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Dielectric Properties of Mixed and Complex Compounds

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ABSTRACT

The average energy gap (E_g) and optical refractive index (n) of mixed and complex crystals are computed from the measured values of (E_g) and (n) of pure crystals. The pure crystals have fixed values of optical and dielectric parameters, which do not in general, match exactly with the values required in opto-electronic compounds for specific use. Thus it is proposed to develop the mixtures of binary compounds which may have their properties matching exactly with the values required in opto-electronic compound. An empirical relation between n and E_g is developed for mixed compound families by using these computed values. This relation shows a fine agreement with ion-dependent dielectric model of compounds. This study is limited to binary solids of I-VII, II-VI and III-V type cross compounds. This prescribed theory can therefore be used for different mixed crystal as well as for complex compounds. The theoretical validity of the relation is also established. This theory is applicable for explaining the intermolecular behaviour of solids of other families of similar nature which can be extended for polar and non-polar liquids too. Certain industrial and technical applications are also proposed.

Keywords: Average energy gap, Optical refractive index, Dielectric model, Opto-electronic compounds, Binary solids, Cross compounds, Polar and Non-Polar liquids.

INTRODUCTION

The dielectric parameters of pure binary crystals are computed using ion-dependent dielectric theory [1,2]. 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 [3]. There was no generalized theory for all ionic and covalent mixed families together [4]. The pure crystals have characteristically fixed values of dielectric constant $\in\propto$ and average energy gap E_g [5,6] which may not match exactly with values required for many recently developed opto-electronic compounds. However, the required values of optical refractive index (n) may be readily obtained by mixing two binary crystals in certain definite proportion [8]. Thus the concept of mixed crystal finds its importances in the electronic modern industries. In the present paper we propose to evaluate the optical refractive index (n) and average energy gap (Eg) 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 of Eg in definite proportion. This prescription can directly be used in preparation of certain compounds of known refractive index [9,10,11]. Since the dielectric

parameters are directly related with intermolecular structure of crystals [12,13]. Therefore this study will be important in defining the intermolecular behaviour of compounds, which can be extended to interpret the molecular interaction of compounds in liquid solutions. [14].

MATERIALS AND METHODS

Theory: The well established isotropic one gap dielectric model for binary solids given by Penn (3), Van-Vechten (4) and frequency dependent dielectric theory of Phillips (7) lead to a generalised expression,

$$n^2 = 1 + (h\omega_\rho / Eg) \quad \text{..... (1)}$$

where ω_ρ is the plasma frequency and Eg is the average energy gap. It is also noticed that Eg is found to have direct bearing on R as,

$$Eg = BR^S,$$

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

$$\in_\infty = n^2 \quad \text{.....} \quad (2)$$

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

$$\in_o{}^{\in} = (\epsilon_o - \epsilon_\infty)_m - [(\epsilon_o - \epsilon_\infty)_1 x_1 + (\epsilon_o - \epsilon_\infty)_2 x_2] \text{ .... (3)}$$

Here x_1 and x_2 are the mixing proportions of respective crystals where as $\in_o$ is static dielectric constant and $\in_\infty$ is limiting dielectric constant 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 compounds (i.e. 50%-50%) which leads to,

$$x_1 = x_2 = 1/2 \quad \text{.....} \quad (4)$$

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

$$\epsilon_\infty = x_1(\epsilon_\infty)_1 + x_2(\epsilon_\infty)_2 \text{ .....} \quad (5)$$

and Inter ionic separation

$$R^3 = x_1 R_1{}^3 + x_2 R_2{}^3 \text{ .....} \quad (6).$$

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

$$n^2 = 1 + CEg^k \quad \text{..... (7)}$$

where C & K are characteristic constants for mixture compounds. Equation (7) infers that (n^2-1) should have a direct dependance on some power of Eg. Thus we propose to plot variations of log (n^2-1) against log Eg 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 each 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 and vice-versa.

RESULTS AND DISCUSSION

A view of fig 1a, 1b and 1c infers that there are parallel straight lines for each family and each parallel line containing the mixture of same cation and same anions respectively. Overall view of these plots suggesting a correlation between n & Eg as

$$\text{Log } (n^2 - 1) = K \log Eg + \text{Log } C \quad \text{..... (8)}$$

Here slope K is obtained as family characteristics and log C (intercept on log n^2-1) is characteristic constant for a particular ion in the given family. Thus equation (8) is extended form of equation (7) which proves the theoretical validity of dielectric behaviour of mixed compounds. It is also clear from table 1a, 1b and 1c 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 compounds 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 and III-V family too. 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 (12). This prescription can be used for developing the compounds of mixed crystals with any value of K & C. On the basis of this theory certain mixed crystals can be prepared with varying value of n & E_g with required proportions. It can also be concluded that dielectric behaviour of solids are directly related with the molecular interaction behaviour of compounds. 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.

Table 1. Mixed Binary Crystals in I – VII Family

Cation	Crystal	n	Log(n2-1)	Eg	Log Eg	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	
	LiBr-LiI	1.87	0.3979	5.76	0.09892	
Na	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
	KCll-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	
	Rbf-RbBr	1.466	0.0607	10.76	1.011	
Rb	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(n2-1)	Eg	logEg	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
	SrSe-SrTe	2.31	0.6370	6.65	0.8228	
Zn	ZnS-ZnSe	2.35	0.6553	7.85	0.8948	
	ZnS-ZnTe	2.50	0.7201	7.12	0.8524	0.175
	ZnSe-ZnTe	2.26	0.6135	6.85	0.8356	
Cd	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 $(n^2 - 1)$	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-lnN	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	
	GaN-InN	2.291	0.6284	10.6	1.0253	
P	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	
	AlP-InP	3.008	0.9058	5.65	0.7520	
	GaP-InP	3.008	0.9058	5.75	0.7596	
As	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	

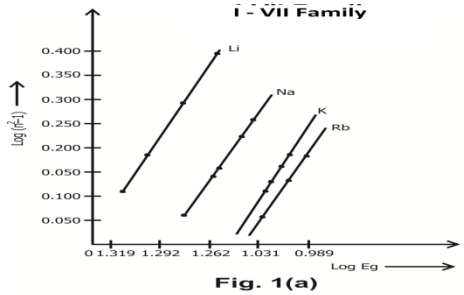

Fig. 1(a)

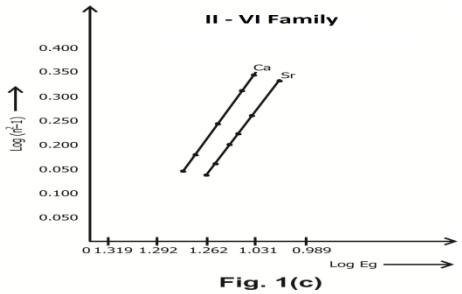

Fig. 1(c)

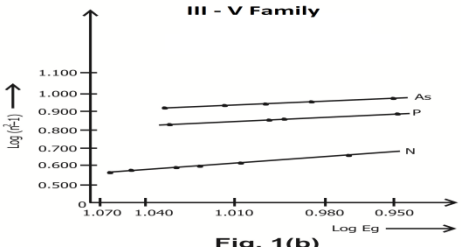

Fig. 1(b)

APPLICATIONS

In view of these results it can be concluded that dielectric behaviour of solids are directly related with the molecular interaction behaviour of crystals. This theory can be extended to interpret the inter-molecular behaviour of solids as well as liquids. On the basis of this theory certain mixed crystals can be prepared with varying value of n and E_g with required proportions as per technological applications. This approach successfully applied for the dielectric study of nano- materials. This prescription can also be useful to define shape, size and nature of constituents in compounds.

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