TEMPERATURE VARIATION OF AVERAGE ENERGY GAP OF III-V GROUP SEMICONDUCTORS

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Abstract:

In this research paper we have proposed a theory to study the effect of heat on the average energy gap of ionic solid families of type A^NB^{8-N} like I-VII,II-VI and III-V family . A generalized formulation has been developed using ion dependent dielectric theory to establish a correlation between average energy gap (Eg) and refractive index (n). On varying the temperature, the dielectric and optical refractive properties of the solids change. We shall therefore modify the formulation for ionic crystals to give proper predictions for the temperature variation of E_g and n.The calculated values of temperature derivatives of average energy gaps, both at constant pressure and constant volume, are found in good agreement with the values estimated. The thermal treatment of solids can vary the average energy gaps (E_g) to any appreciable extent. The semiconducting crystals of III-V family are highly inconclusive and we have not yet been able to seek for any comparison. The predicted values of temperature dependence of the average energy gaps may have a wide range of applications in various industrial and technological applications like photo conducting properties of crystals and solar cell technology etc.

Key Words: Ion dependent, optical dielectric constant, mixed binaries, Average energy gap, photo conducting properties etc.

Introduction:

We intend to put forward a theory to study the effect of heat on the average energy gap of ionic solid family of type A^NB^{8-N}. On varying the temperature the dielectric and optical refractive properties of the solids change .The theory can yield improvements in them. Among many application there are optical semiconducting and photo conducting properties of crystals and solar cell technology. These properties depend widely upon the average energy

gaps (E_g) between bonding and anti bonding states in the crystals .Thus studies of the effects of temperature variations of E_g will be an integral part of the present study.

We will use our formulation of ion dependent correlation between the electronic dielectric constant (ϵ_∞) and average energy gap (E_g). This correlation has found its validity to all ionic and covalent solids, simultaneously. The proposed correlation refer to two parameters, the behavior of which follow anion dependence in covalent solids and cation dependence in ionic crystals. It is also noticed that the temperature variation of the average energy gaps (E_g) for covalent semiconductor vary with optical refractive index. We shall therefore modify the formulation for ionic crystals. Finally we will try to give proper predictions for the temperature variation of E_g and ϵ_∞.

Theory:

To study the temperature variation of optical refractive index for ionic crystals under consideration, we will use our well established ion dependent correlation between optical refractive index and average energy gap .This gives a formulation

$$\epsilon_\infty = 1 + CE_g^p \quad \ldots\ldots\ldots\ldots\ldots(1)$$

Here the parameter p is a family characteristic, said to be different for different simple binary families, such as I-VII, II-VI and III-V family. The other parameter C is a characteristic of cation constant in ionic solids and anion constant in covalent ones.

Differentiating equation (1) with respect to temperature at constant pressure and volume, we get,

$$\left(\frac{d\epsilon_\infty}{dT}\right)_P = (\epsilon_\infty - 1)\left[\frac{P}{E_g}\left(\frac{dE_g}{dT}\right)_P + \frac{1}{C}\left(\frac{dc}{dT}\right)_P\right] \quad \ldots\ldots\ldots\ldots\ldots(2)$$

All terms in this equation are represented with unit per Kelvin and while deriving this correlation, the effect of core-d electron is neglected. In fact the presence of core-d electron affects the number of free electron per atom, which subsequently changes the plasma frequency by small amount (4). It is also noticed that ion characteristic C varies a little from one ionic solid to another with the same cation due to variation in the plasma frequency of the crystals.

$$\left(\frac{d\epsilon_\infty}{dT}\right)_v = (\epsilon_\infty - 1)\left[\frac{P}{E_g}\left(\frac{dE_g}{dT}\right)_v + \frac{1}{C}\left(\frac{dc}{dT}\right)_v\right] \quad \ldots\ldots\ldots\ldots\ldots..(3)$$

The direct temperature derivation of electronic dielectric constant $(d \in_\infty/dT)$ are experimentally measured for almost all binary solids quite conclusively, both for constant pressure and volume (Lowndes and Martin, 1969), we can estimate the experimental values of $\frac{d\in_\infty}{dT}$ for all concerned mixtures in different families through our usual method as

$$\frac{d\in_\infty}{dT} = \lambda_1 \left(\frac{d\in_\infty}{dT}\right)_1 + \lambda_2 \left(\frac{d\in_\infty}{dT}\right)_2 \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

We have enlisted these experimental values of $d \in_\infty/dT$ in different mixing proportions and different families. We expect the value of the derivation of C in equation (2) and (3), i.e. $\frac{1}{c}(dc/dT)$ to remain constant for same cation mixtures in ionic solids and same anion mixtures in covalent solids in each particular mixing proportions. Fernandez and Sarkar (1991) have found the values of $\frac{1}{c}(dc/dT)$ for each cation in ionic solids and each anion in covalent ones. Since its value for a particular ion in individual solids is constant, it remains the same constant in the same ion mixtures too whatsoever the mixing proportions. Quite a few individual binary solids have been subjected to experimental measurement for their temperature derivatives of (E_g) i.e. $\left(\frac{1}{Eg}\right)\left(\frac{dEg}{dT}\right)$ for all concerned proportion. These values; named as 'estimated experimental values'.

Observations:

(A) **Calculated values of $\frac{1}{Eg}\left(\frac{dEg}{dT}\right)$** **Mixing proportion 10% - 90%**

P = -0.770

Mixtures	$(\in_\infty - 1)$	$\left(\frac{d\in_\infty}{dT}\right)_P$ **x $10^{-4}/K$** **Experimental Values**	$\frac{1}{C}\left(\frac{dC}{dT}\right)_P$ **x $10^{-5}/K$**	$\frac{1}{Eg}\left(\frac{dEg}{dT}\right)_P$ **x $10^{-5}/K$** **Present Computation**
GaP – InP	8.49	7.982	4.389	-6.509
InP – GaP	7.61	6.478	4.389	-5.355
GaAs – InAs	11.16	14.081	7.693	-6.390
InAs – GaAs	10.04	12.649	7.693	-6.378

GaSb – InSb	14.57	25.150	11.726	-7.188
GaSb - InSb	18.53	23.790	11.726	-7.606

(B) Calculated values of $\frac{1}{Eg}\left(\frac{dEg}{dT}\right)$ Mixing proportion 20% - 80%

P = -0.678

Mixtures	$(\in_\infty - 1)$	$\left(\frac{d \in_\infty}{dT}\right)_P x\ 10^{-4}/K$ **Experimental Values**	$\frac{1}{C}\left(\frac{dC}{dT}\right)_P x\ 10^{-5}/K$	$\frac{1}{Eg}\left(\frac{dEg}{dT}\right)_P x\ 10^{-5}/K$ **Present Computation**
GaP – InP	8.38	7.794	4.389	-7.244
InP – GaP	7.72	6.666	4.389	-6.262
GaAs – InAs	11.02	13.902	7.693	-7.259
InAs – GaAs	10.18	12.828	7.693	-7.318
GaSb – InSb	14.39	24.980	11.726	-8.220
GaSb - InSb	13.66	23.960	11.726	-8.575

(C) Family III-V p = 0.611 Mixing proportion 30% - 70%

Mixtures	$(\in_\infty - 1)$	$\left(\frac{d \in_\infty}{dT}\right)_P x\ 10^{-4}/K$ **Experimental**	$\frac{1}{C}\left(\frac{dC}{dT}\right)_P x\ 10^{-5}/K$	$\frac{1}{Eg}\left(\frac{dEg}{dT}\right)_P x\ 10^{-5}/K$ **Present Computation**
GaP – InP	8.27	7.606	4.389	7.869
InP – GaP	7.83	6.854	4.389	7.143
GaAs – InAs	10.88	13.723	7.693	8.052
InAs – GaAs	10.32	13.007	7.693	8.037
GaSb – InSb	14.31	24.810	11.726	9.184
GaSb - InSb	13.79	24.130	11.726	9.447

(D) Calculated values of $\frac{1}{Eg}\left(\frac{dEg}{dT}\right)$ Mixing proportion 40% - 60%

P = I0.678

Mixtures	$(\in_\infty - 1)$	$\left(\frac{d \in_\infty}{dT}\right)_P x\ 10^{-4}/K$ Experimental	$\frac{1}{C}\left(\frac{dC}{dT}\right)_P x\ 10^{-5}/K$	$\frac{1}{Eg}\left(\frac{dEg}{dT}\right)_P x\ 10^{-5}/K$ Present Computation
GaP – InP	8.16	7.418	4.389	6.934
InP – GaP	7.94	7.042	4.389	6.607
GaAs – InAs	10.74	13.544	7.693	7.253
InAs – GaAs	10.46	13.186	7.693	7.246
GaSb – InSb	14.18	24.640	11.726	8.334
GaSb - InSb	13.92	24.300	11.726	8.452

(E) Calculated values of $\frac{1}{Eg}\left(\frac{dEg}{dT}\right)$ Mixing proportion 50% - 50%

P = -0.477

Mixtures	$(\in_\infty - 1)$	$\left(\frac{d \in_\infty}{dT}\right)_P x\ 10^{-4}/K$ Experimental Values	$\frac{1}{C}\left(\frac{dC}{dT}\right)_P x\ 10^{-5}/K$	$\frac{1}{Eg}\left(\frac{dEg}{dT}\right)_P x\ 10^{-5}/K$ Present Computation
GaP – InP	8.16	7.200	4.389	-9.549
GaAs – InAs	10.74	13.362	7.693	-10.990
GaSb - InSb	14.05	24.484	4.726	-12.752

Analysis:

The calculated values of $\left(\frac{1}{E_g}\right)\left(\frac{dE_g}{dT}\right)_{p,v}$ by our ion dependent theory using equation (2) and (3) are given in above tables along with available experimental values of the derivatives of average energy gap (E_g) and high frequency dielectric constant ($\in_\infty$). The calculated the values of $\frac{1}{C}(dc/dT)$ at constant pressure and volume are also shown in tables. The calculated

values of temperature derivatives of average energy gaps, both at constant pressure and constant volume, are found in good agreement with the values estimated for III-V semiconductor which are highly inconclusive and we have not yet been able to seek for any comparison. The predicted values of temperature dependences of the average energy gaps (E_g) may have a wide range of applications. Since the optical refractive index (n) is related to high frequency dielectric constant $\in_\infty$, $(n^2 = \in_\infty)$, we can obtain any required amounts of variations in (n) by the application of heat. This can evolve some exciting new properties in the fields of photo-elasticity and photoconductivity. The thermal treatments of solids can vary the average energy gaps (E_g) to any appreciable extent. Some other applications of interest in this field are semiconductor electronics and high power laser technology etc.

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