International Journal of Advanced Research in Engineering and Applied Sciences
ISSN: 2278-6252
Impact Factor: 7.687

The Dependence of Magnetic Susceptibility, Electronic Polarizabilty on Refractive index for the Binary Compounds

Anil Kumar Ojha,
Department of Physics, Govt. College, Tigaon (Faridabad).
E-mail:- ojha97@rediffmail.com

Abstract

An analysis is presented for the electronegativity, fractional ionic character and refractive index of binary compounds with mono-valent, divalent and trivalent atoms in order to calculate the electronic polarizabilty and magnetic susceptibility. The values of electronegativity difference by investigating a relationship between fractional ionic character and electro negativities have been determined .More accurate of ionicity based on the revised energy gap model have been used in the present study to obtain the new results. The values of electronegativity difference are found to be correlated well with the values of refractive index and energy gap in case of I-VII.II-VI and III-V binary compounds. Valance electron plasma energies have also been calculated from the interionic distances for I-VII,II-VI and III-V group binary Compounds based on the assumption that a linear relationship exists between them with in a molecular group of compounds. The estimated valance electron plasma energy values are used in the evaluation of electronic polarizabilty and magnetic susceptibility in the above group of solids .Different new relations are proposed between the magnetic susceptibility and electronic polarizabilty. Good agreements are observed between the computed and literature values of magnetic susceptibility.

Introduction

The magnetic Susceptibility plays a vital role in understanding the nature of the chemical bonding in semiconductor Binary crystals. Interesting relationships between certain physical parameters such as electronic polarizabilty, ionicity parameters, energy gap, refractive index etc. and individual components of lattice susceptibility, Characterizing both bands and bonds in semiconductors, have been reported [1,2].It has been recognized that many of the physical properties of simple and compound semiconductors are governed by the position in the periodic chart of the component atoms. Therefore the search for the key parameters, which characterize both the individual and bound atoms, may be very useful to define and predict some typical properties of a given semiconductor. The average ionic gap is very useful parameters in understanding the trends over the periodic table for a class of semiconductors, provided that the value of the dielectric constant is available. The high frequency dependent dielectric constant is explicity dependent on the valance plasma energy, an average energy gap and Fermi energy. The electronic dielectric constant, the energy gap between bonding and antibonding states and interionic nearest neighbor separation for a given crystal are related to each other With the help of valance electron plasma energy with dielectric constants and energy gap and refractive index some other parameters can be evaluated and these evaluated parameters are used to calculate the values of magnetic susceptibility and electronic polarizabilty for the above crystals. Electronic polarizabilty and Magnetic susceptibility are also related to the electronegativity and ionicity parameters for the crystals. Electronegativity is defined as the power of an atom to attract an electron to itself. Pauling determined the electronegativity of different elements using thermochemical method based on the dissociation energies of molecules

and compounds. Many attempts have been made to find several relationships between physical and chemical parameters both from the point of view of fundamental interest and technological application [1-8]. Batsanov[9,10] proposed a method for calculating the electronegativity from thermochemical and structural parameters of inorganic materials. However electronegativity is also related with Energy gap and ionicity parameters. Singh [19] have used a modified energy gap expression as derived by Grimes and Cowley [4] in order to revise the estimates of ionicity parameters due to Phillips[14] and Vechten [15].Their revised values of ionicity parameters obtained for A^NB^{8-N} type diatomic compounds are shown to exhibit systematic relationships with interatomic separations. Grimes and Cowley [4] removed the shortcomings of the models due to Penn[2] and Srinivasan [5],Penn[2]derived a set of formulae based on an isotropic, nearly free electron model for the energy bands. The work of Penn was extended by Srinivasan. However, the model adopted by Penn as well as Srinivasan [5] was so complicated that the dielectric function could not be evaluated analytically. They obtained approximate analytic expressions for the dielectric function after introducing several simplifications specifically, the square matrix elements were replaced by interpolation formula chosen to reproduce the zero and long wave vector values, and energies near the zone boundary were replaced by constant values rather than the exact expressions. These drawbacks have been rectified by evaluating the sums directly as integrals over the spherical Brillouin zone. Results obtained are sufficiently accurate at small, intermediate and large wave vectors. The modified expression for the energy gap between bonding and antibonding states due to Grimes and Cowley[4] is plausible and consistent with experimental data[22].A simple empirical relationships been established for the estimation of magnetic susceptibility, electronic polarizabilty with the refractive index parameters[25-27].

Method of Analysis:-

The modified expression for energy gap between bonding and anti bonding states evaluated numerically has been found as given by Grimes and Cowley[4]

$$\epsilon_\infty - 1 = \left(\frac{\hbar \omega_p}{E_g} \right) S_0 \quad (1)$$

Where ϵ_∞ is the electronic constant which is related to the refractive index $\epsilon_\infty = n^2$,as ,S_0=0.62 is the correction factor, E_g is the average energy gap between bonding and antibonding states Plasma energy $\hbar \omega_p$ can be related to the interionic distance by following equations, assuming that they are applicable to compound semiconductors and alkali halides [25]

$\hbar \omega_p = -8.08 (r_0 + 39.10$ for alkali Halides I-VII group (2)

$\hbar \omega_p = -6.78 (r_0) + 34.44$ group II-VI semiconductors (3)

$\hbar \omega_p = -8.99 (r_0) + 37.80$ group III-V semiconductors (4)

Where $\hbar \omega_p$ and r_0 are the valance electron plasma energy in eV and interionic distance in A^0. The Energy gap E_g can be split in to an ionic (Heteropolar) part C and Covalent (Homopolar) part E_h such that

$$E^2_g = E^2_h + C^2 \quad (5)$$

The ionicity of chemical bond is expressed in terms of fractional ionic character f_i as follows;

$$f_i = C^2 / E^2_g \quad (6)$$

and fractional covalent character as;

$f_c = 1-f_i = (E^2_h / E^2_g)$ (7)

Following the theory due to Pauling, a relationship between fractional ionic character and electronegativity difference Δ X,

$\Delta X = 2\{ \ln(1-f_i)^{-1}\}^{0.5}$ (8)

The linear relationship between n^2 (refractive index)^2 and Δ X can be represented as[20-21],

$n^2 = A_1 \Delta X + B_1$ (9)

where A_1 and B_1 are constants determined by finding a regression line based on the data for a group of compounds[20]

The relationships between E_g and Δ X can be written as follows

$\ln E_g = A_2 \ln \Delta X + B_2$ (10)

and

$\ln E_g = A_3 \Delta X + B_3$ (11)

Equation (8) gives the power as

$E_g = B_2(\Delta X)^{A_2}$ (12)

Where Equation (9) gives the exponential law

$E_g = B_3 e^{A_3 \cdot \Delta X}$ (13)

The electronic polarizabilty (α) of a material is also related to the refractive index as follows-

$\alpha = [(n^2 -1)/ (n^2 +2)]/(3M/4\pi Nd)$ (14)

Where n is the refractive index of the substance, d is its density at temperature T,M is its molecular weight and N is the Avogadro number . Above equation for refractive index is based on the classical theory of the dielectric constant due to claussius and Mossotti [24,25].

The electronic polarizabilty (α) is also related to the electronegativity difference as follows

$\alpha = A_4(\Delta X) + B_4$ (15)

the constants A_4 and B_4 are cation dependent in case of I-VII and II-VI compounds and independent of cations or anions in III-V compounds [21].

The magnetic susceptibility can be evaluated by using the values of electronic polarizabilty with the help of linear relationships given by Reddy et.al.[26]

$\chi_d = - [8.83x10^{18} (\alpha) + 5.020 x 10^{-6}]$ for alkali Halides (16)

$\chi_d = - [7.82x10^{18} (\alpha) + 8.102x10^{-6}]$ for II-VI compounds (17)

$\chi_d = - [4.56x10^{18} (\alpha) + 0.510 x 10^{-6}]$ for III-VI compounds (18)

χ_d is also obtained by using Kirkwood's equation [27]

$\chi_d = -3.11 x10\text{-}6 (Z \alpha)^{1/2}$ (19)

Kirkwood relationship shows that the susceptibility is proportional to the square root of the polarizabilty but the experimental results supports the linearity between them. In terms of refractive index χ_d and α of the given crystals are also given as,[21].

$\chi_d = 2.01 x 10^{-6} \sum [n^2/(Z-s)^2][1- 3(l+1)-1/5n^2]$ (20)

and

$\alpha = 0.281\sum [(5n^2 + 7n^4)(2l +1)/Z-s)^4]$ (21)

Result and Discussion:-

The necessary interionic distance, and energy gap are taken from the literature [1-10]. The valance plasma energy is calculated from the relationships given in equations(2-4). Using the values of average energy gap E_g the values of electronic dielectric constant ε_∞ has been calculated. The values of E_g has also been calculated from the power law and empirical law relation given in equation (12) and equation (13).The electronegativity difference in terms of fractional ionic character has been formulated by using the equation(8). For calculating

refractive index of the crystals the Moss[24] relation $\varepsilon_\infty = n^2$ and the linear relationship proposed by Singh et.al.[20] given in equation (9) has been utilized. The values of the constants A_1,B_1 ; A_2,B_2; A_3,B_3 and A_4,B_4 reported by Singh et.al.[20] are given in table (1). For calculating electronic polarizabilty its relation with electronegativity given in equation (15) has been used. The values of electronic polarizabilty (α) has been calculated by using a relation given in equation (14) taking the values of refractive index. The value of this parameter can also be calculated from equation (15), reported in tables (2-4). The electronic polarizabilty data obtained from (14) and (15) are inserted in to (16-18) . Calculated values of various above optoelectronic parameters Table (2-4) agrees fairly with experimental results . It is interesting to note that the decrease of interionic distances shows and corresponding increase in χ_d. It is to be noted that all groups of the compounds studied exhibit a linear variation in the value of χ_d. It is pertinent to mention here that Iχ_dI decreases with a corresponding increase in band gap energy and hence decrease with refractive index.

Acknowledgement - I am extremely grateful to Professor Jai Shanker and Prof. B.P. Singh, department of Physics, Institute of Basic Sciences, Khandari, Agra for their valuable guidance, support and discussion.

Table -1

Values of parameters used to evaluate various optoelectronic parameters [21].

Cations	A_1 (eV)	B_1 (eV)	A_2 (eV)	B_2 (eV)	A_3 (eV)	B_3 (eV)	A_4 (eV)	B_4 (eV)
Li	-10.1	34.6	19.7	-20.1	6.31	-17.3	-33.0	106.9
Na	-6.64	25.1	18.6	20.5	5.41	-16.1	-30.2	107.5
K	-12.4	46.8	41.6	-51.1	11.6	-39.4	-108.3	396.2
Rb	-10.8	41.8	43.7	54.5	11.9	-41.4	-130.2	482.9
Cs	-19.7	75.8	54.9	-70.0	14.8	-52.9	-165.6	621.1
Cu	-14.9	39.1	12.4	-8.60	5.26	-10.3	-35.1	89.2
Ag	-5.04	18.4	3.9	-2.05	1.45	-2.11	-13.7	44.8
Mg	-8.18	25.9	5.73	-3.36	2.28	-3.83	-17.4	49.1
Ca	-15.3	47.2	11.3	-9.63	4.09	-9.50	-48.6	141.7
Sr	-13.7	43.9	11.1	-9.98	3.89	-9.34	-42.7	129.8
Ba	-36.7	115.9	8.69	-7.76	2.90	-6.92	-3.09	99.0
Zn	-14.5	33.3	5.69	-1.84	3.01	-3.93	-25.5	55.2
Cd	-4.65	16.0	2.85	-0.49	1.31	-1.14	-25.2	63.7
Al,Ga,In	-8.26	18.8	0.88	1.19	0.93	0.49	-8.61	16.9

Table -2

Calculated values of valance Plasma energies, electronegativity, energy gap, electronic polarizabities, Magnetic Susceptibility and refractive index of Alkali Halides

Crystals	(f_i)	r (A^0) (Interatomic separation)	(ΔX) Eq.8	Energy gap E_g (eV)	Plasma Energy $\hbar\omega_p$ (eV) (Eq.2)	(α) (A^0)^3		χ_d (10^{-} cm^3. mol^{-1}) Eq.16	$\varepsilon_\infty = n^2$ R.I Eq.9
						Eq.14	Eq.15		
LiF	0.926	2.01	3.223	9.49	22.84	0.85	0.72	-12.3	1.93
LiCl	0.909	2.57	3.141	7.02	18.33	3.00	2.82	-30.5	2.75
LiBr	0.915	2.75	3.095	5.91	16.87	4.04	3.98	-39.4	3.16
LiI	0.901	3.09	3.041	4.38	14.62	7.14	6.32	-65.8	3.80
NaF	0.955	2.31	3.527	9.99	20.43	1.34	1.32	-16.5	1.74
NaC1	0.946	2.81	3.419	8.13	16.33	3.75	3.19	-37.0	2.33
NaBr	0.941	2.98	3.381	7.21	14.98	4.93	4.31	-47.0	3.60
NaI	0.939	3.23	3.343	6.00	13.96	7.26	6.42	-66.8	3.01
KF	0.963	2.64	3.631	9.77	18.54	1.80	1.10	-20.4	1.85
KCl	0.962	3.14	3.621	8.59	13.70	4.97	4.13	-47.3	2.17
KBr	0.961	3.31	3.597	7.96	12.46	6.32	6.25	-58.8	2.36
KI	0.959	3.56	3.572	6.88	10.57	8.97	8.19	-81.4	2.65
RbF	0.967	2.77	3.694	9.43	16.32	2.26	2.62	-24.3	1.93
RbC1	0.965	3.27	3.662	8.56	12.52	5.71	4.78	-53.6	2.18
RbBr	0.964	3.44	3.649	8.02	11.32	7.21	6.92	-66.4	2.34
RbI	0.963	2.69	3.637	7.15	17.55	10.12	9.09	-91.1	2.58
CsF	0.969	3.03	3.728	8.65	14.78	2.67	2.58	--27.8	2.16
CsC1	0.969	3.57	3.725	7.50	10.30	5.31	5.24	-50.2	2.63
CsBr	0.968	3.70	3.717	6.95	9.06	5.99	6.61	-56.0	2.78
CSI	0.967	3.95	3.694	5.88	7.13	9.29	9.16	-84.0	3.05
CuF	0.781	1.85	2.464	2.46	18.23	2.71	2.66	-28.1	2.50
CuCl	0.762	2.35	2.397	2.40	15.26	5.41	5.39	-51.0	3.65
CuBr	0.737	2.46	2.312	2.31	13.46	7.18	6.98	-66.1	4.40
CuI	0.728	2.62	2.282	2.82	12.45	9.80	9.60	-88.4	5.50
AgF	0.899	2.46	3.030	3.03	18.95	3.17	3.08	-32.0	2.90
AgCl	0.869	2.77	2.851	2.85	15.23	6.12	6.10	-57.1	4.15
AgBr	0.847	2.89	2.742	2.74	12.45	7.24	7.19	-66.6	5.00
AgI	0.775	2.80	2.443	2.44	12.63	11.32	10.30	-101.3	5.90

Table -3

Calculated values of valance Plasma energies, electronegativity, energy gap, electronic polarizabities , Magnetic Susceptibility and refractive index of II-VI group Binary Compounds

Crystals	(f_i)	r (A^0)	(ΔX) Eq.8	Energy gap E_g (eV) (Eq.3)	(α) (A^0)^3		Plasma Energy $\hbar\omega_p$ (eV) Eq.(3)	χ_d (10^- cm^3. mol^{-1}) Eq.17	$\varepsilon_\infty = n^2$ Refractive index
					Eq.14	Eq.15			
MgO	0.857	2.10	2.79	8.61	4.04	3.96	22.25	-6.1	2.95
MgS	0.806	2.60	2.56	4.31	4.44	4.02	20.36	-41.7	5.10
MgSe	0.790	2.73	2.50	3.66	5.66	5.45	19.65	-51.4	5.90
MgTe	0.730	2.75	2.29	2.76	9.22	8.30	18.39	-79.9	7.00
CaO	0.870	2.40	2.86	6.15	2.22	2.61	18.13	-23.9	3.33
CaS	0.862	2.84	2.81	5.40	5.85	4.89	15.14	-52.9	4.50
CaSe	0.851	2.96	2.76	5.00	7.06	5.93	14.36	-62.6	5.10
CaTe	0.832	3.17	2.67	4.20	7.85	6.67	12.89	-72.6	6.30
SrO	0.888	2.57	2.96	5.80	2.90	3.55	16.95	-29.3	3.30
SrS	0.875	3.01	2.88	4.80	6.56	5.90	14.03	-58.6	4.40
SrSe	0.873	3.12	2.87	4.60	8.05	7.10	13.27	-7.05	4.90
SrTe	0.855	3.24	2.78	4.00	10.73	8.95	11.81	-91.9	5.80
BaO	0.907	2.75	3.08	4.20	3.45	5.29	15.66	-33.7	3.00
BaS	0.886	3.18	2.09	4.00	7.75	7.78	13.78	-68.1	7.10
ZnO	0.880	3.12	2.91	3.47	8.74	3.22	21.22	-76.0	5.06
ZnS	0.876	2.90	2.89	2.75	7.89	4.98	18.44	-86.6	5.20
ZnSe	0.646	1.95	2.04	3.20	2.48	6.37	17.83	-26.0	3.75
ZnTe	0.627	2.36	1.98	3.70	6.43	7.75	16.61	-57.5	5.20
CdO	0.596	2.45	1.90	2.58	7.30	4.41	18.51	-64.5	5.90
CdS	0.551	2.63	1.79	2.10	9.54	7.34	14.57	-82.4	7.30
CdSe	0.789	2.35	1.49	2.60	7.87	9.08	14.03	-61.0	4.63
CdTe	0.706	2.93	2.21	2.40	9.28	9.20	13.98	-69.1	5.20

Table -4

Calculated values of valance Plasma energies, electronegativity, energy gap, electronic polarizabities , Magnetic Susceptibility and refractive index of III-V group Binary Compounds

Crystals	(f_i)	r (A^0)	(ΔX) Eq.8	Energy gap E_g (eV) (Eq.4)	(α) $(A^0)^3$		Plasma Energy $\hbar\omega_p$ (eV) (Equation (4)	χ_d (10^{-} cm^3. mol^{-1}) Eq.18	$\varepsilon_\infty = n^2$ Refractive index Eq.9
					Eq.14	Eq.15			
AlN	0.451	1.86	1.548	2.98	1.86	2.59	21.08	-4.1	4.80
AlP	0.327	2.35	1.260	2.55	5.25	5.43	16.67	-21.4	8.50
AlAs	0.221	2.43	1.000	2.24	7.40	6.94	15.95	-32.4	10.3
AlSb	0.145	2.66	0.792	2.24	10.44	9.48	13.89	-48.0	10.2
GaN	0.469	1.94	1.591	5.45	2.07	2.97	20.36	-5.2	5.00
GaP	0.333	2.36	1.273	2.97	6.74	6.10	16.58	-29.1	8.50
GaAs	0.137	2.43	0.769	2.42	8.22	7.63	15.95	-36.6	11.3
Gasb	0.060	2.65	0.495	1.86	11.29	12.61	13.95	-52.4	14.4
InIN	0.507	2.13	1.682	4.47	3.11	4.59	18.65	-10.5	5.50
InP	0.342	2.54	1.294	2.48	8.95	8.74	14.97	-40.4	9.60
InAs	0.188	2.62	0.913	2.07	10.65	11.40	14.25	-49.1	12.3
InSb	0.078	2.80	0.569	1.64	13.67	14.53	12.63	-64.5	15.7

References :-

[1] Harison W.A. ; Electronic structure and properties of solids (1980)
[2] Penn D.R. ;Phys.Rev.28,2093(1962).
[3] Shanker J. and Dixit S; Phys.State sol. (a) 123.17(1991).
[4] Grmes And Cowley F.R. ;Can.J.Phys 53,2549+ (1975).
[5] Sriniwasan G.;Phys.rev.291244(1969).
[6] Phillips J.C.;Rev.of Mod.Phys.B17,42(1970 .; Phy.Rev.B29.6583(1964) ; ; Phys.State sol.(a)18,55(1966),Phys Rev.Lett.20,550(1968).
[7] Pauling L.;Nature of Chemical Bond,CornwellUniversity,Ithaka,N.Y.(1960); ;Proc.Roy Soc.A1114,181(1927);J.Am.chem.Soc.54,3;Phjy570(1932).
[8} P.Boguslawasi; ; Solid state.Comm.(USA),7,626(1986)
[9] Batsanov S.S. ;Zh Fig Khim,74,331(2000).
[10] Batsanov S.S.*zv Akad Nauk SSSR Neorg Mater,26,679(1990)*
[11] Penn D.R.;Phys.Rev.128,2093(19692)
[12] Shanker J.;Goyal S.C. and Verma M.P. ; Phys.Rev.B14,4669(1976).
{13} Levine B.F.;Phy.Rev.B7,2600(1973),J.chem.Phys.,59(1973);Phys.Rev.:ett.25,44(1970).
[14] Van. Vechten J.A. ;Phys.Rev.89,469(1969);Phys.Rev.B1,3351(1970).
[15] Phillips J.C. and Van. Vechten J.A. Phys Rev. 183,709(1976).
[16] Motfit W.F. ;Proc.Roy Soc. London A196,510(1949) ; A 202,548(1959).
[17] Pentilides S.T.;Phys Rev.B11,5082(1975).
[18] Shanker J.and Aharma O.P.;Philosophical Magzine35,6(1977).
[19] Singh B.P.Phys.stat.sol.(b)162,329(1990).
[20] Singh B.P.,Baghel V.S.and Bhagel K.S.;Ind.J.Pure & applied Phys.12,293(2009).
[21] Singh B.P.,Baghel V.S.and Bhagel K.S.;Ind.J.Pure & applied Phys.47,793(2009).
[22] Singh B.P. and ojha A.K.;Indian J.Phys.76A(3)297(2003).
[23] Singh B.P.,Ojha A.K. And S.Tripti;Physica B,350338(2004).
[24] Moss T.S;Phys,Status Solidi (b) ,131.415(1985),
[25] Singh B.P.,Tripti S.and Singh Vipnesh Indian J.pure & AppliedPhys.46,502(2008).
[26] Reddy R,R,.Nazeer Ahmed Y;Rama Gopal K & Raghuram DV; Opt. Matter. 10,95(1998)
[27] Reddy R,R,.Nazeer Ahmed Y& Ravi Kumar M;Phys, Chem.Solds.56,825(1995).
[28] Reddy R,R,.Nazeer Ahmed Y;Rama Gopal K & Raghuram;Opt.Mater,14,355(2000).
[29] Salem M.A. Turk J.Phys,27,569(2003).
[30] Reddy R,R,.Nazeer Ahmed Y;Rama Gopal K et.al.;Indian J Pure& appl.Phys.,40,471,(2002) [31] Wimples And Didomenics; Phys. Rev.Lett.23,1156(1969).