

# Inter Molecular Behaviour of Mixed and Complex Compounds

K. P. Tiwari

Department of Physics, Agra College, Agra-282002 (Affl. to: Dr. B. R. Ambedkar University, Agra (India))

Email: drkptiwari@rediffmail.com.

**Abstract**— The dielectric behaviour of compounds has gradual change from high cation dependence to high anion dependence for crystals moving from high ionicity to high covalence. The average energy gap ( $E_g$ ) and optical dielectric constant ( $\epsilon_\infty$ ) of mixed and complex crystals are computed from the experimental values of  $E_g$  and  $\epsilon_\infty$  of pure crystals. Generally it is observed that the dielectric parameters of crystals do not match exactly with the values required in optoelectronics for specific use. Thus in this research paper we have developed the mixture of binary compounds with specific concentrations and tried to study their dielectric properties, which are closely related with the values required in optoelectronic compounds. The theoretical validation is in fine agreement with ion dependent dielectric model of compounds. We have tried this prescription on various ionic, covalent and cross compounds with different mixing proportions at certain temperature. This theory leads to explain the intermolecular behaviour of crystals, which can be extended to interpret the molecular interactions of hydroxyl and amino groups in mixture of polar liquids. This approach has proved to be remarkably successful in the study of dielectric parameters of nano- materials. Certain industrial applications are also suggested.

**Keywords**— Optical dielectric constant, optoelectronic, ionicity etc.

## I. INTRODUCTION

The dielectric and refracting properties of mixed binary crystals in mixed and complex compounds are found to be of great scientific and technological importance. Numerous attempts have been made to investigate various properties of mixed crystals in the recent past but all these studies are generally confined only to the ionic and covalent families (1, 2). There was no generalised theory for all ionic and covalent mixed families together. The pure crystals have characteristically fixed values of optical refractive index ( $n$ ) and ( $E_g$ ) which may not match exactly with values required for many recently developed opto-electronic compounds (3). However, the required values of  $n$  may be readily obtained by mixing two binary crystals in certain definite proportion. Thus the concept of mixed crystal finds its importance in the electronic modern industries (4).

In the present paper we propose to evaluate the optical refractive index ( $n$ ) and average energy gap ( $E_g$ ) of a number of mixed crystals in ionic and covalent families, and developed a generalised inter-relationship between them. This relationship is found satisfactory for all solids and one can always develop a material of any required value of  $n$ , knowing the value  $E_g$  of definite proportion. This prescription can directly be used in preparations of certain compounds of known refractive index because the dielectric parameters are directly related with intermolecular structure of crystals.

Therefore this study will be important in defining the intermolecular behaviour of compounds.

## II. MATERIAL AND METHODS

The well-established isotropic one gap dielectric model for binary solids given by Penn (5), Van-Vechten (6) and frequency dependent dielectric theory of Phillips (7, 8, 9) lead to a generalised expression,

$$n^2 = 1 + (h \omega_p / E_g) \quad (1)$$

Where  $\omega_p$  is the plasma frequency and  $E_g$  is the average energy gap. It is also noticed that  $E_g$  is found to have direct bearing on  $R$  as,

$$E_g = BR^S,$$

Where  $S$  is family characteristics and  $B$  is cation characteristics in ionic families and anion characteristics in covalent families. In the dielectric studies of matter, one finds that the optical dielectric constant ( $\epsilon_\infty$ ) of a compound is closely related to its optical refractive index as,

$$\epsilon_\infty = n^2 \quad (2)$$

The values of  $\epsilon_\infty$  for almost all solids in simple binary compounds are experimentally measured. It is also noticed that dielectric constant ( $\epsilon_\infty$ ) of mixture of binary compounds is correlated with concentration as (3, 4, 11),

$$\epsilon_\infty = (\epsilon_\infty)_m - [(\epsilon_\infty)_1 x_1 + (\epsilon_\infty)_2 x_2] \quad (3)$$

Here  $X_1$  and  $X_2$  are the mixing proportions of respective crystals where as  $\epsilon_0$  is static dielectric constant and  $\epsilon_\infty$  is limiting dielectric for binary mixture and suffix  $m$  stands for mixture.

In the present study it is proposed to prepare a mixture of equal concentrations ( $X$ ) of two pure crystals (i.e. 50%-50%) which leads to,

$$x_1 = x_2 = 1/2 \quad (4)$$

Thus at fixed proportion and at constant temperature equation (3) & (4) leads to

$$\epsilon_\infty = x_1(\epsilon_\infty)_1 + x_2(\epsilon_\infty)_2 \quad (5)$$

And Inter ionic separation

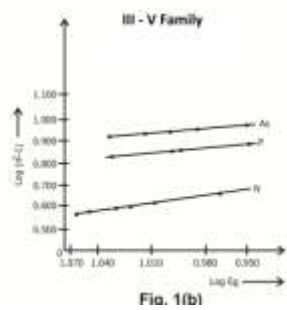
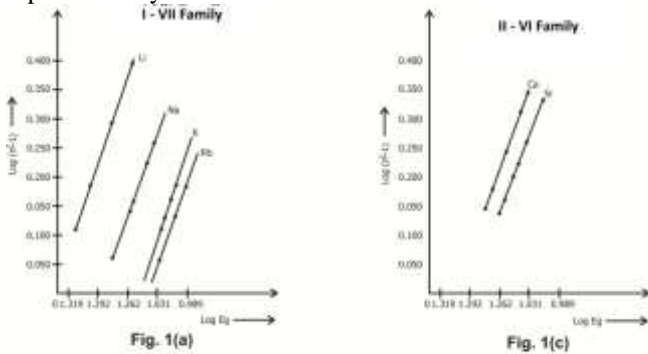
$$R^3 = x_1 R_1^3 + x_2 R_2^3 \quad (6)$$

Thus in the present work, mixtures of same cation solids in equal proportions are mixed together and evaluate their  $n$  and  $E_g$  for mixed binary crystals in I – VII, II – VI and III – V families and reported in the table 1, 2 & 3. A view of equation 1, 2, 3 & 6 leads to

$$n^2 = 1 + CEg^k \quad (7)$$

Where  $C$  &  $K$  are characteristics constants for mixture compounds. Equation (6) infers that ( $n^2-1$ ) should have a direct dependence on some power of  $E_g$  (10, 11). Thus we propose to plot variations of  $\log(n^2-1)$  against  $\log E_g$  for each separate mixture family. The respective plots for each family

are shown in fig. 1(a), 1(b) & 1(c). A perusal of these plots shows parallel straight lines. In I-VII family we get parallel lines and line containing the mixture of same cation where as in III-V family also plots are parallel lines but each line is represented by same anion mixtures.



III. RESULTS AND DISCUSSION

A view of fig 1(a), 1(b) & 1(c) infers that there are parallel straight lines for each family and each parallel line containing the mixture of same cation and same anions respective family. Overall view of these plots suggesting a correlation between n & E<sub>g</sub> as

$$\text{Log}(n^2 - 1) = K \text{ log } E_g + \text{Log } C \tag{8}$$

Here slope K is obtained as family characteristics and log C (intercept on log n<sup>2</sup>-1) is characteristic constant for a particular ion in the given family. Thus equation (8) is a extended form of equation (7) which proves the theoretical validity of dielectric behaviour of mixed crystal.

It is also clear from table 1, 2 and 3 that all mixed compounds in a particular family, constant K is constant but constant C is different for different ions in the same family. It is also noticed that mixtures in I-VII family are formed by same cation solids and all same cation mixed crystals fall on same straight lines. Thereby C should be called an anion characteristic constant for this family. Similar process has been tried with the same anion mixtures in I-VII & III-V family too (12, 13, 14). This concludes that the dielectric behaviour of ionic solid mixtures is purely cation dependent while that of cation solid mixture is purely anion dependent. This inference is quite in agreement with the well established ion dependent model for pure binary crystals (15). This prescription can be used for developing the compounds of mixed crystals with any value of K & C (16).

IV. CONCLUSIONS

On the basis of this theory certain mixed crystals can be prepared with varying value of n & E<sub>g</sub> with required proportions. It can also be concluded that dielectric behaviour of solids are directly related with the molecular interaction behaviour of crystals. Thus this theory can be extended to interpret the inter-molecular behaviour of solids as well as liquids. This study has vast applications in industrial, technological and environmental fields.

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TABLE 1. Mixed Binary crystals in I – VII Family

Cation	Crystal	n	Log(n <sup>2</sup> -1)	E <sub>g</sub>	Log E <sub>g</sub>	C
Li	Lif-LiCl	1.156	0.1139	20.86	1.3192	
	Lif-LiBr	1.596	0.1903	19.62	1.2925	
	Lif-LiI	1.688	0.2672	18.35	1.2636	0.094
	LiCl-LiBr	1.717	0.2896	12.26	1.0884	
	LiCl-LiI	1.802	0.3522	21.99	1.3422	
Na	LiBr-LiI	1.87	0.3979	5.76	0.09892	
	Naf-NaCl	1.414	0.000	19.5	1.2798	
	Naf-NaBr	1.466	0.0607	18.02	1.2557	
	Naf-NaI	1.549	0.1461	16.69	1.2224	0.054
	NaCl-NaBr	1.565	0.1614	12.48	1.0962	
	NaCl-NaI	1.643	0.2304	11.21	1.0496	
	NaBr-NaI	1.688	0.2672	10.18	1.0077	
	Kf-KCl	1.414	0.000	16.09	1.0206	
	Kf-KBr	1.449	0.0414	15.3	1.1846	
	Kf-KI	1.5	0.0969	14.35	1.5668	
K	KCl-KBr	1.516	0.1139	14.39	1.0565	0.035
	KCl-KI	1.565	0.1614	10.44	1.0187	
	KBr-KI	1.596	0.1903	9.65	0.9845	
	Rbf-RbCl	1.431	0.0212	11.21	1.041	
Rb	Rbf-RbBr	1.466	0.0607	10.76	1.011	
	Rbf-RbI	1.516	0.1139	10.36	1.016	0.031
	RbCl-RbBr	1.516	0.1614	10.10	1.0561	
	RbCl-RbI	1.565	0.1614	9.75	1.009	
	RbBr-RbI	1.596	0.1903	9.68	0.999	

TABLE 2. Mixed Binary Crystals in II – VI Family

Cation	Crystals	n	Log(n <sup>2</sup> -1)	E <sub>g</sub>	logE <sub>g</sub>	C
Ca	Cas-CaSe	2.19	0.57933	7.80	0.8920	
	Cas-CaTe	2.32	0.64171	7.10	0.8512	0.077
	CaSe-CaTe	2.38	0.6687	6.80	0.8325	
Mg	MgS-MgSe	2.34	0.6508	8.415	0.9250	
	MgS-MgTe	2.45	0.6991	4.450	0.6483	0.121
	MgSe-MgTe	2.53	0.7324	3.960	0.5976	
Sr	SrS-SrSe	2.15	0.5590	7.52	0.8762	
	SrS-SrTe	2.25	0.6087	7.14	0.8536	0.062

Zn	SrSe-SrTe	2.31	0.6370	6.65	0.8228	
	ZnS-ZnSe	2.35	0.6553	7.85	0.8948	
	ZnS-ZnTe	2.50	0.7201	7.12	0.8524	0.175
Cd	ZnSe-ZnTe	2.26	0.6135	6.85	0.8356	
	SdS-CdSe	2.37	0.6643	6.97	0.8438	
	CdS-CdTe	2.48	0.7118	6.54	0.8155	0.138
	CdSe-CdTe	2.57	0.7485	6.28	0.7979	

TABLE 3. Mixed Binary Crystal in III-V Family

Cation	Crystal	n	Log (n <sup>2</sup> - 1)	Eg	Log Eg	C
N	BN-AlN	2.156	0.5623	11.70	1.0750	
	BN-GaN	2.179	0.574	13.65	1.1350	
	BN-InN	2.236	0.6021	14.35	1.150	2.183
	AlN-GaN	2.213	0.5911	11.75	1.070	
	AlN-InN	2.269	0.6180	10.85	1.0354	
P	GaN-InN	2.291	0.6284	10.6	1.0253	
	BP-AlP	2.924	0.8779	11.21	1.0480	
	BP-Gap	2.924	0.8779	10.60	1.0200	
	BP-InP	3.016	0.9085	10.50	1.0250	3.451
	AlP-GaP	3.016	0.8751	6.00	0.7781	
As	AlP-InP	3.008	0.9058	5.65	0.7520	
	GaP-InP	3.008	0.9058	5.75	0.7596	
	Bas-AlAs	3.209	0.9685	10.98	1.0450	
	Bas-GaAs	3.263	0.9845	13.65	1.1350	
	Bas-InAs	3.368	1.0149	11.70	1.0650	4.236
	AlAs-GaAs	3.368	0.980	5.4	0.73230	
	AlAs-InAs	3.354	1.0107	5.1	0.70750	
	GaAs-InAs	3.405	1.0253	5.1	0.70750	

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