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Relationship between Refractive Index, Electronic Polarizavility, Optical Energy Gap Optical Electronegativity and Plasmon Energy in I-Iii-Vi_2 and Ii-Iv-V_2 Groups of Semi Conductors.

R.S. Indolia[a] and R.K. Verma[a]
Dept. Of Physics Agra College, Agra[a]

ABSTRACT
Refractive index(n), Electronic Polarizability (α_p), Optical Energy Gap(E_g) and optical electronegativity($\Delta\chi^*$), of I-III-VI_2 and II-IV-V_2 groups of ternary semiconductors have been calculated using Plasmon energy data on the basis best fit data, new relations have been proposed for the calculation of refractive index , electronic polarizability, optical energy gap and optical electronegativity. The calculated values of n, $\alpha_{p,}$ E_g and ($\Delta\chi^*$) from the new relations have been compared with the values reported by different researcher. An excellent agreement with calculated values and experimental values has been obtained.

Keywords:
Plasmon energy, Refractive index, Electronic Polarizability optical energy gap and optical electronegativity for I-III-VI_2 and II-IV-V_2 groups of semiconductors.

I. INTRODUCTION

Optical energy gap(E_g), Refractive index(n), Electronic Polarizability(α_p), optical electro-negativity($\Delta\chi^*$) of I-III-VI_2 and II-IV-V_2 groups of semiconductors have been an important parameters to study these ternary semiconductors, because these ternary semiconductors have potential application in a variety of opto-electronic devices such as non-linear optics, Light emitting diodes, photo voltaic cells photo detectors, Lasers, Modulators, Integrated circuits and Filters [1-5, 6,7]. All the methods enumerated in[8-19] for the evaluation of optical energy gap, refractive index, electronic polarizibility involve many experimentally determined parameters and tedious mathematical calculations. It has been established that E_g and n depends on optical electro negativity($\Delta\chi^*$), given by Duffy expressions[20,21,22] and Reddy at al[23] and optical electro negativity have a correlation with Plasmon energy .This shows that there must be correlation between optical energy gap, refractive index and Plasmon energy. Electronic polarizibility associated with electronic structure .(α_p) calculated by different authors [24,25,26] by using various methods, by Ravindra and Srivastav and Kumar et al[27] have developed a relation for electronic polarizibility by using Plasmon oscillation theory of solids.
In the present paper we have proposed a new relations to evaluate optical energy gap(Eg), refractive index(n), and electronic polarizibility(αp) and optical electronegativity (Δχ*) for I-III-VI_2 and II-IV-V_2 Groups of ternary semiconductors. The calculated values of n, Eg, αp and Δχ* are compared with values reported by Ravindra ,Srivastav in table 9.14[28], Reddy at al[28], Jackson, Ohmer[28,29]. The calculated values of n, Eg, are compared with the values reported by Jackson, Ohmer, Reddy and Ravindra ,Srivastav[30]. Although Jackson, Ohmer, Reddy, Ravindra has reported the values of n, Eg, αp and Δχ* only for few semiconductors, the proposed new relations are successfully applied to the both I-III-VI_2 and II-IV-V_2 groups of ternary semiconductors.

II. THEORY

Assuming that there exist a relationship between n, Eg, αp, Δχ* and plasmon energy($\hbar w_p$) for ternary semiconductors. Moss [8,9] proposed a general relationship between Eg and n.

$$E_g = \left(\frac{95}{n^4}\right) eV \qquad (1)$$

The absorption edge or optical energy gap is most interesting and fundamental property of material and it is related with other important optoelectronic properties. We have studied the dependence of optical energy gap on plasmon energy by plotting Eg versus $\hbar w_p$ in figure 1 It is noted from figure that optical energy gap linearly depend on plasmon energy for a particular series of ABC2 semiconductors. Few semiconductors such as CuInTe2, $AgInSe_2$, $AgInTe_2$ of group I-III-VI_2 and $ZnGeS_2$, $CdSiP_2$ of group II-IV-V_2 are exceptions for this trend. On the basis of linear trend found in fig. 1 the relationship between optical energy gap and plasmon energy can be approximated by the following linear relation.

$$Eg = K_{55} \left(\hbar w_p\right) - K_{56} \qquad (2)$$

Where K_{55} (dimensionless) and K_{56} (eV) are constants for a particular series of ternary semiconductors. The numerical values of K_{55} = 0.476, 0.496, 0.648, 0.371; and K_{56}= 4.706, 6.123, 7.750, 4.189; respectively for I-Al-VI_2, Cu-III-VI_2, (III = Ga, In), Ag-Ga-VI_2 and II-IV-V_2. We have calculated the values of optical energy gap for ternary semiconductors under study; and reported in table 1, together with the literature values [28].

Duffy [21, 22] has well established the concept of optical absorption, and introduced it in terms of optical electro negativity ($\Delta\chi^*$) of binary semiconductors. Duffy expression is as follows

$$\Delta \chi^* = 0.2688 \quad E_g \qquad (3)$$

For simple system $\Delta\chi^*$ can easily be estimated, but in case of ternary and complex systems, the $\Delta\chi^*$ estimation is somewhat difficult. In order to overcome the difficulty, Reddy et al. [28] have used equation (3) for the calculation of the optical electronegativity of complex system and got good results. Using equations (2) and (3) we obtained expression for optical electro negativity in terms of plasmon energy as follows

$$\Delta \chi^* = K_{57} \left(\hbar w_p\right) - K_{58} \qquad (4)$$

where K_{57} (eV)–1 and K_{58} are constants for a particular series of ternary semiconductors under study. The numerical values of K_{57} = 0.128, 0.133, 0.174, 0.096; and K_{58} = 1.265, 1.649, 2.083, 1.126; respectively, for I-Al-VI_2, Cu-III-VI_2 (III= Ga, In), Ag-Ga-VI_2) and II-IV-V_2 semiconductor. We have calculated $\Delta\chi^*$ for these ternary semiconductors, and reported in table 1, together with the literature value [28].

The refractive index is also another important fundamental property of the material, and it is related with the many other opto-electronic properties, Reddy et al. [23] related optical electronegativity with the refractive indexby empirical relationship .

$$n = -\ln \left\{0.102 \quad \Delta \chi^*\right\} \qquad (5)$$

using equations (4) and (5) we have obtained an expression for refractive index in terms of plasmon energy as follows

$$n = -\ln \left\{K_{59} \left(\hbar w_p\right) - K_{60}\right\} \qquad (6)$$

where K_{59} (eV)–1 and K_{60} (dimensionless) are constants for a particular series of ternary semiconductors under study. The numerical values of K_{59}= 0.013, 0.014, 0.018, 0.010; and K_{60} = 0.129, 0.168, 0.212, 0.115; respectively, for I-Al-VI_2 Cu-III-VI_2 (III = Ga, In), Ag-Ga-VI_2. We have calculated the values of refractive index for these ternary semiconductors, and reported in table 1 together with the literature value [28,29].

Electronic polarizability is also an important opto-electronic property of semiconductors as it is associated with electronic structure as hardness / softness, acidity / basicity, ionization potential etc. Although electronic poarlizability of ternary semiconductors have been calculated by different authors [6-7, 24-26] by using various methods. Further. Ravindra and Srivastava [31], and Kumar et al [27] have developed relations for electronic polarizability by using plasma oscillations theory of solids. But these relations are limited for binary semiconductors. Therefore we have attempted to correlate electronic polarizability of ternary semiconductor with there plasmon energy. For this purpose we have plotted. $\ln \alpha_p$ versus $\ln \hbar w_p$ in figure 2. We obtained have found linear plots for different series of ternary semiconductors. On the basis of these linear plots the relationship between electronic polarizability and plasma energy can be approximated by the following equation.

$$\alpha_p = K_{61} \left(\hbar w_p\right)^{-K_{62}} \qquad (7)$$

Where K_{61} and K_{62} are constants for a particular series of semiconductors. The numerical values of K_{61} = 1574.20, 1467.44, 4561.97, 3.644 x 107, 20037.28, 69015.75; and K_{62} = 1.890, 1.768, 2.059, 5.457, 2.595, 2.963 respectively for I-III-VI_2 (III-Ga, In and VI = S, Se, Te), I-Al- VI_2, II-IV-V_2 (V = P, As). We have calculated the values of electronic polarizability for these ternary semiconductors, and reported in table 1 together with the literature values [30].

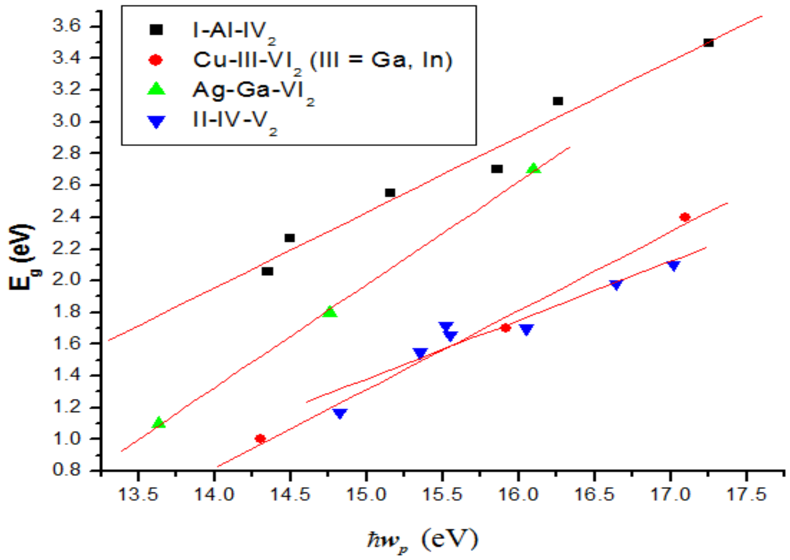
Table 1 The values of optical energy gap E_g *(eV)*, electronegativity $\Delta\chi^*$, plasmonenergy ($\hbar w_p$), refractive index (n) and electronic polarizability α_p (A^{o3}) of ternary semiconductors

S. No.	Compounds I-III-VI$_2$	E_g		$\Delta\chi^*$		n		$\hbar w_p$	α_p	
		[28]	Cal. Eqn. (2)	[28]	Cal Eqn. (4)	[28-29]	Cal. Eqn. (6)	[20] $\hbar w_p$	[30]	Cal. Eqn. (7)
1	CuAIS2	3.50	3.50	0.93	0.943	2.346	2.351	17.25	6.73	6.49
2	CuAISe2	2.70	2.84	0.723	0.765	2.600	2.562	15.86	10.09	10.26
3	CuAITe2	2.06	2.12	0.552	0.572	2.876	2.855	14.35	17.17	17.71
4	CuGaS2	2.40	2.36	0.643	0.628	2.710	2.640	17.10	7.25	7.34
5	CuGaSe2	1.70	1.77	0.455	0.471	3.068	2.903	15.92	10.91	10.98
6	CuGaTe2	1.00	0.97	0.268	0.260	3.590	3.436	14.30	19.20	19.04
7	CulnS2	1.53	1.87	-	0.498	2.600	2.853	16.12	8.42	8.21
8	CulnSe2	-	1.36	-	0.361	-	3.141	15.09	12.47	12.07
9	CulnTe2	0.95	-	0.254	-	3.650	-	13.66	20.86	20.93
10	AgAIS2	3.13	3.03	0.838	0.816	2.458	2.496	16.26	9.02	8.96
11	AgAISe2	2.55	2.51	0.683	0.680	2.660	2.687	15.16	11.31	13.12
12	AgAITe2	2.27	2.20	0.608	0.591	2.779	2.822	14.50	19.35	16.74
13	AgGaS2	2.70	2.69	0.723	0.718	2.606	2.554	16.10	8.22	8.22
14	AgGaSe2	1.80	1.82	0.482	0.485	3.011	2.925	14.76	12.3	12.55
15	AgGaTe2	1.10	1.09	0.294	0.289	3.504	3.401	13.63	20.79	21.02
16	AgInS2	-	-	-	-	-	-	15.21	9.04	9.16
17	AglnSe2	1.24	-	0.332	-	3.384	-	14.23	13.51	13.39
18	AgInTe2	1.00	-	0.268	-	3.699	-	13.04	23.23	23.03

Cont.. Table 1

S. No.	Compounds I-III-VI$_2$	E_g		$\Delta\chi^*$		n		$\hbar w_p$	α_p	
		[28]	Cal. Eqn. (2)	[28]	Cal Eqn. (4)	[28-29]	Cal. Eqn. (6)	[20] $\hbar w_p$	[30]	Cal. Eqn. (7)
19	$ZnSiP_2$	2.10	2.13	0.562	0.558	2.809	2.896	17.02	12.45	12.79
20	$ZnSiAs_2$	1.70	1.77	0.456	0.462	3.160	3.090	16.05	18.12	18.49
21	$ZnGeP_2$	1.98	1.99	0.533	0.522	2.949	3.180	16.64	14.24	13.57
22	$ZnGeAs_2$	1.15	-	0.308	-	3.370	-	15.66	20.52	20.31
23	$ZnSnP_2$	1.66	1.59	0.444	0.414	3.092	3.206	15.55	16.36	16.17
24	$ZnSnAS_2$	-	1.32	-	0.341	-	3.405	14.82	23.84	23.42
25	$CdSiP_2$	2.45	1.51	0.656	-	3.100	-	16.19	14.34	14.56
26	$CdSiAs_2$	1.55	1.58	0.415	0.394	3.161	3.257	15.35	20.71	21.10
27	$CdGeP_2$	1.72	1.35	0.461	0.411	3.190	3.214	15.52	15.95	16.25
28	$CdGeAS_2$	0.57	1.31	-	0.349	3.500	3.381	14.90	23.16	23.05
29	$CdSnP_2$	1.17	1.05	0.313	0.341	3.442	3.405	14.82	18.40	18.32
30	$CdSnAs_2$	-	-	-	0.272	-	3.642	14.12	26.68	27.03

Figure 1



E_g = Optical energy gap

$\hbar w_p$ = plasmon energy

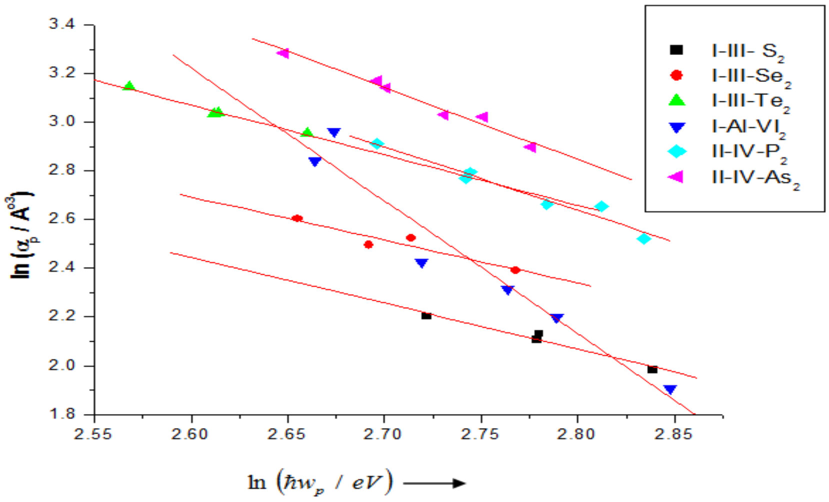


Figure 2

α_p = electronic polarizability

$\hbar w_p$ = Plasmon energy

III. RESULT AND DISCUSSIONS

The present paper reports different correlations between n, E_g, α_p, $\Delta\chi^*$ and $\hbar w_p$ in I-culatIII-VI_2 and II-IV-V_2 groups of teranary semiconductor .The values of optical energy gap and optical electronegativity of these ternary semiconductor s have been calculated using equation s (2,3) . The calculated values are listed in table 1 and compared with the values reported by [28]. Our calculated values of E_g and $\Delta\chi^*$ are in good agreement within 3% with literature values reported by [28]. The values of refractive index of these ternary semiconductors have been calculated by using equation (6) and listed in table 1 ,compared with reported values of[28,29]. The calculated values are in close agreement within 2.8% with the values reported by [28,29]. The values of α_p of these ternary semiconductors have been calculated by using equation (7) and listed in table 1. The calculated values are in close agreement with values reported [30].

IV. CONCLUSION

On the other hand our proposed relations are simple and useful as we can directly relate n , Eg, $\Delta\chi^*$ and α_p with $\hbar w_p$. The relationship between these optoelectronic properties of ternary semiconductors is equally hold good for I-III-VI_2 and II-IV-V_2 groups of semiconductors given by equations (2-3, 6-7) have been proved that the knowledge of Plasmon energy can be used as a parameter to calculate these optoelectronic properties of semiconductors which is of good use in todays semi-condutors devices such as lasers, modulators and light emiting diodes.

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