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Ion Dependent Computation for Electronic Dielectric Constants of Mixed Ionic Crystals

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Abstract

An ion dependent dielectric model is developed for mixed binary crystals. The interionic separation (R) and electronic dielectric constant ($\in_\infty$) of the mixed ionic crystals are computed from the measured values of R and $\in_\infty$ of pure crystals. The values of Electronic dielectric constants ($\in_\infty$) are evaluated for mixed ionic crystals. The results are agree well with the well established Clausius-Mossotti relation also. Thus its gives a strong support to the validity of Ion dependent theory.

Key words: Electronic dielectric constant ($\in_\infty$), interionic separation (R), Mixed Crystals.

1. Introduction

The dielectric properties of mixed binary crystals in both ionic and covalent families are found to be of great scientific and technological importance in electronic Industries. For the study of dielectric behaviour, a number of classical models have been prescribed. Most satisfactory results are obtained through the quantum ion dependent model.[1 to 5]

The model says that the dielectric behaviour of ionic crystals is completely cation dependent. The relation between $\in_\infty$ and R is suggested as [1]

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

Where B is a characteristics 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. [6]

In the present paper we propose to mix the ionic crystals of I-VII family. Mixed crystals in different proportions are taken up and their electronic dielectric constants ($\in_\infty$) and interionic separation (R) are evaluated by using the ion dependent concept.

2. Method of Calculation

Any two crystals A and B with same cation in ionic binary family are mixed in different proportion λ_A and λ_B respectively. The interionic separation of the mixed crystal (R) should be found through the relation

$$R^3 = \lambda_A R_A^3 + \lambda_B R_B^3 \qquad \ldots (2)$$

where R_A and R_B are the interionic separations of the pure crystals A and B respectively. This formula is a accordance with the concept of volume mixing.[7, 8]

According to well established classical Clausius-Mossotti relation for electronic dielectric constants

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

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

For electronic dielectric constant ($\in_\infty$) of mixed crystals, we consider Kamiyoshi and Nigara[9] and Varotsos[10] 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 by equation (3) in modified[11] as

$$\frac{\in_\infty -1}{\in_\infty +2} = \lambda_A \left[\frac{(\in_\infty)_A -1}{(\in_\infty)_A +2}\right] + \lambda_B \left[\frac{(\in_\infty)_B -1}{(\in_\infty)_B +2}\right] \qquad \ldots (4)$$

where $(\in_\infty)_A$ and $(\in_\infty)_B$ are the electronic dielectric constants of pure crystals A and B respectively.

By using equation (2) and (4) we may, thus, find the values of interionic separation (R) and electronic dielectric constant ($\in_\infty$) of the binary crystal mixtures made in different proportions. The calculated values of $\in_\infty$ and R are reported in table 1 to 4 for comparison.

Table – 1

LiF – LiCl % LiCl	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$
0	2.01	1.85	1.90
10	2.08	1.94	1.97
20	2.15	2.04	2.04
30	2.21	2.13	2.11
40	2.27	2.23	2.19
50	2.32	2.31	2.26
60	2.38	2.41	2.34
70	2.43	2.51	2.42
80	2.48	2.60	2.52
90	2.52	2.68	2.61
100	2.57	2.78	2.70

Table – 2

NaCl – NaBr % NaBr	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$
0	2.82	2.34	2.30
10	2.84	2.37	2.33
20	2.85	2.39	2.36
30	2.87	2.42	2.38
40	2.88	2.43	2.41
50	2.90	2.46	2.44
60	2.92	2.49	2.48
70	2.93	2.51	2.51
80	2.95	2.54	2.54
90	2.96	2.56	2.57
100	2.98	2.59	2.60

Table – 3

KBr– KI % KI	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$
0	3.30	2.36	2.40
10	3.33	2.40	2.42
20	3.35	2.43	2.46
30	3.37	2.45	2.48
40	3.40	2.49	2.52
50	3.42	2.52	2.54
60	3.44	2.55	2.57
70	3.46	2.57	2.61
80	3.48	2.60	2.64
90	3.51	2.64	2.67
100	3.53	2.67	2.70

Table – 4

RbI – RbF % RbF	R	$(\varepsilon_\infty)_a$	$(\varepsilon_\infty)_b$
0	3.66	2.67	2.70
10	3.59	2.57	2.61
20	3.52	2.48	2.52
30	3.45	2.40	2.43
40	3.37	2.30	2.35
50	3.30	2.22	2.26
60	3.21	2.12	2.19
70	3.12	2.03	2.11
80	3.03	1.94	2.04
90	2.92	1.85	1.97
100	2.82	1.76	1.90

3. Analysis of the Results

A comparison of $(\in_\infty)_a$ evaluated from quantum ion dependent formulation and $(\in_\infty)_b$ predicted from classical Clausius Mossotti relation shows excellent agreement in table 1 to 4. Close matching of the results from two entirely different approaches proves the reliability of the values of electronic dielectic constants of mixed ionic crystals in I-VII

binary family. Thus quantum ion dependent formulation can be used to predict the electronic dielectric constant of the mixed crystals of II-VI and III-V family also.

Other kinds of quantum approaches for the developments in the theory of mixed crystals have been considered, but only for pure ionic crystals.[12]

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