QUANTUM ION DEPENDENT COMPUTATION FOR REFRACTIVE INDEX AND AVERAGE ENERGY GAPS FOR MIXED BINARY IONIC CRYSTALS

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Abstract

Quantum Ion dependent theory for refractive Index (n) and Average Energy Gaps (Eg) for mixed binary Ionic crystals in different proportions are evaluates, the relation between refractive Index and average energy gaps show the Cation dependent dielectric behaviour of Ionic crystals. Thus, it gives a strong support in the field of photo conductivity and solar cell technology.

Keywords: Refractive Index, Average Energy Gaps, Mixed Binary Ionic Crystals

Introduction

In simple binary semiconductors refractive index (n) and energy gap between bonding and antibonding states of the crystal are the most important optimal properties of them. A correlation between these parameters should be very useful towards the application of semiconductors in various fields as photoelasticity, photoconductivity solar cell technology etc.

What should be the correlation between the refractive index and corresponding energy gap of simple and complex binary solids is a topic of immense interest among a number of scientists. In 1952 Moss started the topic by suggesting a relation between n and Eg. Further the matter had gone through the hands of Penn (1962) using an isotropic one gap model of binary solids, Ziman (1964) has given a frequency dependent dielectric function and finally Phillips (1968) and Van Vechten (1969) came forward with their ionicity and dielectric Co-ordinations. But all these suggested correlations while satisfying for certain experimental observations, kept on failing for some others.

In 1979 Ravindra and his co-workers established a relation between n and Eg. This relation is claimed as the most general one by them. They further put forward sophisticated technological applications of this relation towards solar cell and photoconductivity fields but the correlation had to face a number of criticism at a later stage.

After that Vishnu Gipal (1982) tried to correlate electronic dielectric constant and minimum energy gap (E_0) with two arbitrary taken characteristics constant but these relations had been put forward without any theoretical explanation. Moreover, his correlations were shown to be deviating for his own considered compounds like Cd Te etc. by Sarkar (1978, 1980, 1982, 1985) who inturn extended an ion dependent dielectric theory in this field, that gave excellent agreement in many experimental optical and thermal properties of binary and polyatomic compounds.

Quantum Ion Dependent Theory for Mixed Binary Crystals

According to quantum ion dependent model the relation between refractive indices (n) and average energy gap for all $A^N B^{8-N}$ type binary crystals is given as

$$n^2 = 1 + CEg^p \qquad \ldots.(1)$$

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

To show the dependence of refractive indices (n) on average energy gap (Eg) we rearranging the equation (1) into the logarithmic from, we get

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

Equation (2) is similar to equation of straight line. In I-VII family, we get parallel straight line for each cation. This inference is quite in agreement with our ion dependent model.

From equation (2), we also calculate the value of P and C for I-VII family.

Computation of Refractive Index (n) and Average Energy Gaps (Eg) for Mixed Binary Crystals

According to Quantum Ion Dependent Theory the correlation between n and $E_g$is given earlier in equation (1) as

$$n^2 = 1 + C\, E_g^p \qquad \ldots(3)$$

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

$$n = \lambda_x n_x + \lambda y\, n_y \quad \ldots(4)$$

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:

$$Eg = \lambda x\, (Eg)_x + \lambda y\, (Eg)_y \quad \ldots(5)$$

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 calculated values of refractive index (n) and average energy gap (Eg) are reported in Table (1) to (6).

Table – 1

S.No.	% of LiF in LiCl	n	Eg (in ev)	$n^2 - 1$	log (n^2-1)	Log Eg
1	0	1.64	13.50	1.6896	0.228	1.130
2	25	1.57	17.18	1.465	0.166	1.235
3	50	1.51	20.85	1.280	0.107	1.319
4	75	1.45	24.53	1.102	0.042	1.390
5	100	1.38	28.21	0.904	-0.044	1.450

Table – 2

S.No.	% of LiF in LiBr	n	Eg (in ev)	$n^2 - 1$	log (n^2-1)	Log Eg
1	0	1.79	11.02	2.204	0.343	1.042
2	25	1.69	15.32	1.856	0.266	1.185
3	50	1.59	19.61	1.496	0.175	1.292
4	75	1.48	23.91	1.190	0.075	1.378
5	100	1.38	28.21	0.904	-0.044	1.450

Table – 3

S.No.	% of LiCl in LiBr	n	Eg (in ev)	$n^2 - 1$	log (n^2-1)	Log Eg
1	0	1.79	11.02	2.204	0.343	1.042
2	25	1.75	11.64	2.062	0.314	1.066
3	50	1.71	12.26	1.924	0.284	1.088
4	75	1.68	12.88	1.822	0.260	1.110
5	100	1.64	13.50	1.690	0.228	1.130

Table – 4

S.No.	% of NaF in NaCl	n	Eg (in ev)	$n^2 - 1$	log (n^2-1)	Log Eg
1	0	1.51	13.51	1.280	0.107	1.131
2	25	1.46	16.28	1.132	0.054	1.212
3	50	1.40	19.05	0.960	-0.018	1.280
4	75	1.35	21.82	0.822	-0.085	1.339
5	100	1.30	24.59	0.690	-0.161	1.391

Table – 5

S.No.	% of NaF in NaBr	n	Eg (in ev)	$n^2 - 1$	log (n^2-1)	Log Eg
1	0	1.61	11.45	1.592	0.202	1.059
2	25	1.53	14.73	1.341	0.127	1.168
3	50	1.45	18.02	1.102	0.042	1.256
4	75	1.38	21.30	0.904	-0.044	1.328
5	100	1.30	24.59	0.690	-0.0161	1.391

Table – 6

S.No.	% of NaCl in NaBr	n	Eg (in ev)	$n^2 - 1$	log (n^2-1)	Log Eg
1	0	1.61	11.45	1.592	0.202	1.059
2	25	1.58	11.96	1.496	0.175	1.078
3	50	1.56	12.48	1.434	0.156	1.096
4	75	1.53	12.99	1.341	0.127	1.114
5	100	1.51	13.51	1.280	0.107	1.131

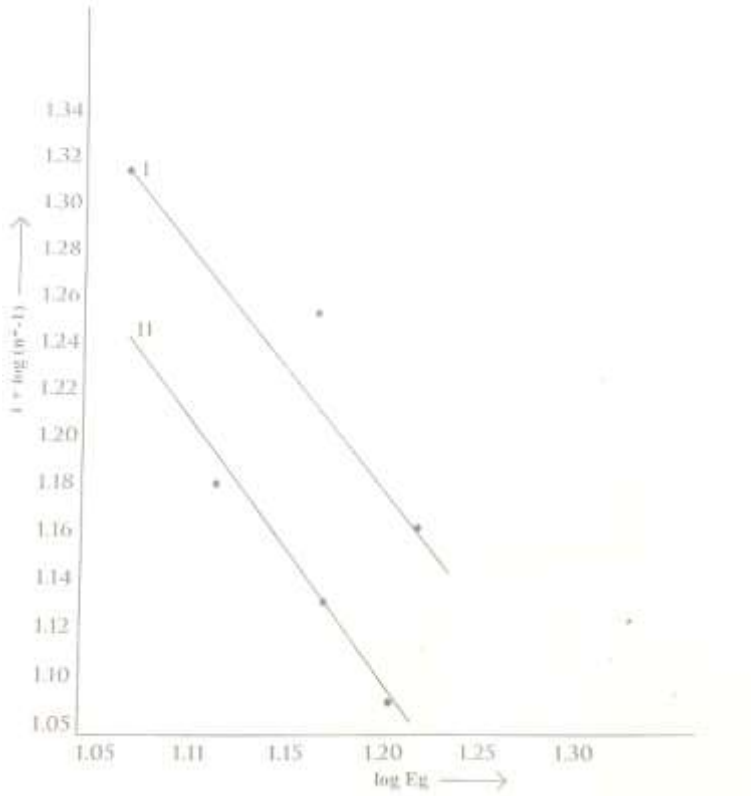

Fig. – 1

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

1. **Line I represent the Lithium Cation in the mixture of**
   - **(a) LiF – LiCl**
   - **(b) LiF – LiBr**
   - **(c) LiCl – LiBr**
   - **in the proportion of 25% - 75%**

2. **Line II represent the Sodium Cation in the mixture of**
   - **(a) NaF – NaCl**
   - **(b) NaF – NaBr**
   - **(c) NaCl – NaBr**
   - **in the proportion of 25% - 75%**

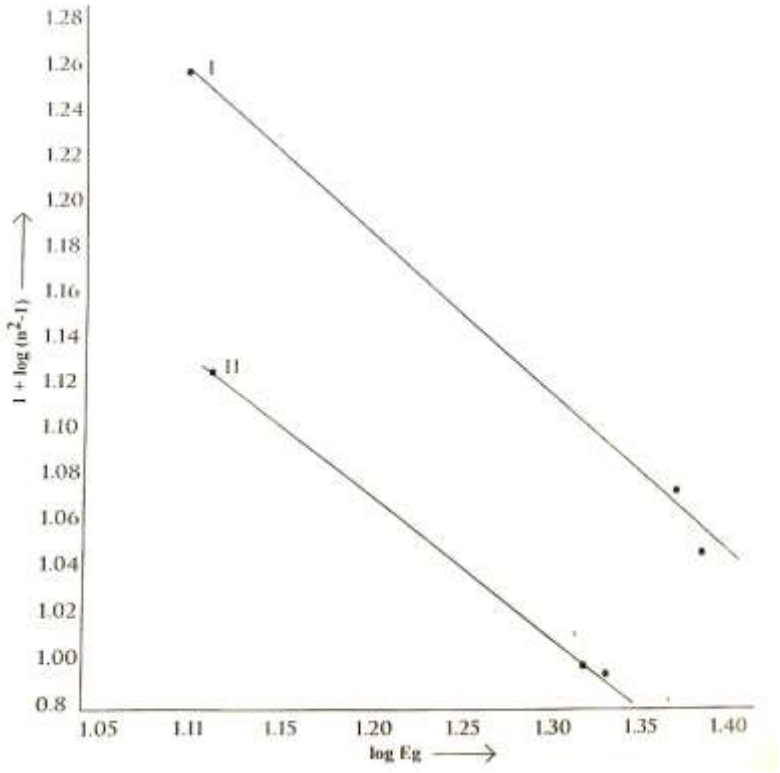

Fig. - 2

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

1. Line I represent the Lithium Cation in the mixture of

(a) LiF – LiCl

(b) LiF – LiBr

(c) LiCl – LiBr

in the proportion of 75% - 25%

2. Line II represent the Sodium Cation in the mixture of

(a) NaF – NaCl

(b) NaF – NaBr

(c) NaCl – NaBr

in the proportion of 75% - 25%

Analysis of the Result

The dielectric behaviour of mixed binary ionic crystals are explained by using the relation between refractive Index (n) and average energy gap (Eg). According to equation (2), if we plot the graph between log (n^2 – 1) and log Eg.Then we find the Parallel straight

lines for the ionic crystals of I-VII family which 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 Cation dependence of mixed binary ionic crystals.

References:

1. Moss T.S. Phys. Stat. Sol. (b) **131**, 415 (1985)
2. Moss T.S., Photoconductivity in the elements, Butterworths, London (1952)
3. Penn D.R., Phys. Rew. **128**, 2093 (1962)
4. Phillips J.C., Phys. Rev. **166**, 832 (1968 'b')
5. Phillips J.C., Phys. Rev. Lett. **20**, 550 (1968 'a')
6. Sarkar K.K. and Goyal S.C., Jour. Chem Phys. **68**, 3232 (1978 'a')
7. Sarkar K.K. and Goyal S.C. Phys. Rev. **21**, 879 (1985)
8. Singh P. and Sarkar K.K., sol. Stat. Comm. **55**, 439 (1985)
9. Sarkar K.K. and Goyal S.C., Phys. Rev. **21** 879 (1980)
10. Van Vechten J.A., Phys. Rev. **182**, 891 (1969 'a')
11. Van Vechten J.A., Phys. Rev. **187**, 1007 (1969 'b')
12. Ziman J.M., Principles of the theory of solids (Cambridge University Press, London, 1964)