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ION DEPENDENT ELECTRONIC DIELECTRIC THEORY FOR STRAIN POLARISABILITY FOR MIXED BINARY CRYSTALS

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Abstract

According to ion dependent electronic dielectric theory the effect of application of hydrostatic pressure on the mixed binary crystals, gives the relations for the volume derivative of electronic dielectric constants for mixed binary crystals. By the using of these derivatives the strain polarisabilities are derived for mixed binary crystals. The calculated values of the volume derivatives are compared with the works of some other physicists.

Key words: volume derivatives, strain polarisability, Electronic dielectric theory.

INTRODUCTION

The volume and pressure dependences of optical dielectric constant of crystalline solids are the subjects of great interest in the last decade since they give variations in dielectric constant and refractive indices of materials. In the present paper we intend to put forward a theory to study the effect of hydrostatic pressure on the electrostatic dielectric properties of ionic and covalent A^NB^{8-N} types mixed binary crystals. Application of pressure on these crystals appreciably change their dielectric properties. It, therefore, renders term useful in a large number of ways such as the variations in photo conducting properties of crystals, high power laser beams and solar cell technology (Pitha 1972 and Bendow et al., 1974). These properties depend widely upon the average energy gaps (E_g) between bonding and anti-bonding states in the crystals. Many theories have come up for presenting dielectric behaviour of strained crystals in order to explain experimental results properly, but none of the theories so far have given very satisfactory agreement with the experimental results of pure crystals.

In this paper we will put forward a general quantum ion dependent model for the effect of hydrostatic pressure on the dielectric properties of mixed ionic and

covalent crystals. Since the application of hydrostatic pressure introduces a reverse change in the volume of crystals, we can consider volume parameters of a crystal instead of pressure ones. Thus, we will derive a formulation for the volume derivatives of dielectric properties for mixed crystals.

VOLUME DERIVATIVE OF ELECTRONIC DIELECTRIC CONSTANT ($\in_\infty$) AND STRAIN POLARISABILITY (λ) FOR MIXED BINARY CRYSTALS

In the simple binary solids as we move from rocksalt to Wurtzite and Zinc blende and finally to diamond structures, a gradual transition from high ionicity to high covalency takes place (Van Vechten, 1969). Ion dependent model shows that the dielectric behaviour has gradual change from high cation dependences to high anion dependences for crystals with high ionicity to high covalency (Sarkar et al. 1980).

In order to predict the volume derivatives of mixed binary crystals, we have used this well established ion dependent electronic dielectric theory. According to this theory the relation between $\frac{d \in_\infty}{dV}$ and $\left(\frac{dB'}{dV}\right)$ given as

$$V \frac{d \in_\infty}{dV} = (\in_\infty - 1)\left[\frac{S'}{3} + \frac{V}{B'}\left(\frac{dB'}{dV}\right)\right] \qquad \ldots(1)$$

Here $B' = CB^{(3/S-2)}$ and $S' = (2S - 3)$ are the ion and family characteristics respectively.

The electronic dielectric constant ($\in_\infty$) is related to the optical refractive index (n) as

$$\in_\infty = n^2 \qquad \ldots(2)$$

This leads to

$$V \frac{d \in_\infty}{dV} = V \frac{dn^2}{dV}$$

$$V \frac{d \in_\infty}{dV} = V.2n. \frac{dn}{dV}$$

Or

$$\frac{V}{2n} \cdot \frac{d \in_\infty}{dV} = V \frac{dn}{dV}$$

According to Lorentz-Lorentz relation

$$V\left(\frac{dn}{dV}\right) = \frac{-(n^2 - 1)(n^2 + 2)}{6n}(1 - \lambda)$$

Now substituting the value of $V\frac{dn}{dV}$, we get

$$\frac{1}{2n}V\frac{d\in_\infty}{dV}=-\frac{\left(n^2-1\right)\left(n^2+2\right)}{6n}\left(1-\lambda\right)$$

or

$$V\frac{d\in_\infty}{dV}=\frac{\left(n^2-1\right)(n^2+2)}{3}(1-\lambda)$$

So,

$$\lambda=1+\frac{3V\left(\frac{d\in_\infty}{dV}\right)}{\left(n^2-1\right)\left(n^2+2\right)} \qquad \ldots (3)$$

The particular family I – VII, which is highly ionic, shows the cation dependent dielectric behaviour and thus the value of $\frac{V}{B'}\left(\frac{dB'}{dV}\right)$ should remain constant in same cation solids. Similarly III-V family, which is highly covalent in nature, shows anion dependent dielectric behaviour and thus the value of $\frac{V}{B'}\left(\frac{dB'}{dV}\right)$ should remain constant in same anon solids. Thus, the value of $V\left(\frac{d\in_\infty}{dV}\right)$ can be estimated from equation (1) and using that the value of strain polarisability (λ) can be calculated from equation (3).

COMPUTATIONS FOR VOLUME DERIVATIVE OF ELECTRONIC DIELECTRIC CONSTANT ($\in_\infty$) AND STRAIN POLARISABILITY (λ) FOR MIXED BINARY CRYSTALS

For input data we have the experimental values of $\in_\infty$ and R. Through ion dependent formulation we find the values of S' and B' and $\frac{V}{B'}\left(\frac{dB'}{dV}\right)$.

Here we form mixture of same cation I-VII solids in 50%-50% proportion. The values of $\in_\infty$ (and hence n) are calculated and we use equation (1) and (3) to calculate the values of $V\left(\frac{d\in_\infty}{dV}\right)$ and λ respectively. The calculated values are reported in table (1).

In a similar manner we can predict the volume derivative of $\in_\infty$and strain polarisability constant (λ) for mixed binary crystals in III-V family. Since III-V family shows purely anion dependent dielectric behaviour due to a large covalent contribution, same anion solids are taken in the mixture. The calculated values of mixed binary crystals of same anion N, P, As and Sb in III-V family are reported in table (2).

Table – 1: Calculated values of volume derivative of electronic dielectric constant ($\in_\infty$) and strain polarisability (λ) for I-VII mixed binary crystals (S' = 3.00)

Cations	Crystals 50%-50%	$\in_\infty$	Refractive index (n)	$\left(\frac{V}{B'}\right)\left(\frac{dB'}{dV}\right)$	Values of $V\left(\frac{d \in_\infty}{dV}\right)$ calculated from ion dependent model	λ from present theory
Li	LiF-LiCl	2.30	1.52	-1.406	-0.5278	0.719
	LiF-LiBr	2.55	1.60	-1.406	-0.6293	0.735
	LiF-LiI	2.85	1.69	-1.406	-0.7511	0.750
	LiCl-LiBr	2.95	1.72	-1.406	-0.7917	0.755
	LiCl-LiI	3.25	1.80	-1.406	-0.9135	0.766
	LiBr-LiI	3.50	1.87	-1.406	-1.0150	0.778
Na	NaF-NaCl	2.00	1.41	-1.690	-0.6900	0.482
	NaF-NaBr	2.15	1.47	-1.690	-0.7935	0.501
	NaF-NaI	2.40	1.55	-1.690	-0.9660	0.529
	NaCl-NaBr	2.45	1.56	-1.690	-1.0005	0.535
	NaCl-NaI	2.70	1.64	-1.690	-1.1730	0.559
	NaBr-NaI	2.85	1.69	-1.690	-1.2765	0.573
K	KF-KCl	2.00	1.41	-1.640	-0.6400	0.520
	KF-KBr	2.10	1.45	-1.640	-0.7040	0.532
	KF-KI	2.25	1.50	-1.640	-0.8000	0.548
	KCl-KBr	2.30	1.52	-1.640	-0.8320	0.553
	KCl-KI	2.45	1.56	-1.640	-0.9280	0.568
	KBr-KI	2.55	1.60	-1.640	-0.9920	0.578
Rb	RbF-RbCl	2.05	1.43	-1.620	-0.6510	0.541
	RbF-RbBr	2.15	1.47	-1.620	-0.7130	0.552
	RbF-RbI	2.30	1.52	-1.620	-0.8060	0.567
	RbCl-RbBr	2.30	1.52	-1.620	-0.8060	0.567
	RbCl-RbI	2.45	1.56	-1.620	-0.8990	0.582
	RbBr-RbI	2.55	1.60	-1.620	-0.9610	0.591

Table – 2: Calculated values of volume derivative of electronic dielectric constant ($\in_\infty$) and strain polarisability (λ) for III-V mixed binary crystals (S' = 1.45)

Anions	Crystals 50%-50%	$\in_\infty$	Refractive index (n)	$\left(\frac{V}{B'}\right)\left(\frac{dB'}{dV}\right)$	Values of $V\left(\frac{d \in_\infty}{dV}\right)$ calculated from ion dependent model	λ from present theory
N	AlN-GaN	4.90	2.213	0.4795	3.755	1.419
	AlN-InN	5.15	2.269	0.4795	3.996	1.404
	GAN-InN	5.25	2.291	0.4795	4.092	1.398
P	AlP – GaP	8.50	2.915	0.6069	8.176	1.312
	AlP – InP	9.05	3.008	0.6069	8.776	1.296
	GaP – InP	9.05	3.008	0.6069	8.776	1.296
As	AlAs-GaAs	10.55	3.248	1.396	17.947	1.450
	AlAs-InAs	11.25	3.354	1.396	19.263	1.425
	GaAs-InAs	11.60	3.406	1.396	19.920	1.414
Sb	AlSb-GaSb	12.30	3.507	1.386	21.123	1.392
	AlSb-InSb	12.95	3.599	1.386	22.338	1.375
	GaSb-InSb	15.05	3.879	1.386	26.264	1.329

ANALYSIS OF THE RESULT

The predicted values of the volume derivative of high frequency dielectric constant may have a vast range of applications. Since the optical refractive index (n) is directly related to $\in_\infty$ as $n^2 = \in_\infty$, we can get any desired amount of variations in the refractive index by applying different amounts of strains on the mixed crystals. This may lead to an exciting revolution in the field of photoelectricity and photo conductivity. The other fields of interest are of semiconductor electronics and high power laser technology as well as the solar cell technology.

A single crystal can be used in many ways by using its strained characteristics. By varying different gaps and thus E_g and $\in_\infty$, a require form of semiconductor can be obtained. At different pressure, a single semiconductor can be used with varying photoelastic and photo conducting properties.

There is a considerable variation in the energy levels of various conduction and valence bands with changes in pressure. This can induce the shift in energy gaps. Thus, hydrostatic pressure may change the behaviour of one semiconductor into that of

another. Likewise strain derivatives of optical dielectric constant are also useful to get required resonance frequency of the compounds. The change is refractive index may be useful in many different fields of linear and non-linear optics.

By using pressure and volume derivatives of dielectric constant, the volume dependence of energy gap and electronegativity parameters can be easily estimated. Volume dependent study of refractive index directly leads to frequency dependence of photoelastic constants.

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