Ion Dependent Computation for Electronic Dielectric Constants of Mixed Crystals in Rocksalt and Zinc blende Structures

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Abstract

Quantum ion dependent theory for electronic dielectric constants of $A^N B^{8-N}$ binary solids has been extended to the II-VI crystals mixed in different proportions. The values of optical dielectric constants (ε_∞) are evaluated for a number of mixed crystals, which are found to agree with available experimental values. The results agree well with the predictions from well established Clausius-Mossotti relation also. Thus, it gives a strong support to the validity of ion dependent formulation for mixed crystals.

Key words: *Electronic Dielectric Constant (ε_∞), Interionic Separation (R), Mixed Crystals*

Introduction

The electronic dielectric behaviour of binary crystals remained a topic of great interest in last few decades as it is a subject of great experimental importance in electronic industry. The varied values of optical dielectric constants (ε_∞) and average energy gaps (E_g) of ionic and covalent crystals have helped in developing many components for photo elastic, photo conducting and solar cell devices. 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[1 to 5] established in last two 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 ε_∞ and the interionic separation R is suggested as[1]

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

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 Moss[6].

In the present paper we propose to mix the solids of rocksalt and zinc blende structures, specially in partial ionic- covalent family II-VI. Mixed solids in different proportions are taken up and their electronic dielectric constants are evaluated by using the ion dependent concept.

Theory and Method of Calculation

Any two crystals X and Y with same cation in binary II-VI family are mixed in different proportion λ_x and λ_y respectively. The interionic separation of the mixed crystal (R) is found through the relation

$$R^3 = \lambda_x R_x^3 + \lambda_y R_y^3 \qquad (2)$$

where R_x and R_y are the interionic separations of the pure II-VI crystals X and Y respectively. This formula is in accordance with the concept of volume mixing[7, 8]. Calculated values of R for mixed crystals in different proportions are reported in tables 1 to 6. Since we are mixing two same cation solids, values of characteristic constants B and S for same cations are directly taken up from the tables, earlier predicted for pure II-VI family through ion dependent formulation[1]. Thus, by using the values of R obtained from eqn. (2), we predict the values of ε_∞ for different mixed crystals through eqn. (1). Tables 1 to 6 show the calculated values of ε_∞ through ion dependent calculations.

In order to check the validity of the results we call back the well established classical Clausius Mossotti relation for electronic dielectric constants

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

where α and V are the polarisability and volume per ion pair of the crystal respectively.

Kamiyoshi and Niagra[9] and Varotsos[10] considered the polarisability of mixed crystal to be equal to the sum of polarisabilities of the pure crystals taken in the proportion of mixing ratio. Thus eqn. (3) in modified[11] as

$$\frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 2} = \lambda_x \left[\frac{(\varepsilon_\infty)_x - 1}{(\varepsilon_\infty)_x + 2}\right] + \lambda_y \left[\frac{(\varepsilon_\infty)_y - 1}{(\varepsilon_\infty)_y + 2}\right] \qquad (4)$$

using experimental values of $(\varepsilon_\infty)_x$ and $(\varepsilon_\infty)_y$ for pure II-VI crystals[1], ε_∞ for mixed crystals are evaluated from eqn (4). These values are also reported in table 1 to 6 for comparison.

Table – 1 : Rocksalt Structure

MgS – MgSe (% MgSe)	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$	$(\varepsilon_\infty)_{Exp.}$
0	2.60	5.09	5.09	**5.1**
10	2.61	5.16	5.16	-
20	2.63	5.22	5.25	-
30	2.64	5.29	5.32	-
40	2.65	5.35	5.38	-
50	2.67	5.42	5.46	-
60	2.68	5.48	5.56	-
70	2.69	5.54	5.63	-
80	2.70	5.61	5.71	-
90	2.72	5.67	5.79	-
100	**2.73**	**5.74**	**5.89**	**5.9**

Table – 2 : Rocksalt Structure

CaO – CaS (%CaS)	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$	$(\varepsilon_\infty)_{Exp.}$
0	2.40	3.21	3.30	**3.3**
10	2.45	3.36	3.40	-
20	2.50	3.50	3.50	-
30	2.55	3.65	3.61	-
40	2.59	3.79	3.71	-
50	2.64	3.94	3.84	-
60	2.68	4.08	3.96	-
70	2.72	4.23	4.08	-
80	2.76	4.37	4.21	-
90	2.80	4.52	4.35	-
100	**2.84**	**4.66**	**4.49**	**4.5**

Table – 3 : Rocksalt Structure

SrSe – SrTe (% SrTe)	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$	$(\varepsilon_\infty)_{Exp.}$
0	3.12	5.04	4.90	**4.9**
10	3.13	5.09	4.98	-
20	3.14	5.14	5.06	-
30	3.16	5.18	5.14	-
40	3.17	5.23	5.23	-
50	3.18	5.28	5.32	-
60	3.19	5.33	5.41	-
70	3.20	5.38	5.50	-
80	3.22	5.42	5.59	-
90	3.23	5.47	5.69	-
100	**3.24**	**5.52**	**5.79**	**5.8**

Table – 4 : Zinc blende Structure

BeS – MeSe (% BeSe)	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$	$(\varepsilon_\infty)_{Exp.}$
0	2.10	6.48	7.09	**7.1**
10	2.11	6.56	7.11	-
20	2.12	6.65	7.13	-
30	2.13	6.73	7.15	-
40	2.14	6.81	7.17	-
50	2.15	6.89	7.19	-
60	2.16	6.97	7.21	-
70	2.17	7.06	7.23	-
80	2.18	7.14	7.25	-
90	2.19	7.22	7.27	-
100	**2.20**	**7.30**	**7.29**	**7.3**

Table – 5 : Zinc blende Structure

ZnS – ZnSe (% ZnSe)	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$	$(\varepsilon_\infty)_{Exp.}$
0	2.36	5.38	5.19	**5.2**
10	2.37	5.43	5.26	-
20	2.38	5.48	5.32	-
30	2.39	5.53	5.39	-
40	2.40	5.58	5.46	-
50	2.40	5.64	5.53	-
60	2.41	5.69	5.60	-

70	2.42	5.74	5.67	-
80	2.43	5.79	5.74	-
90	2.44	5.85	5.82	-
100	**2.45**	**5.90**	**5.89**	**5.9**

Table – 6 : Zinc blende Structure

CdS – CdTe (% CdTe)	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$	$(\varepsilon_\infty)_{Exp.}$
0	2.52	5.53	5.19	**5.2**
10	2.55	5.68	5.35	-
20	2.58	5.84	5.52	-
30	2.60	5.99	5.70	-
40	2.63	6.15	5.88	-
50	2.66	6.30	6.07	-
60	2.68	6.46	6.28	-
70	2.71	6.61	6.49	-
80	2.73	6.77	6.72	-
90	2.75	6.92	6.95	-
100	**2.78**	**7.08**	**7.20**	**7.2**

Analysis of Results

A comparison of $(\varepsilon_\infty)_a$ evaluated from quantum ion dependent formulation and $(\varepsilon_\infty)_b$ predicted from classical Clausius Mossotti relation in tables 1 to 6 shows excellent agreement. Close matching of the results from two entirely different approaches proves the reliability of the values of electronic dielectric constants of mixed crystals in II-VI 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 covalent III-V semiconductors also, since the basic cation anion dependent theory covers all subsets of binary $A^N B^{8-N}$ family[1].

Other kinds of quantum approaches for the developments in the theory of mixed crystals have been considered, but only for pure ionic crystals[12]. 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 semiconductors also. In a wider arena, a huge range of values of ε_∞ can be obtained by mixing the crystals in different proportions, which can be used for many different purposes. The electronic dielectric constant has a direct bearing on the optical refractive index (n) as

$$\varepsilon_\infty = n^2 \qquad (5)$$

Thus one can derive proper crystal mixture for any definitely required refractivity in opto-electronic systems.

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