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SHORT COMMUNICATION

Dependence of Physical Parameters of Compound Semiconductors on Refractive Index

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ABSTRACT

Interesting relationships have been found between refractive index, plasmon energy, electronic polarisability, bond length, microhardness, bulk modulus, force constants and lattice energy. An attempt has been made for the first time to correlate only one physical parameter with others. The calculated values are in good agreement with the experimental values as well as with the values reported in the literature. Refractive index data is the only one parameter required to estimate all the above parameters.

Keywords: Refractive index, plasmon energy, electronic polarisability, bond length, microhardness, bulk modulus, force constants, and lattice energy

1. INTRODUCTION

Recently, much attention has been given to the study of binary tetrahedral semiconductors because of their potential applications in linear and nonlinear optics, solar cells, light-emitting diodes, laser diodes, and integrated optical devices, such as switches, modulators, filters, etc. The evaluation of refractive indices of a semiconductor is of considerable importance for different applications, where the refractive index of the material is the key parameter for the device design. On the basis of Phillips and Van Vechten's[1] quantum dielectric theory, the refractive index, plasmon energy, and energy gap are interrelated. Kumar,[2] *et al.* have successfully developed several empirical relationships between plasmon energy, microhardness, and bulk modulus. Reddy,[3-5] *et al.* have given a relationship between refractive index and bulk modulus, nuclear effective charge, microhardness, optical electronegativity and electronic polarisability of semiconductor materials.

Recently, Kumar[6] estimated interatomic force constants and bond lengths for various semiconductors using plasmon energy. Kumar[7], *et al.* have reported interesting relationships between the electronic polarisability, lattice energy and plasmon energy. Ravindra and Srivastava[8] have developed Clausius-Mossotti equation, through a phenomenological approach, involving plasmon energy and average Penn gap. Most of the correlations discussed above are directly linked with plasmon energy. Plasmon energy and refractive index are well related with each other. Sincere efforts have been made for correlating the above parameters, but still many uncertainties exist, on how different physical parameters affect the structural, elastic and solidstate properties of semiconductor materials. In this paper, a number of equations have been proposed to estimate plasmon

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energy ($n\omega_p$), electronic polarisability (α_{pol}), bond length (d), force constants (α, β), microhardness (H), bulk modulus (B) and lattice energy (U). The calculated values of these parameters are in good agreement with the values reported by different investigators, as well as with experimental values. Some compounds of this family are potential candidates for infrared detectors used in military applications. Since the optical properties of semiconducting compounds play an important role in device development and fabrication, it is worthwhile to discuss the optical properties in terms of structure, stability, bonding, and other physical parameters.

2. THEORY & CALCULATIONS

Phillips and Van Vechten's[1] quantum di-electronic theory has been used to correlate refractive index, plasmon energy, and energy gap. Therefore, it was thought to be of interest to give an expression for refractive index and plasmon energy. Based on the above, the following relationship for the plasmon energy ($n\omega_p$) has been proposed:

$$n\omega_p = m \exp(bn) \tag{1}$$

Here, n is the refractive index, and m and b are the constants. The numerical values of these constants for $A^{II}B^{VI}$ semiconductors are 22.079, – 0.1779, respectively, and for $A^{III}B^{V}$ semiconductors are 47.924, – 0.3546, respectively.

Ravindra and Srivastava[8] have derived a relationship similar to that of Clausius-Mossotti in which $n\omega_p$ is involved. Replacing $n\omega_p$ with the above relation, one may get the electronic polarisability (α_{pol}) as

$$\alpha_{pol} = \left(\frac{S_0 K_1 \exp(K_2 n)}{S_0 K_1 \exp(K_2 n) + 3E_p^2} \right) \times \frac{M}{\rho} 0.396 \times 10^{-24} \tag{2}$$

$$S_0 = 1 - \left(\frac{E_P}{4E_F} \right) + \frac{1}{3} \left(\frac{E_P}{4E_F} \right)^2$$

$$E_P = \frac{n\omega_p}{\left(n^2 - 1\right)^{1/2}} \; eV$$

$$E_F = 0.2948 \times \left(n\omega_p\right)^{4/3} eV$$

Here, S_0, E_p, E_F, M and ρ have the same meaning as described by Ravindra and Srivastava[8]. K_1 and K_2 are constants and are listed in Table 1 for $A^{II}B^{VI}$ and $A^{III}B^{V}$ semiconductors.

Table 1. Numerical values of constants K_1, K_2, K_3, K_4, K_5

Parameter	Semiconductors	K_1	K_2	K_3	K_4	K_5
d	$A^{II}B^{VI}$	1.944	0.1186	----	----	----
(Eqn 3)	$A^{III}B^{V}$	1.159	0.2364	----	----	----
α_{pol}	$A^{II}B^{VI}$	487.480	– 0.3558	----	----	----
(Eqn 2)	$A^{III}B^{V}$	2296.709	– 0.7092	----	----	----
H	$A^{II}B^{VI}$	9.273	– 0.1779	4.97	----	----
(Eqn 4)	$A^{III}B^{V}$	104.953	– 0.3546	26.82	----	----
B	$A^{II}B^{VI}$	275.330	– 0.1779	124.33	----	----
(Eqn 5)	$A^{III}B^{V}$	648.890	– 0.3546	130.33	----	----
α	$A^{II}B^{VI}$	76.670	– 0.3024	----	----	----
(Eqn 6)	$A^{III}B^{V}$	286.300	– 0.6028	----	----	----
U	$A^{II}B^{VI}$	421.224	1338.9960	– 0.3546	408.814	– 0.7092
(Eqn 8)	$A^{III}B^{V}$	421.224	616.8800	– 0.1779	86.771	– 0.3558

Recently, Kumar[6] has proposed a relationship between bond length and plasmon energy for the $A^{II}B^{VI}$ and $A^{III}B^{V}$ groups of semiconductors. In the present study, the following relationship has been proposed for the estimation of bond length, d (Å) using refractive index of the material:

$$d\ (Å) = K_1 \exp (K_2 n) \quad (3)$$

The relevant values of K_1 and K_2 are listed in Table 1 for $A^{II}B^{VI}$ and $A^{III}B^{V}$ groups of semiconductors. Kumar[2], *et al.* have proposed some relationship between microhardness, bulk modulus and plasmon energy. Using the relationship proposed by Kumar[2], *et al.*, the following expressions have been obtained for microhardness and bulk modulus:

$$H(GPa) = K_1 \exp (K_2 n) - K_3 \quad (4)$$

$$B(GPa) = K_1 \exp (K_2 n) - K_3 \quad (5)$$

Though the above equations appear to be the same yet the nature of the linearity and their constants K_1, K_2 and K_3 have different magnitudes. These values are listed in Table 1.

Recently, Kumar[6] has proposed a simple relationship between the interatomic force constants α and β in terms of $n\omega_p$. In the present calculations, α and β are expressed in terms of n by the following equations:

$$\alpha\ (N/m) = K_1 \exp (K_2 n) \quad (6)$$

$$\beta\ (N/m) = 0.28\ (1 - fi)\ \alpha \quad (7)$$

Neumann's[9] expression Eqn (7) is used for the estimation of β. f_i is the ionicity of the semiconductor. The bond-stretching force constant (α) values are obtained using Eqn (6) in Eqn (7) to estimate the bond-bending force constant β. Kumar[7], *et al.* have developed a simple relationship between lattice energy and plasmon energy. Based on curve fitting, the following equation is proposed for calculating the lattice energy in terms of refractive index (n):

$$U = K_1 + K_2 \exp (K_3 n) - K_4 \exp (K_5 n) \quad (8)$$

Here, K_1, K_2, K_3, K_4 and K_5 are listed in Table 1 for $A^{II}B^{VI}$ and $A^{III}B^{V}$ groups of semiconductors.

The proposed correlations are empirical in nature and the numerical constants involved in the equations are unique in the sense that they represent the best fit with the experimental data. The relevant input data n, M, ρ and fi values have been taken from literature[10-12] to estimate, plasmon energy ($n\omega_p$), electronic polarisability (α_{pol}), bond length (d), microhardness (H), bulk modulus (B), force constants (α,β) and lattice energy (U). One can estimate the above physical parameters with the knowledge of refractive index (n) only.

3. RESULTS & DISCUSSION

The present paper reports different trends between refractive index (n), $n\omega_p$, α_{pol}, d, α, β, H, B and U in $A^{II}B^{VI}$ and $A^{III}B^{V}$ groups semiconductors. The above physical parameters are computed using Eqns (1-8) and are listed in Tables 2 to 5. The relevant K values are listed in Table 1. Figures 1-6 show the graphical representation of refractive index versus different physical parameters for II-VI and III–V groups of semiconductors. An excellent agreement has been observed between the calculated values of the above parameters and the values reported by different workers[2-5,7-15] as well as the available experimental values. The accuracy of the estimated physical parameters $n\omega_p$, α_{pol}, d, force constants (α,β), H, B and U mainly depend on the reliability and precision of the refractive index (input data). The calculated values of $n\omega_p$ for *SrTe*, *MgTe*, *SrSe*, *BaS*, *BaSe* and *ZnS* are deviating more in comparison with others[6,10]. The obtained plasmon energy values from Eqn (1) in the case of III-V groups of semiconductors are in good agreement with the literature values[6,10]. The bond length values listed in Table 2 are in reasonable agreement (except *BaS* and *BaSe*) with the corresponding values given by Kumar[6,7], *et al.* Experimental results confirm the present empirical rule. The proposed relationships between refractive index and electronic polarisability and bond length give an access to study the nature of bonding. Pauling has first established the nature of chemical bonding using the electronegativity concept. It can be observed from the tables that as the electronegativity difference for the groups of semiconductors and bulk modulus with common cation decrease with

Table 2. Plasmon energy and bond length of binary semiconductors

Compound	Refractive index n [10 – 12]	Plasmon energy, $n\omega_p$ (eV)		Bond length, d (Å)	
		Eqn (1)	Ref (6,10)	Eqn (3)	Ref (6,7)
$A^{II}B^{VI}$					
CaS	2.05	15.331	15.16	2.479	----
CaSe	2.09	15.223	14.10	2.490	----
CaTe	2.17	15.008	13.86	2.514	----
SrS	2.11	15.169	14.32	2.496	----
SrSe	2.13	15.115	13.20	2.502	----
SrTe	2.21	15.901	12.20	2.419	----
BaS	2.21	14.901	13.09	2.526	3.18
BaSe	2.38	14.457	12.41	2.578	3.31
MgSe	2.03	15.386	16.45	2.473	----
MgTe	2.12	15.142	12.99	2.499	2.75
ZnS	2.27	14.743	16.71	2.544	2.36
ZnSe	2.43	14.329	15.78	2.593	2.45
ZnTe	2.70	13.659	14.76	2.677	2.63
CdS	2.38	14.457	14.88	2.578	2.52
CdSe	2.49	14.177	14.01	2.611	2.62
CdTe	2.70	13.657	13.09	2.677	2.78
$A^{III}B^{V}$					
BN	2.10	22.758	24.53	1.905	1.56
AlN	2.16	22.278	22.97	1.932	1.86
AlP	2.75	18.073	16.65	2.221	2.35
AlAs	3.00	16.540	15.75	2.356	2.43
AlSb	3.19	15.462	13.72	2.465	2.66
GaN	2.40	20.462	21.98	2.045	1.94
GaP	2.90	17.137	16.50	2.301	2.36
GaAs	3.30	14.871	15.35	2.530	2.43
GaSb	3.79	12.499	13.38	2.840	2.65
InP	3.10	15.964	14.76	2.413	2.54
InAs	3.50	13.853	14.07	2.652	2.59
InSb	3.95	11.810	12.73	2.950	2.80

the refractive index and hence electronic polarisability increases. This trend is noticed in the case of II-VI and III-V groups of semiconductors. The ionic character can be understood from the proposed relations. Electronegativity difference of the two atoms forming a compound and band gap (E_g) are interrelated[4]. Compounds with ionic bonding have the largest band gaps and covalent bonding have the smallest ones. Electronegativity describes the pre-desposition of an atom to absorb electrons; its units are the square root of bond strength. Thus an atom with higher electronegativity will be more reactive chemically than one with a lower electronegativity. When the electronegativities with an atom engaged with covalent bonding are similar, this factor has little influence on bonding. However, when the difference of the electronegativities of the two species is equal or more than about 0.2 units, small amounts of ionic bonding may take place along with the covalent bonding.

Longer electronegativity difference involves the higher degree of ionicity in the bonding. It is probable that perfectly pure covalent bonding normally

Table 3. Electronic polarisability and lattice energy of binary semiconductors

Compound	Refractive index n [10 – 12]	Electronic polarisability $[\alpha_{pol}(\text{Å})^3]$				Lattice energy, U (kcal/mol)	
		Eqn (2)	Known+	Ref (7)	Ref (8,13,14)	Eqn (8)	Ref (7)
$A^{II}B^{VI}$							
CaS	2.05	5.25	6.15	----	5.90	808	----
CaSe	2.09	6.25	7.63	----	6.98	805	----
CaTe	2.17	6.82	8.70	----	7.53	800	----
SrS	2.11	6.15	6.80	----	6.85	804	----
SrSe	2.13	7.34	8.51	----	8.15	803	----
SrTe	2.21	9.08	10.86	----	9.95	709	----
BaS	2.21	7.87	8.42	----	8.64	709	----
BaSe	2.38	9.61	9.88	----	----	788	----
MgSe	2.03	4.39	6.04	----	----	809	----
MgTe	2.12	7.56	----	9.95	10.62, 11.05	803	754
ZnS	2.27	5.03	5.46	5.35	5.46, 5.65, 5.69	794	838
ZnSe	2.43	6.08	6.54	6.16	6.54, 6.81, 6.50	785	818
ZnTe	2.70	7.72	8.15	7.26	8.16, 8.00, 8.11	770	795
CdS	2.38	6.68	7.22	7.12	7.22, 7.78, 7.05	788	798
CdSe	2.49	7.93	8.27	8.25	8.27, 9.12, 7.91	782	778
CdTe	2.70	----	10.98	----	----	770	756
$A^{III}B^{V}$							
BN	2.10	2.11	2.45	2.75	2.32,2.45	965	999
AlN	2.16	2.51	2.74	3.22	2.74, 2.94, 2.94	955	969
AlP	2.75	6.21	6.50	6.88	6.50, 5.92, 7.08	868	837
AlAs	3.00	7.42	8.16	7.83	8.16, 7.51, 8.33	835	817
AlSb	3.19	10.19	10.10	10.75	10.23, 9.59, 10.10	811	771
GaN	2.40	3.12	3.80	3.58	3.33, 3.33, 3.18	918	949
GaP	2.90	6.59	6.87	7.03	6.24	848	834
GaAs	3.30	8.02	8.27	8.31	7.66	797	808
GaSb	3.79	10.79	10.72	11.38	10.34	743	763
InP	3.10	8.64	8.94	9.09	8.66	822	795
InAs	3.50	10.21	10.48	9.72	9.53	774	779
InSb	3.95	13.20	13.46	12.74	14.27	726	748

+ Calculated from the Clausius-Mossotti relation $[(n^2-1)/(n^2+1)]\, M/\rho = 2.53 \times 10^{24}$, taking n, M and ρ values from Ref [10-12]

does not exist in compounds because no two atoms have identical electronegativities, small degree of ionicity are present. The percentage of ionic bonding, based on Pauling's criterion, is estimated to be 22 per cent in *CdS* and *ZnS*. After careful examination of the crystal structure, it is known that the wurzite structure is more favourable for crystals with large charge difference of electronegativity between the two kinds of atoms. In other words, the general tendency is such that the wurzite structure is more proven than the zinc blende structure having a higher degree of ionicity. The nature of the bonding is clearly evident from this discussion.

Estimated physical parameters in the present study are in good agreement with the values reported by the different investigators. Several other workers have also estimated these parameters with distinct ideas. But, all the methods enumerated in the literature involves tedious or too many experimental parameters[3-5,8-10]. The main advantage of the present model is the simplicity of the formulae, which do

Table 4. Microhardness and bulk modulus of binary semiconductors

Compound	Refractive index n [10–12]	Microhardness, H (GPa)			Bulk modulus, B (GPa)		
		Eqn (4)	Expt Ref (2)	Ref (2, 15)	Eqn (5)	Expt Ref (2)	Ref (2-5,9)
$A^{II}B^{VI}$							
CaS	2.05	1.469	----	----	67	----	----
CaSe	2.09	1.423	----	----	66	----	----
CaTe	2.17	1.333	----	----	63	----	----
SrS	2.11	1.440	----	----	65	----	----
SrSe	2.13	1.378	----	----	64	----	----
SrTe	2.21	1.708	----	----	74	----	----
BaS	2.21	1.288	----	----	62	----	----
BaSe	2.38	1.101	----	----	56	----	----
MgSe	2.03	1.492	----	----	68	----	----
MgTe	2.12	1.389	----	0.48	65	----	37
ZnS	2.27	1.222	1.70,2.80,3.50	2.05	60	77	84
ZnSe	2.43	1.048	1.30-1.80	1.66	54	62	72
ZnTe	2.70	0.766	0.80-1.10	1.23	46	51	60
CdS	2.38	1.101	1.20	1.28	56	62	61
CdSe	2.49	0.984	0.70-1.20	0.91	52	53	50
CdTe	2.70	0.765	0.40-0.74	0.53	46	42	39
$A^{III}B^{V}$							
BN	2.10	23.020	34.30-73.00	26.90	178	----	202
AlN	2.16	21.968	12.30	23.48	171	----	181
AlP	2.75	12.759	5.50	9.64	114	86	95
AlAs	3.00	9.402	4.8-5.00	7.67	94	77	83
AlSb	3.19	7.041	4.00	4.43	79	58	55
GaN	2.40	17.991	----	21.32	146	----	167
GaP	2.90	10.71	9.45	9.32	102	89	93
GaAs	3.30	5.747	7.50	6.79	71	75	78
GaSb	3.79	0.552	4.48	2.48	39	57	51
InP	3.10	8.141	4.10	5.5	86	71	70
InAs	3.50	3.518	3.30	3.99	57	60	64

not require any experimental data except refractive index of the semiconductors. In the case of calcium, strontium, barium atoms linked with selenium (*Se*) and tellurium (*Te*), the estimated $n\omega_p$, and bond length values are not in good agreement with the reported values[6,7,8]. This may be due to the strong electronegative Se^- and Te^- ions.

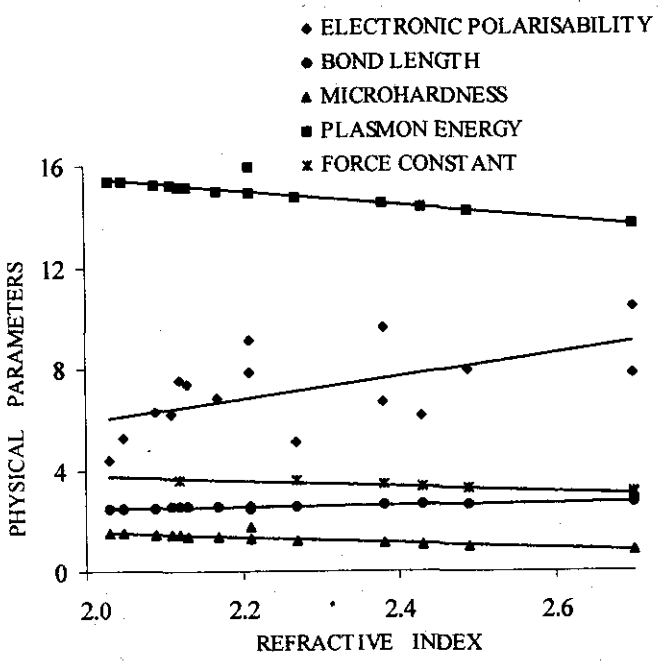

Figure 1. Plot shows the graphical representation of refractive index versus different physical parameters for II–VI groups of semiconductors.

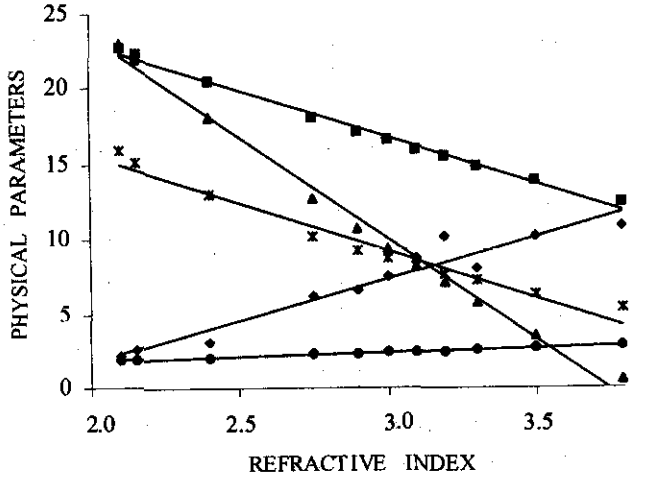

Figure 2. Plot shows the graphical representation of refractive index versus different physical parameters for III–V groups of semiconductors.

In terms of the bonding, Reddy[14], *et al.* have reported that the electronegativity difference ($\Delta\chi$) in the groups of semiconductors with common cation decreases, the optical susceptibility and electronic polarisability increase. The magnitude of $\Delta\chi$ indicates the nature of the bonding[12,14] (ionic or covalent). $\Delta\chi$ Values are slightly higher for II-VI groups of

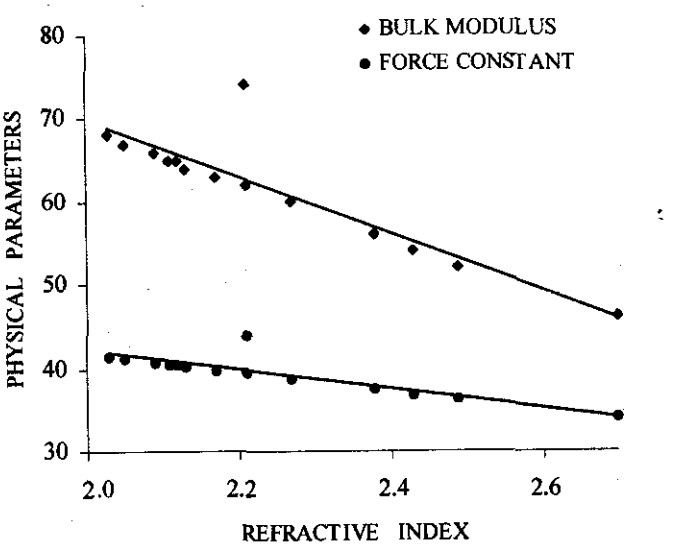

Figure 3. Plot shows the graphical representation of refractive index versus physical parameters for II–VI groups of semiconductors.

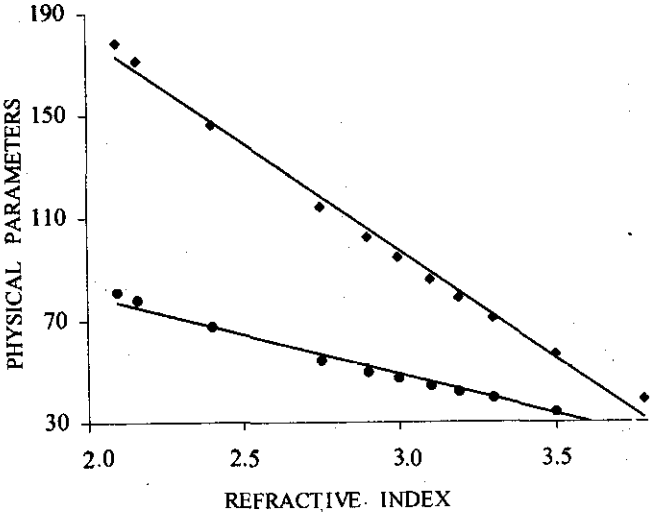

Figure 4. Plot shows the graphical representation of refractive index versus physical parameters for III–V groups of semiconductors.

compounds[14]. It indicates that the ionicity in these compounds is more in comparison to III-V groups of compounds. Equation (2) has its special significance. It connects Penn gap, Fermi energy, plasmon energy, refractive index and electonic polarisability. Moreover, it is similar to that of Clausius-Mossotti relationship. Except *MgTe* and *ZnS* values of α, β, the other estimated values are in good agreement with others[6]. The empirical relationship proposed in the present study will stimulate basic research in describing

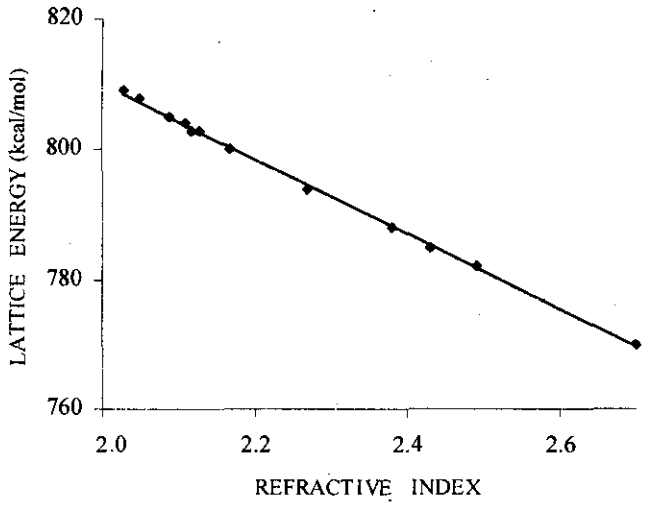

Figure 5. Plot shows the graphical representation of refractive index versus lattice energy for II–VI groups of semiconductors.

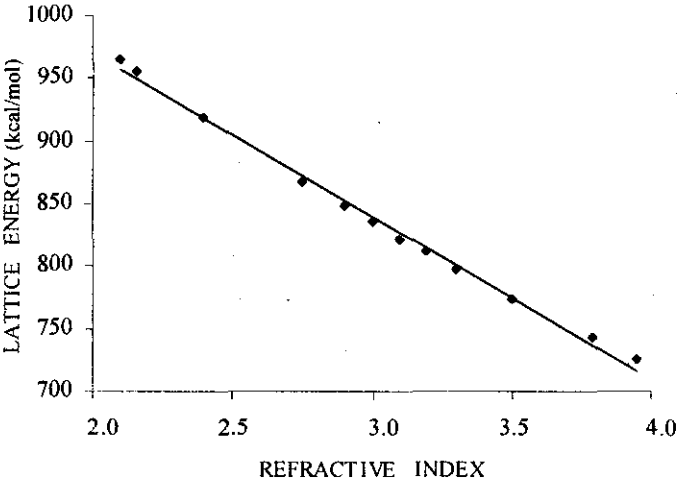

Figure 6. Plot shows the graphical representation of refractive index versus lattice energy for III–V groups of semiconductors.

the physical characterisation of compound semiconductors. In most of the cases, the values coincide with the others. Hence, it is possible to predict the above parameters of the compound semiconductors with the knowledge of only one parameter called refractive index.

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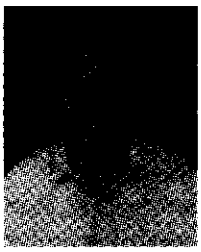
Contributors



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