2[39],60.3[33]
	0.01	0.346	0.346	60.58	60.61		
	0.025	0.348	0.348	60.76	60.83		
	0.05	0.35	0.35	61.07	61.20		
	0.075	0.352	0.353	61.38	61.57		
	0.1	0.354	0.356	61.69	61.95		
	0.2	0.364	0.367	62.97	63.43		
	0.3	0.374	0.378	64.30	64.92		
	0.4	0.384	0.389	65.68	66.40		
	0.5	0.394	0.4	67.12	67.89		
	0.75	0.423	0.427	71.00	71.60		
	0.9	0.441	0.443	73.53	73.83		
	1	0.454	0.454	75.31	75.31	77.1	73.3[39], 72[50]

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Table 11. Bond hardness, H_{ab} (in GPa) and microhardness, H (in GPa) of $ZnS_{1-x}Se_x$ and $Zn_{1-x}Cd_xS$ along with reported values and those obtained from Vegard's law

Sytems	X	Bond hardness, H_{ab} (in GPa)		Microhardness, M (inGPa)			
		This work	Using Vegards law	This work	Using Vegards law	Exp.(Ref. 36)	Reported
ZnS_{1-x} Se_x	0	0.454	0.454	2.33	2.33	1.7,2.8,3.5	1.75[20],3.3[39]
	0.01	0.454	0.453	2.32	2.32		
	0.025	0.452	0.452	2.31	2.32		
	0.05	0.450	0.451	2.30	2.30		
	0.075	0.449	0.449	2.28	2.29		
	0.1	0.447	0.447	2.26	2.27		
	0.2	0.439	0.440	2.20	2.21		
	0.3	0.432	0.433	2.14	2.15		
	0.4	0.424	0.426	2.07	2.09		
	0.5	0.417	0.420	2.01	2.04		
	0.75	0.400	0.402	1.87	1.89		
	0.9	0.391	0.392	1.79	1.80		
	1	0.385	0.385	1.74	1.74	1.3,1.8	1.36[20],1.66[40]
$Cd_{1-x}Zn_xS$	0	0.345	0.345	1.4	1.4		
	0.01	0.346	0.346	1.41	1.41		
	0.025	0.348	0.348	1.42	1.42		
	0.05	0.35	0.35	1.44	1.45		
	0.075	0.352	0.353	1.46	1.47		
	0.1	0.354	0.356	1.48	1.49		
	0.2	0.364	0.367	1.56	1.59		
	0.3	0.374	0.378	1.64	1.68		
	0.4	0.384	0.389	1.73	1.77		
	0.5	0.394	0.4	1.82	1.87		
	0.75	0.423	0.427	2.06	2.1		
	0.9	0.441	0.443	2.22	2.24		
	1	0.454	0.454	2.33	2.33	1.7,2.8,3.5	1.75[20],3.3[39]

4.Conclosion

Bond strength of elemental and binary semiconductors and their alloys has been calculated. Linear correlation between microhardness and bond hardness, and bulk modulus and bond hardness has been proposed. Also an empirical formula is proposed for estimation of microhardness of group- IV, IV-IV, III-V and II-VI semiconductors in terms of bulk modulus. Microhardness of Sn, SiC, GeC, SnC, SiGe,SiSn and GeSn has been predicated for the first time. The proposed relation has also been utilised to predict the bulk modulus of BeO

which is in reasonable agreement with the reported value, and its applicability can also be extended to other ternary and quaternary alloys.

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