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# QUANTAM ION DEPENDENT COMPUTATION FOR ELECTRONIC DIELECTRIC CONSTANTS OF MIXED CRYSTALS IN TETRAHEDRAL STRUCTURES

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## Abstract

Quantum Ion dependent theory for electronic dielectric constants of $A^NB^{8-N}$ binary solids has been extended to III-V crystals mixed in different proportions. The calculated values of electronic dielectric constants for mixed crystals, which are found to agree with experimental values. The results are also agree well with the well established Clausis-Mossotti relation. Thus, it gives a strong support to the validity of ion dependent formulation for mixed crystals.

**Key words:** Electronic Dielectric Constant ($\in_\infty$), Interionic Separation (R), Mixed Crystals

## INTRODUCTION

The dielectric properties of mixed binary crystals are found to be of great scientific and technological importance. Numerous 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 families Fancher and Barch (1969), J.R. Ferraro et al. (1971), Kamiyoshi and Nigara (1971), Rao and Babu (1980), U.C. Shrivastava (1980), Varotsos (1980), J. Shanker and G.D. Jain (1982, 1983), J. Shanker and S.C. Sharma (1986)). Covalent compounds are rarely touched and no generalized theory for all ionic and covalent families together has been prescribed.

For the study of dielectric behaviour, a number of classical models have been prescribed. However, the average energy gap is a quantum concept, hence a good number of quantum theories are also prescribed. Most satisfactory results are obtained through the quantum ion dependent model Sarkar and Goyal (1978, 1980), Goyal and Sarkar (1976), R.P. Singh et al. (1986) established in last few decades. The model says that the dielectric behaviour of ionic crystals and partial ionic-covalent solids (with

dominating ionic contribution) is completely cation dependent. The relation between $\in_\infty$ and the interionic separation R is suggested by Sarkar and Goyal (1980) as

$$\in_\infty = 1 + B\, R^S \qquad \ldots (1)$$

where B is a characteristic constant of a particular cation and S is a family characteristic constant. This ion dependent model is well appreciated in the review article of T.S. Moss (1985).

In the present paper we propose to mix the solids III-V families. Mixed solids in different proportions are taken up and their electronic dielectric constants are evaluated by using the ion dependent concept. We also develop a generalized inter-relationship between electronic dielectric constant ($\in_\infty$) and the inter atomic separation (R) of a number of mixed crystals in ionic, partial ionic-covalent and covalent families, when they are mixed in a definite proportions.

## THEORY AND METHOD OF CALCULATION

According to Clausius-Mossotti relation the static or electronic dielectic constant and the corresponding polarizability are related to each other as

$$\frac{\in -1}{\in +2} = \frac{4\pi}{3}.\frac{\alpha}{V} \qquad \ldots(2)$$

where $\alpha$ and V are the polarizability and volume per ion pair respectively. Here for the static dielectric constant, $\in$ is replaced by $\in_\infty$. Similarly $\alpha_0$ represents the static polarizability and the electronic polarizability is represented by $\alpha_\infty$. Hence, equation (2) reduced as

$$\frac{\in_\infty -1}{\in_\infty +2} = \frac{4\pi}{3}\frac{\alpha}{V} \qquad \ldots (3)$$

For electronic dielectric constant ($\in_\infty$) of mixed crystals, we consider Kamiyoshi and Nigara (1971) and Varotsos (1980) theory. According to above theory the polarisability of mixed crystal should be equal to the sum of polarisabilities of the pure crystals taken in the proportion of mixing ratio. Thus, electronic dielectric constant ($\in_\infty$) of the mixture should be given as

$$\frac{\in_\infty -1}{\in_\infty +2} = \lambda_X \left[\frac{(\in_\infty)_X -1}{(\in_\infty)_X +2}\right] + \lambda_Y \left[\frac{(\in_\infty)_Y -1}{(\in_\infty)_Y +2}\right] \qquad \ldots (4)$$

where $(\in_\infty)_X$ and $(\in_\infty)_Y$ are the electronic constants of pure crystal X and Y respectively. The interionic separation of the mixed crystal (R) should be found through the relation

$$R^3 = \lambda_X R_X^3 + \lambda_Y R_Y^3 \qquad \ldots(5)$$

where $R_X$ and $R_Y$ are the interionic separations of the pure crystals X and Y respectively. This formula is in accordance with the concept of volume mixing (U.V. Rao & V.H. Babu (1980) and P. Varotsos (1980)).

Thus, we calculate the values of $\in_\infty$ for different mixed crystals from equation (1) and the values of (R) obtained from equation (5). Hence the calculated values of $\in_\infty$ by using Quantum Ion Dependent theory are reported in table 1 to 3.

In order to check the validity of the result we call back the well established classical Clausius-Mossotti relation for electronic dielectic constants by equation (3) as

$$\frac{\in_\infty - 1}{\in_\infty + 2} = \frac{4\pi}{3} \cdot \frac{\alpha}{V}$$

Where $\in_\infty$ is the electronic dielectric constant for mixed crystal, $\alpha$ and V are their polarisability and volume per ion pair respectively.

**Table – 1**

| **BN-AIN % AIN** | **R** | $(\varepsilon_\infty)_a$ | $(\varepsilon_\infty)_b$ | $(\varepsilon_\infty)_{Exp.}$ |
|---|---|---|---|---|
| 0 | 1.45 | 3.59 | 4.49 | 4.5 |
| 10 | 1.50 | 3.72 | 4.52 | - |
| 20 | 1.55 | 3.86 | 4.55 | - |
| 30 | 1.60 | 3.99 | 4.58 | - |
| 40 | 1.64 | 4.10 | 4.61 | - |
| 50 | 1.68 | 4.21 | 4.64 | - |
| 60 | 1.72 | 4.32 | 4.68 | - |
| 70 | 1.76 | 4.44 | 4.71 | - |
| 80 | 1.79 | 4.53 | 4.74 | - |
| 90 | 1.83 | 4.63 | 4.77 | - |
| 100 | 1.86 | 4.72 | 4.80 | 4.8 |

**Table – 2**

| **AIP-InP % InP** | **R** | $(\varepsilon_\infty)_a$ | $(\varepsilon_\infty)_b$ | $(\varepsilon_\infty)_{Exp.}$ |
|---|---|---|---|---|
| 0 | 2.35 | 8.62 | 8.49 | 8.5 |
| 10 | 2.37 | 8.70 | 8.60 | - |
| 20 | 2.39 | 8.82 | 8.68 | - |
| 30 | 2.41 | 8.90 | 8.79 | - |

| | | | | |
|---|---|---|---|---|
| 40 | 2.43 | 8.99 | 8.91 | - |
| 50 | 2.45 | 9.10 | 8.99 | - |
| 60 | 2.47 | 9.19 | 9.11 | - |
| 70 | 2.48 | 9.23 | 9.23 | - |
| 80 | 2.51 | 9.39 | 9.36 | - |
| 90 | 2.52 | 9.43 | 9.45 | - |
| 100 | 2.54 | 9.52 | 9.58 | 9.6 |

**Table – 3**

| **GaAs-InAs % InAs** | **R** | **$(\varepsilon_\infty)_a$** | **$(\varepsilon_\infty)_b$** | **$(\varepsilon_\infty)_{Exp.}$** |
|---|---|---|---|---|
| 0 | 2.43 | 10.37 | 10.87 | 10.9 |
| 10 | 2.45 | 10.50 | 10.99 | - |
| 20 | 2.47 | 10.60 | 11.16 | - |
| 30 | 2.49 | 10.70 | 11.27 | - |
| 40 | 2.51 | 10.83 | 11.39 | - |
| 50 | 2.53 | 10.94 | 11.51 | - |
| 60 | 2.55 | 11.04 | 11.70 | - |
| 70 | 2.56 | 11.12 | 11.82 | - |
| 80 | 2.58 | 11.22 | 11.95 | - |
| 90 | 2.60 | 11.35 | 12.15 | - |
| 100 | 2.62 | 11.45 | 12.28 | 12.3 |

**ANALYSIS OF THE RESULT**

A comparison of $(\in_\infty)_a$ evaluated from quantum ion dependent formulation and $(\in_\infty)_b$ predicted from classical Kamiyoshi relation (extended from Clausius Mossotti theory), in the table (1) to (3), shows excellent agreement. Close matching of the results from two entirely different approaches proves the reliability of the values of electronic dielectic constants of mixed crystals in III-V binary family. Thus quantum ion dependent formulation can be used to predict the electronic dielectric constant of the mixed crystals in ionic I-VII solids as well as II-VI solids also, since the basic cation anion dependent theory covers all group of binary $A^N B^{8-N}$ family.

In the modern computerized world, the electronic industries are pioneering over any other technologcial and industrial fields. The products in electronic industries are obtained mainly from the materials in solid state, which cover the optical, photoelastic, photo conducting and many other properties along with their electronic applications. The solar cell technology is one of the topic of highest interest. All such devices and products

use many different kinds of solid state materials with different properties of varied interests.

Other kinds of quantum approaches for the development in the theory of mixed crystals have been considered, but only for pure ionic crystals (Manfred Bucher, 1993). Covalent semiconductors have not been touched at all till to date. The present approach through quantum ion dependent formulation can be well applied for covalent semi conductors also. In a wider arena, a huge range of values of $\in_\infty$can be obtained by mixing the crystals in different proportions, which can be used for many different purposes. Thus, one can derive proper crystal mixture for any definitely required refractivity in opto-electronic system. The prescribed theory can therefore be used to form different mixed crystals with particular values of required in any specific opto-electronic devices.

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