Relationship between Refractive Index, Electronic Polarizability, Optical Energy Gap Optical Electronegativity and Plasmon Energy in I-III-VI$_2$ and II-IV-V$_2$ Groups of Semi Conductors.

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ABSTRACT

Refractive index(n), Electronic Polarizability ($\alpha_p$), 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($\alpha_p$), 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 ($\alpha_p$) 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($E_g$), refractive index(n), and electronic polarizibility($\alpha_p$) and optical electronegativity ($\Delta\chi^*$) for 1-III-VI$_2$ and II-IV-V$_2$ Groups of ternary semiconductors. The calculated values of n, Eg, $\alpha_p$ and $\Delta\chi^*$ 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, $\alpha_p$ and $\Delta\chi^*$ only for few semiconductors, the proposed new relations are successfully applied to the both 1-III-VI$_2$ and II-IV-V$_2$ groups of ternary semiconductors.

II. THEORY

Assuming that there exist a relationship between n, Eg, $\alpha_p$, $\Delta\chi^*$ and plasmon energy($\frac{\hbar \omega}{r}$) for ternary semiconductors. Moss [8,9] proposed a general relationship between Eg and n.

$$E_g = \left( \frac{95}{n^2} \right) eV$$

(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 \( \text{Eg} \) versus \( \hbar \omega_p \) 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, AgInS2, AgInTe2 of group I-III-VI2 and ZnGeS2, CdSiP2 of group II-IV-V2 are exceptions for this trend. On the basis of linear trend found in fig. 1 the relationship between optical gap and plasmon energy can be approximated by the following linear relation.

\[
\text{Eg} = K_{55} \left( \hbar \omega_p \right) - K_{56}
\]

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-VI2, Cu-III-VI2, (III = Ga, In), Ag-Ga-VI2 and II-IV-V2. 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

\[
\Delta \chi^* = 0.2688 \ E_g
\]

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

\[
\Delta \chi^* = K_{57} \left( \hbar \omega_p \right) - K_{58}
\]

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-VI2, Cu-III-VI2 (III= Ga, In), Ag-Ga-VI2 and II-IV-V2 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 index by empirical relationship.

\[
n = - \ln \left[ 0.102 \ \Delta \chi^* \right]
\]

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

\[
n = - \ln \left[ K_{59} \left( \hbar \omega_p \right) - K_{60} \right]
\]

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-VI2, Cu-III-VI2 (III= Ga, In), Ag-Ga-VI2. 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 polarizability 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 \( \ln \hbar \omega_p \) 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.

\[
\alpha_p = K_{61} \left( \hbar \omega_p \right)^{-K_{62}}
\]

Where \( K_{61} \) and \( K_{62} \) are constants for a particular series of semiconductors. The numerical values of \( K_{61} = 1574.20, 1467.44, 4561.97, 3.644 \times 107, 20037.28, 69015.75; \) and \( K_{62}= 1.890, 1.768, 2.059, 5.457, 2.595, 2.963 \) respectively for I-III-VI2 (III-Ga, In and VI = S, Se, Te), I-Al- VI2, II-IV-V2 (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 $\Delta \chi^*$, plasmon energy ($\hbar \nu_p$), refractive index ($n$) and electronic polarizability $\alpha_p (A^3)$ of ternary semiconductors.

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Compounds 1-III-(\tilde{V})_l</th>
<th>$E_g$</th>
<th>$\Delta \chi^*$</th>
<th>$n$</th>
<th>$\hbar \nu_p$</th>
<th>$\alpha_p$</th>
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<td>1</td>
<td>CuAsS_2</td>
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<td>14</td>
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<td>18</td>
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<td>1.00</td>
<td>0.268</td>
<td>0.289</td>
<td>2.600</td>
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Continued Table 1

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Compounds 1-III-(\tilde{V})_l</th>
<th>$E_g$</th>
<th>$\Delta \chi^*$</th>
<th>$n$</th>
<th>$\hbar \nu_p$</th>
<th>$\alpha_p$</th>
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<td>1.35</td>
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<td>0.308</td>
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<td>-</td>
<td>0.341</td>
<td>3.405</td>
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<td>0.516</td>
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<td>1.58</td>
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<tr>
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<td>1.31</td>
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<td>0.349</td>
<td>3.500</td>
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<tr>
<td>29</td>
<td>GaSeTe_2</td>
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<td>1.05</td>
<td>0.313</td>
<td>0.341</td>
<td>3.442</td>
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<td>30</td>
<td>GaSeAs_2</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.375</td>
<td>3.642</td>
</tr>
</tbody>
</table>

Figure 1

- $E_g$ = Optical energy gap
- $\hbar \nu_p$ = Plasmon energy

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$\alpha_p =$ electronic polarizability

$h_{wp} =$ Plasmon energy

III. RESULT AND DISCUSSIONS

The present paper reports different correlations between $n$, $E_g$, $\Delta \chi^*$ and $h_{wp}$ in I-culantIII-VI$_2$ and II-IV-V$_2$ groups of ternary semiconductor. The values of optical energy gap and optical electronegativity of these ternary semiconductors have been calculated using equations (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 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 $\alpha_p$ of these ternary semiconductors have been calculated 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 $n$, $E_g$, $\Delta \chi^*$ and $\alpha_p$ with $h_{wp}$. 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 today’s semiconductor devices such as lasers, modulators and light emitting diodes.

REFERENCES