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An Empirical Relation for Calculation of Plasmon Energy of Ternary-Chalcopyrite Semi-conductors

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Abstract: ***In this paper a simple empirical relation has been proposed to estimate the Plasmon energy of I-III-VI$_2$ and II-IV-V$_2$ type chalcopyrite semi-conductors. This relation is based on the principal quantum number of atoms of compounds and the electro-negativities of the constituent atoms. The computed values of Plasmon energy from the present relation are found to be in good agreement with the known values.***
Index Terms: Plasmon energy, Principal quantum number, Electronegativity.

I. INTRODUCTION-

Ternary Chalcopyrite is a type of semi-conductor with the general formula $A^{I}B^{III}C_2^{VI}$ (A=Li, Cu, Na, Ag; B=Al, Ga, In; C=S, Se, Te) and $A^{II}B^{IV}C_2^{V}$ (A=Zn, Cd; B=Si, Sn, Ge; C=P,As). These type of semi-conductors are widely used in solar energy converters, light emitting diodes (LEDs), detectors, electro-optic devices, lasers and in many other fields[1-5]. Due to their potential applications, numerous researches are going on them. Plasmon energy is one of the most important properties of such compounds. Several researchers have proposed different theoretical models for calculating Plasmon energy of ternary chalcopyrites. Different researchers have derived different theoretical models for Plasmon energy of semi-conductors based on the dependence of Plasmon energy on different factors. Kumar et al.[6-7] have derived a formula for Plasmon energy of ternary chalcopyrites on the basis of the relation between the Plasmon energy, molecular weight, density and number of valence electrons taking part in the collective oscillation. Reddy et al.[8-9] have derived a formula for Plasmon energy of ternary chalcopyrites on the basis of the inter-atomic distances between the atoms of the compounds. In this paper a simple relation between Plasmon energy, electronegativity of constituent atoms and average principal quantum number of atoms constituting the compounds has derived on the basis of least square fitting graphical method.

II. THEORY

A Plasma oscillation in a metal is a collective longitudinal excitation of the conduction electron gas. A Plasmon is a quantum of a plasma oscillation; one may excite a Plasmon by passing an electron through a thin metallic film or by reflecting an electron or a photon from a film. The charge of the electron couples with the electrostatic field fluctuations of the plasma oscillations. The reflected or the transmitted electrons will show an energy loss equal to the integral multiples of the Plasmon energy. It is equally possible to excite collective plasma oscillations in ternary chalcopyrites. In a ternary chalcopyrite semiconductor the plasma oscillation is physically the same as in a metal. The entire valence electron gas oscillates back and forth with respect to the ion cores[10]. Plasmons are studied by the means of Electron Energy Loss Spectroscopy (EELS) and have reported in recent years. Jackson[11] has proposed a model for Plasmon energy on the basis of the relation between Plasmon energy, molecular weight and density. From the model, Plasmon energy is

$$\hbar\omega_p = 28.8\,(Z\rho/M)^{1/2} \qquad \text{.....(1)}$$

where Z atomic number,$\boldsymbol{\rho}$ is molecular weight and M is the molecular weight of the compound. Reddy et al[12]. have derived a model for Plasmon energy of semiconductors and alkali halides based on the interionic distance. The relation is as follows,

$$\hbar\omega_p = -a_1(r_0) + b_1 \qquad \text{.....(2)}$$

where $r_0$is inter-ionic distance, $a_1$and b_1 are constants. Reddy et al[8]. have proposed an empirical relation between Plasmon energy and electronegativity difference (ΔX^*) of alkali halides as follows,

$$\hbar\omega_p = A(\Delta X^*) + B \qquad \text{.....(3)}$$

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where A and B are constants. Plasmon energy can also be calculated from the refractive index of the materials using the empirical relation[13],

$$\hbar\omega_p = K_1 e^{-K_2 n} \quad \text{.....(4)}$$

where K_1 and K_2 are constants. Gorai et al[14-15]. have proposed a relation for Plasmon energy as-

$$\hbar\omega_p = \hbar\sqrt{\frac{4\pi Ne^2}{m}} \quad \text{.....(5)}$$

where N is the valance electron density, e is the charge and m is the mass of the electron.
The present study for the formation of an empirical relation for Plasmon energy of ternary chalcopyrite is based on the chemical bond theory. From the chemical bond theory, one can easily co-relate Plasmon energy with electro-negativity and principal quantum number. We know that, in a crystal homopolar energy gap is related to bond length and so bond length is related to Plasmon energy as

$$d = 15.30\,(\hbar\omega_p)^{-2/3} \quad \text{.....(6)}$$

as homopolar energy gap depends on Plasmon energy as,

$$E_P = \hbar\sqrt{\frac{ne^2}{m\epsilon_0}} = \hbar\omega_p. \quad \text{.....(7)}$$

With increase in the value of principal quantum number the distance between the nuclei and the valence electron increases, this increases the bond length which is related with Plasmon energy.
For I-III-VI_2 and II-IV-V_2 type chalcopyrite semi-conductors, graphs (fig.1 and fig.2) has been plotted between Plasmon energy and the ratio of average principal quantum number of atoms constituting compounds and electro-negativity of atoms. In this case least square fitting method has been used.

Figure.1: Graph between Plasmon energy and ratio of average value of principal quantum number and electronegativity of constituting atoms of compound I-III-VI_2.

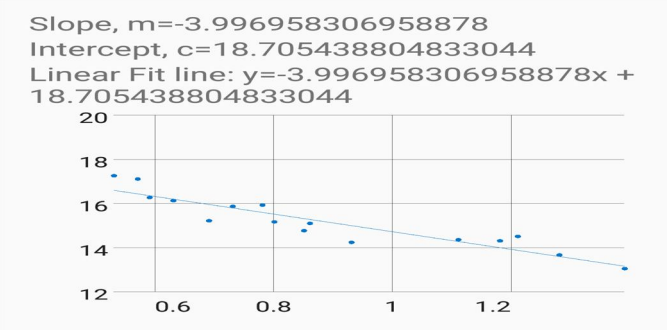
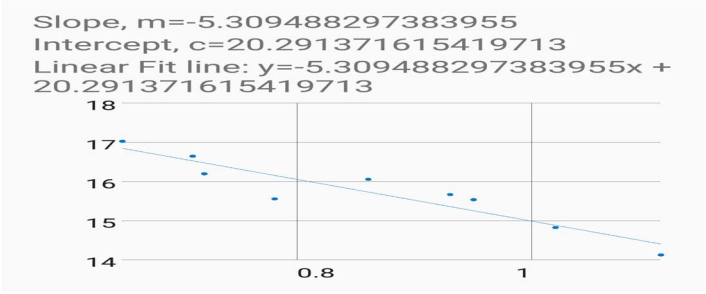


Figure.2: Graph between Plasmon energy and ratio of average value of principal quantum number and electronegativity of constituting atoms of compound II-IV-V_2.



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The graph shows that Plasmon energy is linearly related with the ratio of principal quantum number and electro-negativity in both types of ternary chalcopyrites. Thus this variation can be used to derive an empirical relation for the determination of Plasmon energy of the compounds. For ternary chalcopyrites structure solids, the Plasmon energy is assumed to be co-related to the contribution of three atoms A,B and C_2. Let $\eta_{av} = \frac{(\eta_A+\eta_B+2\eta_C)^{1/4}}{4}$ is the average principal quantum number of the four constituents' atoms in ABC_2. The Plasmon energy of ternary chalcopyrite semi-conductors using the graphs can be expressed as-

$$\hbar\omega_p = \propto \left[\frac{\eta_{av}}{(\chi_A\chi_B)^{\frac{1}{4}} \ (\chi_C)^{1/2}}\right] + \beta \qquad \text{.....(8)}$$

where $\alpha = -3.996958306958878$ and $\beta = 18.705438804833044$ for I-III-VI_2 type semiconductors and $\alpha = -5.309488297383955$ and $\beta = 20.291371615419713$ for II-IV-V_2 type semi-conductors.

III. RESULTS AND DISCUSSION

The Plasmon energy of I-II-VI_2 and II-IV-V_2 type chalcopyrite structure solids is estimated using Equation(8). In Table-1, the estimated values for I-II-VI_2 and in Table-2 estimated values for II-IV-V_2 are listed along with the results of earlier researchers. It is observed that the calculated values are in better agreement with the other reported values. It is observed that in I-II-VI_2 ,$CuAlS_2$ has highest Plasmon energy and $AgInTe_2$ has lowest Plasmon energy. In II-IV-V_2, $ZnSiP_2$ has highest Plasmon energy and $CdSnAs_2$ has lowest Plasmon energy.

Table-1 : Plasmon energy $(\hbar\omega_p)$ in $(eV)$of I-III-VI_2 type chalcopyrite semiconductors-

Compounds	Calculated from Eq.(8)	Ref.[14]	Ref.[15]
$CuAlS_2$	16.58	17.25	16.67
$CuAlSe_2$	15.78	15.86	15.89
$CuAlTe_2$	14.26	14.32	14.40
$CuGaS_2$	16.42	17.10	16.52
$CuGaSe_2$	15.58	15.92	15.69
$CuGaTe_2$	13.98	14.30	14.12
$CuInS_2$	16.18	16.12	16.28
$CuInSe_2$	15.26	15.09	15.38
$CuInTe_2$	13.58	13.66	13.73
$AgAlS_2$	16.34	16.26	16.44
$AgAlSe_2$	15.50	15.16	15.61
$AgAlTe_2$	13.86	14.50	14.00
$AgGaS_2$	16.18	16.10	16.28
$AgGaSe_2$	15.30	14.76	15.42
$AgGaTe_2$	13.58	13.63	13.73
$AgInS_2$	15.94	15.21	16.05
$AgInSe_2$	14.98	14.23	16.05
$AgInTe_2$	13.14	13.04	13.30

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Table-2 : Plasmon energy ($\hbar\omega_p$) in (eV)of II-IV-V_2 type chalcopyrite semiconductors-

Compounds	Calculated from Eq.(8)	Ref.[14]	Ref.[15]
$ZnSiP_2$	16.84	17.02	16.20
$ZnGeP_2$	16.52	16.64	15.97
$ZnSnP_2$	16.14	15.55	15.69
$ZnSiAs_2$	15.72	16.05	15.38
$ZnSeAs_2$	15.35	15.66	15.10
$ZnSnAs_2$	14.87	14.82	14.75
$CdSiP_2$	16.46	16.19	15.93
$CdGeP_2$	16.14	15.52	15.69
$CdSnP_2$	15.72	14.82	15.38
$CdSiAs_2$	15.24	15.53	15.02
$CdGeAs_2$	14.87	14.90	14.75
$CdSnAs_2$	14.39	14.12	14.40

IV. CONCLUSION

It is clear from the above calculations that Plasmon energy of ternary chalcopyrites depends on principal quantum number and electronegativity of the constituting atoms of the compounds. It is evident from the above relation, that no experimental data is essential for the determination of Plasmon energy of ternary chalcopyrite compounds. Just by knowing electronegativity and principal quantum number of atoms, one can easily determine the Plasmon energy of ternary chalcopyrite compounds from the above relation.

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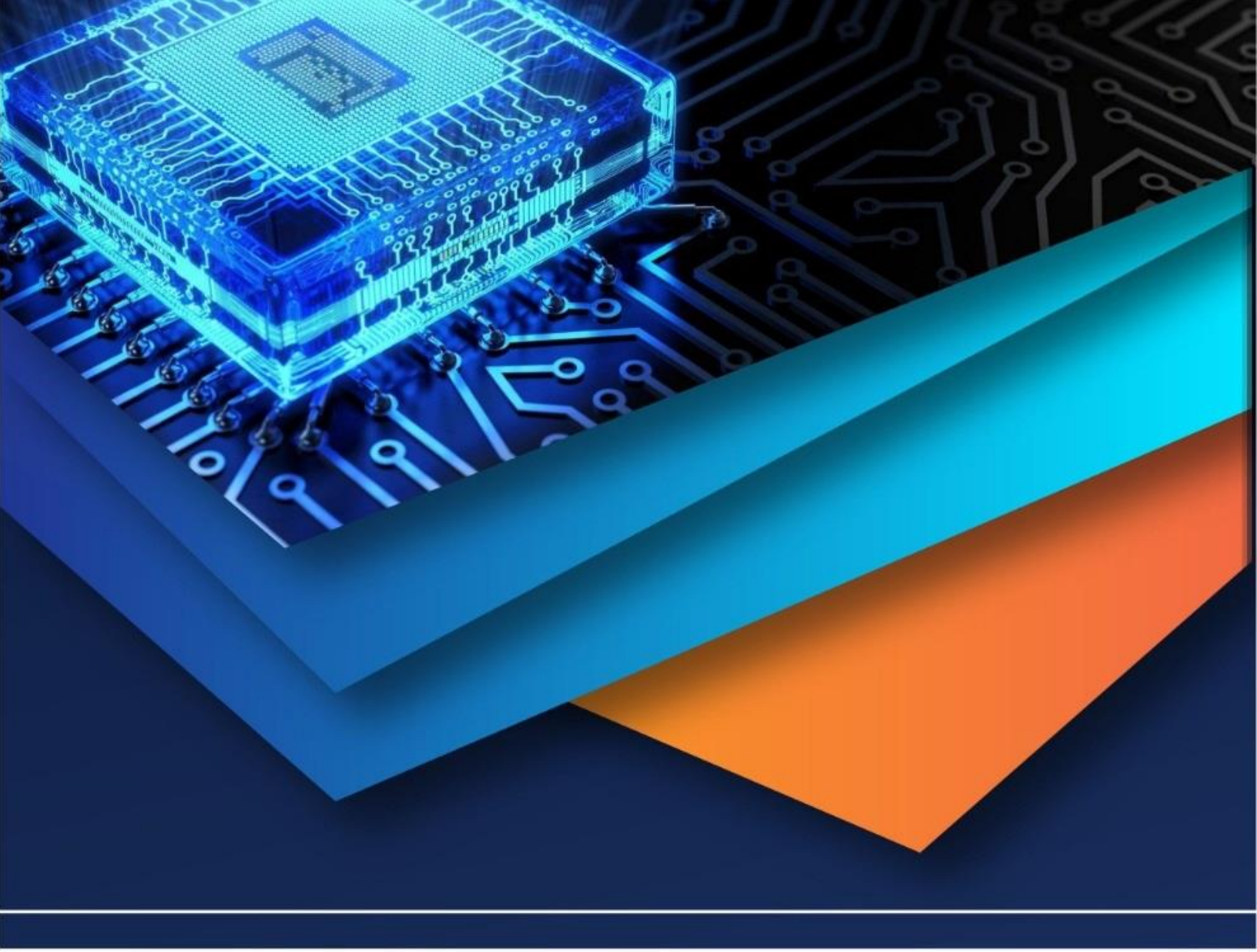

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