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INTER – RELATIONSHIP BETWEEN REFRACTIVE INDEX AND AVERAGE ENERGY GAPS OF MIXED COVALENT BINARY CRYSTALS

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Abstract

The quantum ion dependent formulation for optical refractive indices and average energy gaps for solids gives the evidence that more covalent solids show anion dependent behaviour. This Quantum ion dependent model was also used to predict average energy gaps in solids of simple and complex binary families. Later it was applied in the fields of photoelasticity, photo conductivity, solar cell technology etc. and have been successfully approved.

Key words: Average energy Gaps, Refractive Index, Mixed Binary covalent crystals.

INTRODUCTION

The correlation between average energy gap (Eg) and optical dielectric constant $\in_\infty$ was established by Moss on the very general ground that all the energy levels in a solid element are scaled down by a factor $1/\in_\infty^2$ and the relation between $\in_\infty$ and refractive index (n) given as-

$$\in_\infty = n^2 \qquad \ldots(1)$$

According to our quantum ion dependent model the relation between refractive index (n) and Eg was established with the help of relation between average energy gap and interionic separation (R) (Goyal and Sarkar 1976, Sarkar 1980), as-

$$Eg = BR^{-S} \qquad \ldots(2)$$

This follow the same ion dependent behaviour while exponent s remains family characteristic constant and B is cation characteristic constant for ionic families and anion characteristic constant for covalent families.

The above equation gives:

$$R^3 = B^{3/s}. Eg^{-3/s} \qquad \ldots(3)$$

According Van Vechten (1969)

$$n^2 = 1 + \frac{b}{R^3 E_g^2} \qquad \ldots(4)$$

Here, b is a single parameter which should be a characteristics of either cation in ionic crystals or anion in covalent ones.

By using eg. (3) and (4), we get-

$$n^2 = 1 + \frac{b}{B^{3/s}\ E_g^2 E_g^{-3/s}}$$

or

$$n^2 = 1 + \frac{b\ B^{-3/s}}{E_g^{(2-3/s)}}$$

or

$$n^2 = 1 + C\ Eg^P \qquad \ldots(5)$$

Where C b B^{-3}/s gives the ion characteristic constant and P = (3/s-2) give the family characteristic. Thus in the relation between n^2 and Eg we must have different exponent (P) of Eg in different families and different values of proportionality constent C for different ions.

Thus correlation between n and Eg given by equation (5) is provided through theoretical consideration and hence our established ion dependent theories for relative variance between n and Eg gets a solid base.

To show the dependence of refractive Index (n) and Average energy Gap (Eg), we rearranging the Equation (5), we get

$$\text{Log}\ (n^2\text{-}1) = P\ \text{Log}\ Eg + \text{Log}\ C \qquad \ldots(6)$$

COMPUTATION OF REFRACTIVE INDEX (n) AND AVERAGE ENERGY GAPS (Eg) FOR MIXED COVALENT BINARY CRYSTALS

According to Quantum Ion Dependent Theory the correlation between n and E_g is given earlier in equation (5) as

$$n^2 = 1 + C\ E_g^P$$

Here C and P are Ion characteristic constant and family characteristic constant respectively.

To calculate the value of refractive index (n) and average energy gap (Eg) we use the first assumptions of Clausius Mossotti relation. According to this relation refractive indices and average energy gaps of binary crystals are said to vary linearly with their

concentration i.e. the refractive index (n) of mixed binary crystals can be calculate by following relation

$$n = \lambda x\, n_x + \lambda y\, n_y \qquad \ldots(7)$$

Here λx and λy are proportions of binary crystals x and y respectively and n_x and n_y are the refractive index of pure binary crystals x and y. Similarly we can calculate the value of average energy gaps (Eg) for mixed binary crystals as follows.

$$Eg = \lambda x\, (Eg)_x + \lambda y\, (Eg)_y \qquad \ldots(8)$$

Here λx and λy are the proportions of pure binary crystals x and y and $(Eg)_x$ and $(Eg)_y$ are the average energy gaps of pure crystals x and y.

The values of refractive Index (n) and Average energy Gaps (Eg) of pure binary crystals of III-V family are reported in Table 1.

The calculated values of refractive index (n) and average energy gap (Eg) are reported in Table 2 to 7.

Table – 1

S.No.	Family	Binary Crystal	n	Eg (in ev)
1	III – V	AlN	2.16	3.80(a)
		GaN	2.40	3.25(a)
		InN	2.35	9.70
		AlP	2.75	3.00(a)
		GaP	2.92	6.10
		InP	3.09	5.40

(a) T.S. Moss (1985)

Table – 2

S.No.	% of AIN in GaN	n	Eg (in ev)	n^2 -1	log (n^2-1)	log Eg
1	0	2.40	3.25	4.76	0.678	0.512
2	25	2.34	3.39	4.47	0.651	0.530
3	50	2.28	3.52	4.20	0.623	0.547
4	75	2.22	3.66	3.93	0.594	0.564
5	100	2.16	3.8	3.66	0.564	0.580

Table –3

S.No.	% of AIN in InN	n	Eg (in ev)	n^2 -1	log (n^2-1)	log Eg
1	0	2.35	9.70	4.52	0.655	0.986
2	25	2.30	8.22	4.29	0.632	0.915
3	50	2.25	6.75	4.08	0.611	0.829
4	75	2.21	5.27	3.88	0.589	0.722
5	100	2.16	3.80	3.66	0.564	0.580

Table –4

S.No.	% of GaN in InN	n	Eg (in ev)	n^2 -1	log (n^2-1)	log Eg
1	0	2.35	9.70	4.52	0.655	0.986
2	25	2.36	8.09	4.58	0.661	0.908
3	50	2.37	6.47	4.64	0.666	0.811
4	75	2.38	4.86	4.70	0.672	0.687
5	100	2.40	3.25	4.76	0.678	0.512

Table –5

S.No.	% of AlP in GaP	n	Eg (in ev)	n^2 -1	log (n^2-1)	log Eg
1	0	2.92	6.10	7.526	0.876	0.785
2	25	2.88	5.32	7.280	0.862	0.726
3	50	2.83	4.55	7.037	0.847	0.658
4	75	2.79	3.78	6.798	0.832	0.577
5	100	2.75	3.00	6.562	0.817	0.477

Table –6

S.No.	% of AlP in InP	n	Eg (in ev)	n^2 -1	log (n^2-1)	log Eg
1	0	3.09	5.40	8.548	0.932	0.732
2	25	3.00	4.80	8.030	0.905	0.681
3	50	2.92	4.20	7.526	0.876	0.623
4	75	2.83	3.60	7.037	0.847	0.556
5	100	2.75	3.00	6.562	0.817	0.477

Table –7

S.No.	% of GaP in InP	n	Eg (in ev)	n^2 -1	log (n^2-1)	log Eg
1	0	3.09	5.40	8.548	0.932	0.732
2	25	3.05	5.57	8.287	0.918	0.746
3	50	3.00	5.75	8.030	0.905	0.760
4	75	2.96	5.92	7.776	0.891	0.772
5	100	2.92	6.10	7.526	0.876	0.785

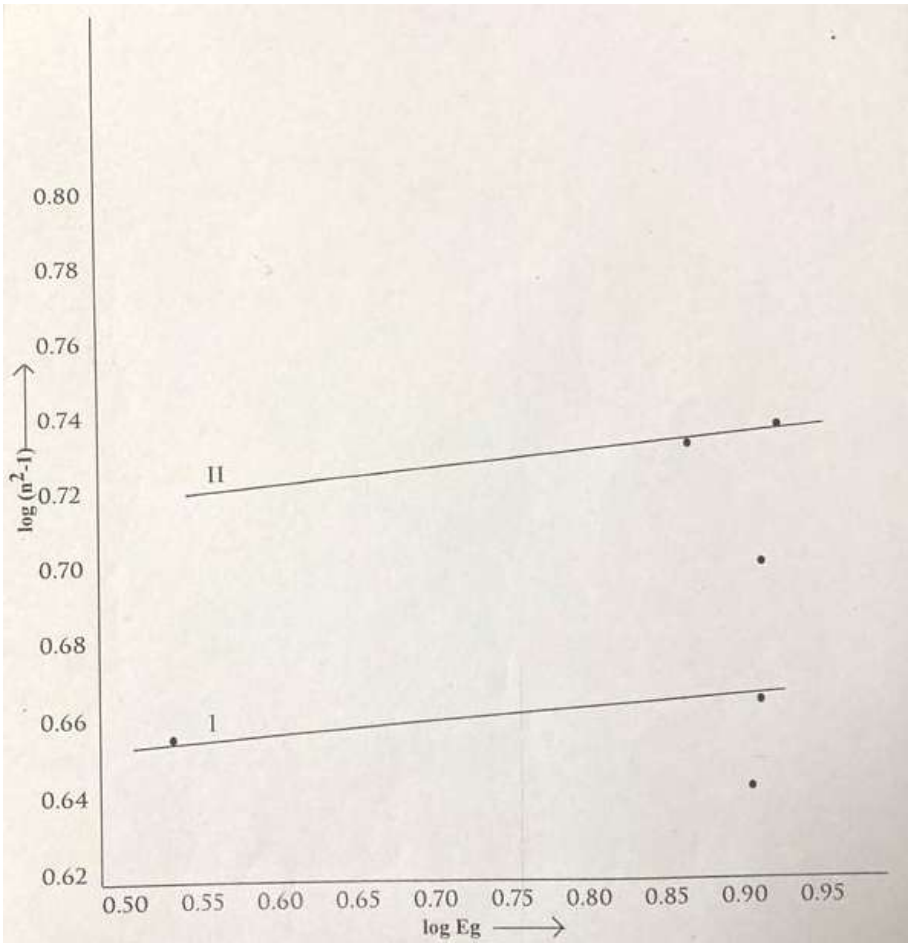

Fig – 1

Graph plot between log (n^2 – 1) and log Eg for Mixed Binary Crystals of III – V family

1. Line I represent the Nitrogen Anion in the mixture of

   (a) AlN – GaN

   (b) AlN – InN

   (c) GaN – InN

   in the proportion of 25% - 75%

2. Line II represent the Phosphorus Anion in the mixture of

   (a) AlP – GaP

   (b) AlP – InP

   (c) GaP – InP

   in the proportion of 25% - 75%

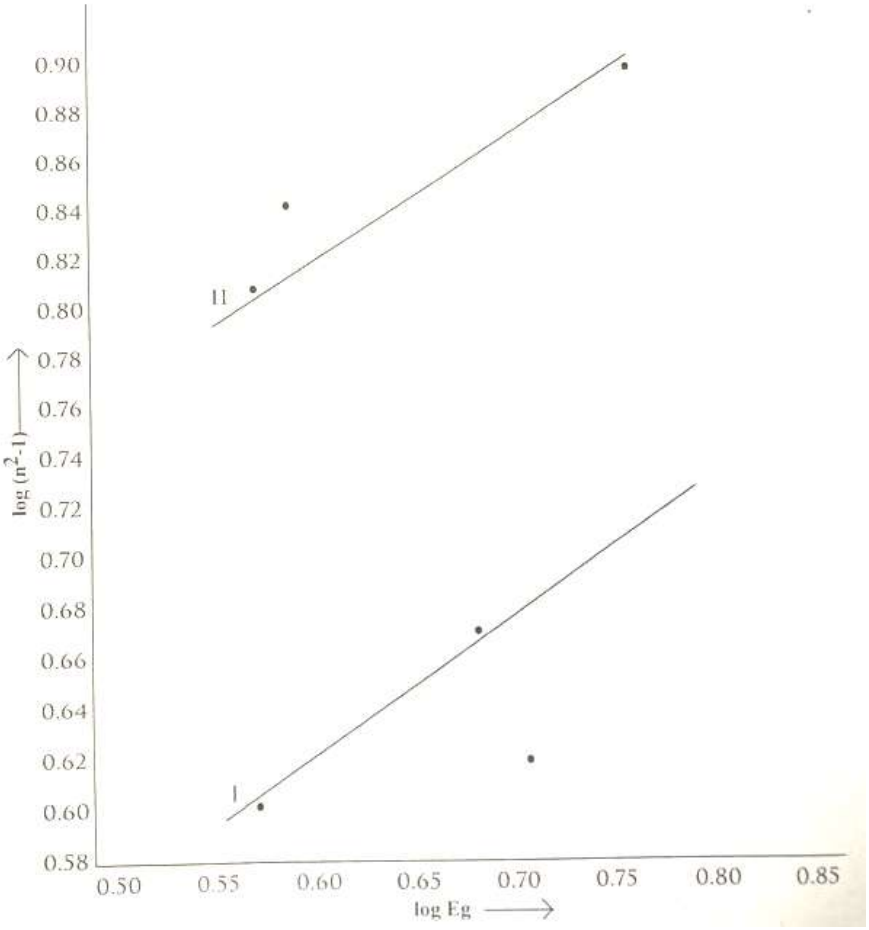

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Fig – 2

Graph plot between log (n^2 – 1) and log Eg for Mixed Binary Crystals of III – V family

1. Line I represent the Nitrogen Anion in the mixture of

   (a) AlN – GaN

   (b) AlN – InN

   (c) GaN – InN

   in the proportion of 75% - 25%

2. Line II represent the Phosphorus Anion in the mixture of

   (a) AlP – GaP

   (b) AlP – InP

   (c) GaP – InP

   in the proportion of 75% - 25%

ANALYSIS OF THE RESULT

The dielectric behaviour of mixed binary crystals are explained by using the relation between refractive index (n) and average energy gap (Eg). According to Ion Dependent Theory n and Eg are related as

$$\mathbf{n^2 = 1 + C\ E_g^{\ P}}$$

Now, taking log on both sides, we get

$$\log (n^2 - 1) = \log C + P \log Eg$$

Above equation represents the equation of straight line. Hence, if we plot the graph between log $(n^2 - 1)$ and log Eg then we find the parallel straight lines for the anions of III – V family is shown in fig. (1) and fig. (2). Since the lines are parallel hence the value of slope (P) of these lines have a constant value. This constant is called Family Characteristic Constant. The value of log C can be found from the intercept on log $(n^2 - 1)$ axis. These parallel lines shows Anion dependence of III – V binary family.

The proposed correlation between n and Eg can be used to calculate electronic dielectric constant ($\in_\infty$) of the complex compounds, if the experimentally observed values of average energy gaps of these compound are known. Its reverse is also true. The knowledge of average energy gaps have many applications in the field of photoconductivity. Photoelasticity and solar cell technology etc. The proposed correlation can also be applied to explain photoemission from strained crystals.

References

1. Moss T.S., Phys. Stat. Sol. (b) **131**, 415 (1985).
2. Philips J.C. and Pandey K.C., Phys. Rev. Lett. **30**, 787 (1973).
3. Phillips J.C., Bonds and Bands in Semiconductors (Academic Press, N.Y., 1973).
4. Philips J.C., Phys. Rev. **166**, 832 (1968 'b')
5. Philips J.C., Phys. Rev. Lett. **20**, 550 (1968 'a')
6. Sarkar K.K. and Goyal S.C., Jour. Chem. phys. **68**, 3231 (1978 'a')
7. Sarkar K.K. and Goyal S.C., Phys. Rev. **21**, 879 (1980).
8. Sarkar K.K. and Goyal S.C., Sol. Stat. Commun. **18**, 1595 (1976)
9. Sarkar K.K., Ph.D. Thesis, Agra University, Agra, (1978).
10. Singh P. and Sarkar K.K., Sol. Stat. Comm. **55,** 439 (1985).
11. Van Vechten J.A., Phys. Rev. **182**, 891 (1969 'a')
12. Van Vechten J.A., Phys. Rev. **187**, 1007 (1969 'b')