An Empirical Relation Showing the Variation of Refractive Index With Energy Gap for $A^{I}B^{III}C_2^{VI}$ & $A^{II}B^{IV}C_2^{V}$ Type Ternary Chalcopyrite Semiconductors

Ajay Kumar Sharma
Assistant Professor, Department of Physics, Bidhan Chandra College, Asansol, West Bengal, India
(Research Scholar, JRU, Ranchi)

***Abstract*- In this paper a simple empirical relation has been proposed to estimate the refractive index of I-III-VI2 and II-IV-V2 type chalcopyrite semi-conductors. This relation is based on the dependence of refractive index on energy gap of the chalcopyrite crystals. The computed values of refractive indices from the present relation are found to be in good agreement with the known values.**

Index Terms- Ternary chalcopyrite, Refractive Index, Energy gap.

I. INTRODUCTION

Ternary Chalcopyrite semi-conductors are becoming the back bone of modern electronic industries. They are widely applicable in opto-electronic devices, photovoltaic solar cells, LEDs, LDs, photo-detectors (PDs), non-linear optical devices (NLO) and in many other fields. The energy gap and refractive index of ternary chalcopyrite represent two fundamental physical aspects that characterize their optical and electronic properties. The nature and magnitude of these two elementary properties determine the optical and electronic applications of ternary chalcopyrite. Many devices such as detectors, solar cells, wave-guides etc. are based on the refractive index and energy gap of the crystals[1-5].

The refractive index of a semi-conductor crystal generally decreases with increase in energy gap (Eg). Several researchers have proposed different theoretical models based on the relation between refractive index and energy gap of the ternary chalcopyrite. In this work a simple empirical model has been derived to co-relate refractive index and energy gap of the ternary chalcopyrite.

II. THEORY

There are a number of theoretical models based on the relation between refractive index and energy gap of ternary chalcopyrite. In 1950 Moss[6] predicted the first ever relation between the refractive index and energy gap of ternary chalcopyrite crystals. The relation is as,

$$n^4 E_g = 95\ e^V \qquad (1)$$

where n and Eg are refractive index and energy gap respectively.

In 1992 Reddy et al. proposed the relation between refractive index(n) and energy gap(Eg) for ternary chalcopyrite crystals as,

$$E_g e^n = 36.6\ e^V \qquad (2)$$

The model of Herve and vandemme[7] given as:

$$n^2 = 1 + \left(\frac{A}{E_g + B}\right)^2 \qquad (3)$$

where A is the hydrogen ionization energy equal to 13.6eV and B =3.4eV is a constant to be the difference between UV resonance energy and band gap energy and Eg is energy gap.

The model of Reddy *et al*[8]. given as:

$$n^2 = \left(\frac{12.417}{E_g - 0.365}\right) \qquad (4)$$

Equation (4) is the modified form of the original Moss equation.

The model of Ravindra *et al*[9]. given as:

$$n = 4.084 + \beta E_g \qquad (5)$$

where $\beta = -0.62\ eV^{-1}$.

The model of Anani *et al*[10]. given as:

$$n^4 = 1 + \frac{A}{{E_g}^2} \qquad (6)$$

where A = 40.8 $A = 40.8e^V$.

The model of Kumar and Singh[11] given as:

$$n = K {E_g}^c \qquad (7)$$

where K = 3.3668 and C = −0.32234 are the constants. They used simulation software and simulated experimental values of energy gap and

refractive index and obtained the relation between n and Eg.

The model of Ahmad and Haq[12] given as:

$$n = \left(\frac{44}{E_g}\right)^{1/3} \quad (8)$$

where n is the refractive index and Eg is the energy gap.

Tripathy[13] fitted an exponential empirical formula to the experimental values of refractive index and energy gap of some elemental and binary semiconductor over a wide range of energy gap ranging from low value of Eg= 0.1eV to a reasonably high value Eg = 8.5 eV.

The proposed relationship for those data is:

$$n = n_0 + n_1 e^{\left(\frac{-E_g}{\mu}\right)} \quad (9)$$

The parameters of the above relation for the best fit are found to be n_0 = 1.65752 ± 0.14605, n_1 = 3.78368 ± 0.21302, and μ = 1.85447 ± 0.25777eV. However, in order to provide the formula to a better shape, equation (9) can be rewritten as:

$$n = n0\ [1 + \alpha e^{-\beta Eg}\ ] \quad (10)$$

The new parameters α, β and n_0 appearing in the above equation are adjusted so as to get good agreement with the experimental values of elemental and binary semiconductors over a wide range of energy gap. The parameters of the modified relation are $n_0 = 1.73$, $\alpha = 1.9017$ and $\beta = 0.539(eV)^{-1}$.

In the present work, I have plotted graphs between refractive indices and energy gap of both types of ternary chalcopyrite with their experimental values. Fig.1 and Fig.2 shows the variation of n Vs Eg for I-III-V_2 and II-IV-VI_2 type semi-conductors respectively. The graphs show that n bears a linear relation with Eg.

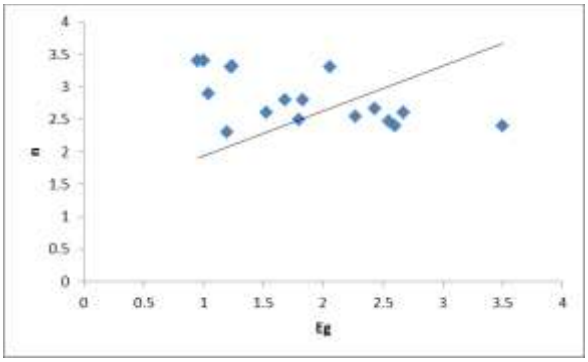

Fig.1: Plot of refractive index (n) Vs energy gap (Eg) for I-III-VI2 type chalcopyrite crystals.

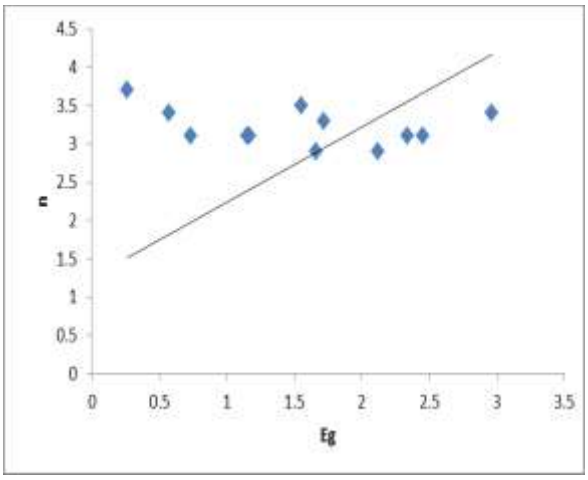

Fig.2: Plot of Refractive index (n) Vs Energy gap (Eg) for II-IV-V_2.

Using the nature of the graphs, I have proposed the following relation:

$$n = \alpha E_g + \beta \quad (11)$$

where α and β are constants. The value of α for I-III-VI_2 is 0.69 and for II-IV-V_2 is 0.9867. The value of β for both crystals is 1.25.

III. RESULTS AND DISCUSSION

The Refractive-index of I-II-VI_2 and II-IV-V_2 type chalcopyrite structure solids is estimated using Equation (11) and by implementing the values of Eg calculated by Harrison et al[14]. and Joshi et al[15].. In Table-1, the estimated values of refractive index for I-II-VI_2 and in Table-2 the estimated values of refractive index 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 experimentally reported values and values estimated by other researchers.

Table-1: Refractive index of I-III-VI2 type chalcopyrite semiconductors

Compounds	Calculated from Eq.(11)	Eq.[1]	Eq.[3]	Eq.[7]	Eq.[8]	Eq.[4]	Eq.[6]	n[16-17]
$CuAlS_2$	3.66	2.28	2.21	2.25	2.33	1.99	1.44	2.40
$CuAlSe_2$	3.09	2.44	2.45	2.45	2.55	2.32	1.61	2.60
$CuAlTe_2$	2.67	2.61	2.68	2.67	2.78	2.71	1.81	3.30

$CuGaS_2$	2.92	2.50	2.54	2.53	2.63	2.45	1.68	2.67
$CuGaSe_2$	2.40	2.74	2.86	2.85	2.97	3.07	1.98	2.80
$CuGaTe_2$	2.09	1.06	3.10	3.15	3.30	3.79	2.30	3.30
$CuInS_2$	2.30	2.81	2.93	2.94	3.06	3.27	2.07	2.60
$CuInSe_2$	1.96	3.09	3.22	3.33	3.48	4.29	2.50	2.90
$CuInTe_2$	1.90	3.16	3.28	3.42	3.59	4.61	2.61	3.40
$AgAlS_2$	-	-	-	-	-	-	-	-
$AgAlSe_2$	3.00	2.47	2.50	2.49	2.58	2.38	1.64	2.47
$AgAlTe_2$	2.81	2.54	2.60	2.59	2.69	2.55	1.73	2.54
$AgGaS_2$	3.04	2.46	2.48	2.47	2.57	2.36	1.63	2.40
$AgGaSe_2$	2.51	2.68	2.79	2.77	2.89	2.91	1.91	2.80
$AgGaTe_2$	2.07	2.98	3.12	3.18	3.32	3.86	2.33	2.30
$AgInS_2$	2.49	2.70	2.80	2.79	2.90	2.94	1.92	2.50
$AgInSe_2$	2.10	2.96	3.10	3.14	3.29	3.77	2.29	3.32
$AgInTe_2$	1.94	3.12	3.25	3.37	3.53	4.42	2.54	3.40

Table-2 :Refractive index of II-IV-V_2 type chalcopyrite semiconductors-

Compounds	Calculated from Eq.(11)	Eq.[1]	Eq.[3]	Eq.[7]	Eq.[8]	Eq.[4]	Eq.[6]	n^{16-17}
$ZnSiP_2$	4.17	2.38	2.36	2.37	2.46	2.19	1.54	3.40
$ZnGeP_2$	3.55	2.52	2.57	2.56	2.66	2.51	1.71	3.10
$ZnSnP_2$	2.88	2.75	2.87	2.86	2.98	3.10	1.99	2.90
$ZnSiAs_2$	3.34	2.59	2.66	2.64	2.75	2.66	1.78	2.90
$ZnGeAs_2$	2.38	3.02	3.15	3.22	3.37	3.98	2.38	3.10
$ZnSnAs_2$	1.97	3.38	3.44	3.73	3.92	5.83	2.91	3.10
$CdSiP_2$	3.66	2.50	2.53	2.52	2.62	2.44	1.67	3.10
$CdGeP_2$	2.94	2.73	2.84	2.83	2.95	3.03	1.96	3.30
$CdSnP_2$	2.40	3.00	3.14	3.20	3.35	3.93	2.36	3.10
$CdSiAs_2$	2.77	2.80	2.92	2.92	3.05	3.24	2.06	3.50
$CdGeAs_2$	1.81	3.59	3.57	4.04	4.26	7.78	3.35	3.40
$CdSnAs_2$	1.50	4.37	3.85	5.20	5.53	-	4.96	3.70

IV. CONCLUSION

It is clear from the above calculations that refractive index of ternary chalcopyrite semiconductors depend on the energy gap. It is evident from the above relation, that no experimental data is essential for the determination of refractive index of ternary chalcopyrite compounds. Just by knowing energy gap, one can easily determine the refractive index of ternary chalcopyrite compounds from the above relation.

REFERENCES

[1] Shay J L, Wernic J H 1975 Ternary chalcopyrite semiconductors growth, in: Electronic properties and application, pergamon press, Newyork

[2] Kazmerski L L, 1983 NuovoCimento 20 2013

[3] Deab S K and Zunger A, 1987 Ternary Multinary Compounds.Mater.Res.SocConf.Proc.37

[4] Yan C and Xue D 2008 Funct.Mater.Lett.1 37

[5] Zhu Y 2008 Funct.Mater.Lett.1239.

[6] Moss, T.S. (1985). Relationship between the refractive index and energy gap of

semiconductors. Physica Status Solidi(b),131(2) :415-427.
[7] Herve, P., and Vandamme, K,L,J. (1994). Infrared Phys,35 609
[8] Reddy,R,R,Nazeer,Ahammed,Y,Rama,Gopal,K, et al.(1998). Opt. Mat.,10 95
[9] Ravindra,N,M,Srivastva,V,K. (1979). Infrared Phys. 19 603
[10] Anani,M,Mathieu,C,Lebid,S,et al. (2008).Computational matter SC,41 570
[11] Kumar, V., and Singh, J.K. (2010). Model for calculating the refractive index of different materials. Indian Pure Applied Physics, 48, 571-574
[12] Ahmad, S., & Haq, M.M. (2014). A study of energy gap, refractive index and electronic polarizability of ternary chalcopyrite semiconductors. Iranian Journal of Physics, 14(3): 89-93
[13] Tripathy, S, K. (2015). Refractive indices of semiconductors from energy gap. Optical Materials, 46 240-246
[14] Harrison,W,A. (1980). Electronic structure and properties of solids.Freeman,W,H, San Fransisco
[15] Joshi,N,V. (1990). Photoconductivity. Merida Veneznela, Marcel Dekker lnc, New York
[16] Reddy,R,R,et al. (2003). Opt.Mat. 22 7
[17] Reddy,R,R,et al.(2009). J.Alloys Comp. 473 28.