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Volume Derivatives of the Electronic Dielectric Constants for Mixtures of I-VII Rocksalt Binary Crystals

Dr. Yogesh Kumar Vashistha
Lecturer in Physics
M.A.J. Govt. (P.G.) College, Deeg (Bharatpur)Rajasthan, India

Abstract

Ion dependent dielectric theory is proposed to the effect of hydrostatic pressure on the mixed crystals. This theory gives the relations for the volume derivative of the electronic dielectric constants for mixed binary crystals. The application of pressure on these crystals gives the variation of the photoelastic and photoconducting properties of the crystals by which the volume dependence of energy gap and electronegativity parameters can be easily estimated.

Key words: Volume derivatives, Electronic dielectric constant, Mixed Crystals.

1. Introduction

The volume and pressure dependences of electronic dielectric constant of crystalline solids are the subjects of great interest in the last few decades. In the present paper we intend to put forward a theory to study the effect of hydrostatic pressure on the dielectric properties of ionic mixture of I-VII 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 photoconducting properties of crystals and high power laser beams and solar cell technology. These properties depend widely upon the average energy gaps (Eg) between bonding and antibonding states in the crystals.[1-4]

In this paper we will put forward a general quantum ion dependent theory for the effect of hydrostatic pressure on the dielectric properties of mixed ionic crystals. Since the application of hydrostatic pressure introduces a reverse change in the volume of crystals, we can consider volume parameters of a crystals instead of pressure ones. Thus, we will derive a formulation for the volume derivatives of dielectric constant for mixed crystals.

2. Computation for volume derivative of electronic dielectric constants

In order to predict the volume derivative of the dielectric properties of I-VII rocksalt structured solids, we make use of a well established ion dependent electronic dielectric theory. It has been established that the dielectric behaviour of binary families with high ionicity is cation dependent while that with high covalancy is anion dependent. According to quantum ion dependent theory the relation between electronic dielectric constant ($\in_\infty$) and interionic separation (R) is given as[5-9]

$$\in_\infty = 1 + BR^S \qquad \ldots (1)$$

Where B is a characteristic constant of a particular cation and S is a family characteristic constant.

The volume of a unit cell is given by

$$V = \frac{1}{2} KR^3 \qquad \ldots (2)$$

Where K is a structural constant.

Now on differentiating equation (2), we get

$$\frac{dV}{dR} = \frac{3}{2} KR^2 = \frac{3V}{R} \qquad \ldots (3)$$

On application of hydrostatic pressure the interionic separation (R) changes, thereby varying the volume (V) of a crystal. Hence, now on differentiating equation (1) with respect to V, we get

$$\frac{d \in_\infty}{dV} = S\, BR^{S-1} \left(\frac{dR}{dV}\right) + R^S \left(\frac{dB}{dV}\right) \qquad \ldots (4)$$

Now substituting the value of $\left(\frac{dR}{dV}\right)$ from equation (3) in equation (4), we get

$$V\left(\frac{d \in_\infty}{dV}\right) = (\in_\infty - 1)\left[\frac{S}{3} + \frac{V}{B}\left(\frac{dB}{dV}\right)\right] \qquad \ldots (5)$$

Equation (5) shows that all the terms are dimensionless. The family characteristic constant(s) have different value for different families. The value of this constant(s) for I-VII binary family is 3.00. The value of $\frac{V}{B}\left(\frac{dB}{dV}\right)$ will be constant for same cation in I-VII family. The value of $\frac{V}{B}\left(\frac{dB}{dV}\right)$ are calculated to put the measured values of $V\left(\frac{d \in_\infty}{dV}\right)$ for the cation Li, Na, K and Rb [10].

Now, on putting the values of $\frac{V}{B}\left(\frac{dB}{dV}\right)$ in equation (5), we can calculate the value of volume derivative of $\in_\infty$ for all the cations of I-VII family. These calculated values are reported in table 1 to 4.

Table – 1

Cation	LiF-LiCl %LiCl	$\in_\infty$	$\frac{V}{B}\left(\frac{dB}{dV}\right)$	$V\left(\frac{d\in_\infty}{dV}\right)$
Li	0	1.85	- 1.406	- 0.3451
	20	2.04	- 1.406	- 0.4222
	40	2.23	- 1.406	- 0.4994
	60	2.41	- 1.406	- 0.5725
	80	2.60	- 1.406	- 0.6496
	100	2.78	- 1.406	- 0.7227

Table – 2

Cation	NaCl-NaBr % NaBr	$\in_\infty$	$\frac{V}{B}\left(\frac{dB}{dV}\right)$	$V\left(\frac{d\in_\infty}{dV}\right)$
Na	0	2.34	- 1.690	- 0.9246
	20	2.39	- 1.690	- 0.9591
	40	2.43	- 1.690	- 0.9867
	60	2.49	- 1.690	- 1.0281
	80	2.54	- 1.690	- 1.0626
	100	2.59	- 1.690	- 1.0971

Table – 3

Cation	KBr - KI % KI	$\in_\infty$	$\frac{V}{B}\left(\frac{dB}{dV}\right)$	$V\left(\frac{d\in_\infty}{dV}\right)$
K	0	2.36	- 1.640	- 0.8704
	20	2.43	- 1.640	- 0.9152
	40	2.49	- 1.640	- 0.9536
	60	2.55	- 1.640	- 0.9920
	80	2.60	- 1.640	- 1.0240
	100	2.67	- 1.640	- 1.0688

Table – 4

Cation	RbI- RbF % RbF	$\in_\infty$	$\frac{V}{B}\left(\frac{dB}{dV}\right)$	$V\left(\frac{d\in_\infty}{dV}\right)$
Rb	0	2.67	- 1.620	- 1.0354
	20	2.48	- 1.620	- 0.9176
	40	2.30	- 1.620	- 0.8060
	60	2.12	- 1.620	- 0.6944
	80	1.94	- 1.620	- 0.5828
	100	1.76	- 1.620	- 0.4712

3. Analysis of the Results

The predicted values of volume derivatives of electronic dielectric constant ($\in_\infty$) may have a vast range of application in the field of photoelectricity, photoconductivity and semiconductor electronics etc. By applying hydrostatic pressure on the solids, the interionic separation R varies. It decreasing on increasing the hydrostatic pressure. At different pressure, a single semiconductor can be used with varying photoelastic and photoconducting properties.

By using of hydrostatic pressure on mixed crystals may lead to photon emission from deformed semiconductors, which refers to the fact that the band gap of semiconductors increases the energy related to the photon emission during the increment in deformation.

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