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TEMPERATURE DEPENDENCE OF ELECTRONIC DIELECTRIC CONSTANT AND AVERAGE ENERGY GAPS FOR MIXED BINARY CRYSTALS

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Abstract

The quantum ion dependent model is utilized to derive an expressions for the temperature derivative of electronic dielectric constant and Average Energy Gap. Thus, our proposal brings out and exciting method by which a single mixed crystal can be used for many different purpose in the present day electronic world.

Key words: Electronic Dielectric Constant ($\in_\infty$), Average energy Gap (E_g), Temperature variation.

INTRODUCTION

The temperature dependence of electronic dielectric constant ($\in_\infty$) and average energy gap (E_g) separately at constant pressure and constant volume of mixed binary crystals have been a subject of great interest industrially due to wide ranging properties in optical, semiconducting, photoconducting, photoelastic and solar cell applications. The application of temperature on a family of crystals appreciable changes the electronic dielectric constant ($\in_\infty$) and modifies the average energy gap (E_g), thus, providing to be an asset in the mentioned applied fields. The temperature derivatives of dielectric constant of ionic crystals are useful to estimate the temperature dependences of some useful parameters like electronegativity parameter etc.

Samara (1976) computed temperature derivatives of dielectric constant and average energy gap by using macroscopic Clausius Mossotti relation as the base. But he failed to establish a general correlation for temperature derivatives of $\in_\infty$ and E_g, which could be applicable to all the simple and complex compounds.

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Thus, in the present paper, we will summarize all the earlier recent theories and examine their validity in the beginning for different simple binary families. We will extend the prediction of temperature dependence for mixed binary crystals of I-VII, II-VI and III-V families which would enables us to know how a particular family can be treated thermally so as to have different applications in the mentioned applied fields. In the next step of this chapter we will put forward a general quantum ion dependent model for temperature derivatives of mixed binary crystals and check the validity of proposed theory with its applications. We will show that the proposed theory and formulation are in quite good agreement for all the families under consideration as far as the analytical and experimental results are concerned.

QUANTUM ION DEPENDENT THEORY FOR TEMPERATURE DERIVATIVE OF ELECTRONIC DIELECTRIC CONSTANT AND AVERAGE ENERGY GAP FOR MIXED BINARY CRYSTALS

According to ion dependent quantum theory for simple and complex binary families, the correlation between $\in_\infty$ and E_g is given

$$\in_\infty = n^2 = 1 + C\, E_g^K \qquad \ldots (1)$$

Here the parameter K is said to be different for different simple binary families like I – VII, II – VI, III – V etc. or for different complex AB_2, A_2B, A_3B and A_3B_2 families, while the other parameter C is a characteristic of cation in ionic solids or of anion in covalent one in a particular family. However, while deriving this correlation, the effect of core-d electrons was neglected. Differentiation of equation (1) with respect to temperature at constant pressure and at constant volume separately lead to

$$\left(\frac{d \in_\infty}{dT}\right)_P = (\in_\infty - 1)\left[\frac{K}{E_g}\left(\frac{dE_g}{dT}\right)_P + \frac{1}{C}\left(\frac{dC}{dT}\right)_P\right] \qquad \ldots (2)$$

and

$$\left(\frac{d \in_\infty}{dT}\right)_V = (\in_\infty - 1)\left[\frac{K}{E_g}\left(\frac{dE_g}{dT}\right)_V + \frac{1}{C}\left(\frac{dC}{dT}\right)_V\right] \qquad \ldots (3)$$

Equation (2) and (3) are applicable to all types of crystals families. These equations are quite useful due to the fact that the quantity $\frac{1}{C}\left(\frac{dC}{dT}\right)$ has the simple unit K^{-1}.

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expected to have quite complicated dimensions. All terms in these equations are represented with the unit per Kelvin.

COMPUTATION FOR TEMPERATURE DERIVATIVES OF ELECTRONIC DIELECTRIC CONSTANT ($\in_\infty$) AND AVERAGE ENERGY GAP (E_G) FOR MIXED BINARY CRYSTALS

The mixed binary crystals under study are in I-VII, II-VI and III-V families. The I – VII family is purely ionic with high percentage of heteropolar contribution and negligible homopolar part, it shows pure cation dependent dielectric behaviour (Pantelides 1975, Sarkar 1976, 1980).

In II-VI family the heteropolar energy contribution is large in comparison to homopolar contribution. Thus, solids in II-VI family may be considered ionic and hence they also show cation dependent dielectric behaviour. In III-V family, solids are highly covalent in nature and show purely anion dependent dielectric behaviour (Sarkar et al. 1980). The homopolar energy contribution is very large while the heteropolar part is negligible in III-V solids. Thus, we form same cation solid mixtures in I-VII and II-VI families and same anion solids mixtures in III-V family. For generalized discussion on final results, we use 50%-50% mixtures every where.

(A) COMPUTATION FOR I-VII MIXTURE FAMILY

The values of $\left(\frac{d \in_\infty}{dT}\right)_P$ and $\left(\frac{d \in_\infty}{dT}\right)_V$ for pure crystals are already found through generalized ion dependent formulations (Fernandez and Sarkar (1991)). Fo 50%-50% mixture we estimate the values of $\left(\frac{d \in_\infty}{dT}\right)_P$ and $\left(\frac{d \in_\infty}{dT}\right)_V$ by averaging the values of pure crystals. These, along with values of K, $\in_\infty$ and $\frac{1}{C}\left(\frac{dC}{dT}\right)$ are enlisted in tables (1) and (2) as input data. Finally the temperature derivatives of average energy gaps $\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)_P$ and

$\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)_V$ are evaluated through equations (2) and (3) respectively and are enlisted in table (1) and (2)

(B) COMPUTATIONS FOR II-VI AND III-V MIXTURE FAMILIES

In order to show complete generalization of theory, we propose to make a reverse computation in these families. The values of $\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)$ for pure crcylstals are recently estimated upto fairly good agreement by Tiwari (1998) . For 50% - 50% mixtures, we estimate the value of $\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)$ by averaging the values of pure crystals. These, along with the values of K, $\in_\infty$ and $\frac{1}{C}\left(\frac{dC}{dT}\right)$ are enlisted in table (3) as input data. Finally the temperature derivations of $\in_\infty$ i.e. $\left(\frac{d\in_\infty}{dT}\right)$ are evaluated through equation (2) for variations at constant pressure and are reported in table (3). Similar computations can be readily done for variations at constant volume also.

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Table – 1: Calculated values of $\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)$ at constant pressure for I-VII mixed binary crystals

(K = -1.00)

Cations	Crystals 50%-50%	$\in_\infty$	$\frac{1}{C}\left(\frac{dC}{dT}\right)_P$ $X10^{-5}/K$	$\left(\frac{d\in_\infty}{dT}\right)_P$ $X10^{-4}/K$ Estimated (a)	$\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)_P$ $X10^{-5}/K$ Calculated
Li	LiF-LiCl	2.30	+5.92	+0.820	-0.388
	LiF-LiBr	2.55	+5.92	+1.165	-1.596
	LiCl-LiBr	2.95	+5.92	+1.735	-2.977
Na	NaF-NaCl	2.00	+2.20	+0.520	-3.000
	NaF-NaBr	2.15	+2.20	+0.870	-5.365
	NaF-NaI	2.40	+2.20	+1.390	-7.728
	NaCl-NaBr	2.45	+2.20	+1.040	-4.972
	NaCl-NaI	2.70	+2.20	+1.560	-6.976
	NaBr-NaI	2.85	+2.20	+1.910	-8.124
K	KF-KCl	2.00	+3.96	+0.695	-2.990
	KF-KBr	2.10	+3.96	+0.695	-2.358
	KF-KI	2.25	+3.96	+0.695	-1.600
	KCl-KBr	2.30	+3.96	+1.040	-4.040
	KCl-KI	2.45	+3.96	+1.040	-3.212
	KBr-KI	2.55	+3.96	+1.040	-2.750
Rb	RbF-RbCl	2.05	+2.72	+0.520	-2.232
	RbF-RbBr	2.15	+2.72	+0.520	-1.802
	RbF-RbI	2.30	+2.72	+0.695	-2.626
	RbCl-RbBr	2.30	+2.72	+0.690	-2.588
	RbCl-RbI	2.45	+2.72	+0.865	-3.245
	RbBr-RbI	2.55	+2.72	+0.865	-2.861

(a) Obtained for 50%-50% mixtures of compounds from measured values of individuals (Fernandez and K.K.Sarkar, 1991)

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Table – 2: Calculated values of $\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)$ at constant volume for I-VII mixed binary crystals

(K = -1.00)

Cations	Crystals 50%-50%	$\in_\infty$	$\frac{1}{C}\left(\frac{dC}{dT}\right)_V$ $X10^{-5}/K$	$\left(\frac{d\in_\infty}{dT}\right)_V$ $X10^{-4}/K$ Estimated (a)	$\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)_V$ $X10^{-5}/K$ Calculated
Li	LiF-LiCl	2.30	-1.58	-0.260	+0.420
	LiF-LiBr	2.55	-1.58	-0.490	+1.581
	LiCl-LiBr	2.95	-1.58	-0.870	+2.881
Na	NaF-NaCl	2.00	+1.52	+0.220	-0.680
	NaF-NaBr	2.15	+1.52	-0.015	+1.650
	NaF-NaI	2.40	+1.52	-0.280	+3.520
	NaCl-NaBr	2.45	+1.52	+0.085	+0.934
	NaCl-NaI	2.70	+1.52	-0.180	+2.579
	NaBr-NaI	2.85	+1.52	-0.415	+3.763
K	KF-KCl	2.00	+0.44	+0.080	-0.360
	KF-KBr	2.10	+0.44	+0.200	-1.378
	KF-KI	2.25	+0.44	+0.455	-3.200
	KCl-KBr	2.30	+0.44	+0.110	-0.406
	KCl-KI	2.45	+0.44	+0.365	-2.077
	KBr-KI	2.55	+0.44	+0.485	-2.689
Rb	RbF-RbCl	2.05	+1.59	+0.275	-1.029
	RbF-RbBr	2.15	+1.59	+0.400	-1.888
	RbF-RbI	2.30	+1.59	+0.450	-1.871
	RbCl-RbBr	2.30	+1.59	+0.495	-2.218
	RbCl-RbI	2.45	+1.59	+0.545	-2.169
	RbBr-RbI	2.55	+1.59	+0.670	-2.732

(a) Obtained for 50%-50% mixtures of compounds from measured values of individuals (A.O. Fernandez and K.K.Sarkar, 1991)

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Table – 3 : Calculated value of $\left(\frac{d \in_\infty}{dT}\right)$ at constant pressure for mixed binary crystals of II-VI and III-V families

Family	Crystals 50%-50%	K (a)	$\in_\infty$	$\frac{1}{C}\left(\frac{dC}{dT}\right)_P$ $X10^{-5}/K$	$\frac{1}{E_g}\left(\frac{dE_g}{dT}\right)_P$ $X10^{-5}/K$ (b)	$\left(\frac{d \in_\infty}{dT}\right)_P$ $X10^{-4}/K$
II-VI	ZnS-ZnSe	-1.000	5.55	2.012	-6.639	+3.936
	ZnS-ZnTe		6.25	2.012	-8.250	+5.387
	ZnSe-ZnTe		6.60	2.012	-8.716	+6.008
III-V	GaP-InP	-0.6552	9.05	4.389	-6.987	+7.200
	GaAs – InAs		11.60	7.693	-7.536	+13.362
	GaSb-InSb		15.05	11.726	-8.743	+24.484

(a) Singh R.P. et al. (1986)

(b) Obtained for 50% - 50% mixtures of compounds from measured values of individuals (Tsay Y.F. et al., 1973 and Sarkar K.K. et. al., 1980)

ANALYSIS OF THE RESULT

The average energy gap between bonding and antibonding states, calculated through quantum ion dependent dielectric model for mixed solids, are used in finding out photo conducting properties, Which lead to predict photo current per photon. It is found by us that at very low temperatures, some of the mixed crystals are highly photo conducting in a very small range of wave lengths, but the study is in an inconclusive stage at present.

The variation in the average energy gap with temperature plays and important role in the fields of fabrication of many components in semiconductor electronics.

The temperature derivative of electronic dielectric constant at constant volumes are used to estimate the magnitudes of anharmonic contribution to different optical properties.

The temperature dependent studies of dielectric constant and average energy gap separate out the insulators and semiconductors in mixtures of complex cross compounds.

The efficiency of solar cells widely depends upon the average energy gaps of parent fabricating material. By application of temperature, one can vary the average energy gap of any special mixed crystal pair so as to prepare a material for best efficient solar cell.

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