

QUANTUM ION DEPENDENT THEORY FOR TEMPERATURE VARIATION OF REFRACTIVE INDICES FOR MIXED BINARY CRYSTALS

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Abstract

The quantum Ion dependent theory for the mixtures of ionic and covalent crystals, firmly established in the present paper have given us a way to predict definite expressions for temperature variation of refractive index (n). These variation effect will lead to many exciting properties in the field of photo elasticity photo conductivity and solar cell technology etc.

Key words: Refractive Index (n), Ionic and Covalent Crystals, Temperature dependence.

Introduction

The temperature variation of refractive index (n) at constant pressure and constant volume of mixed binary crystals have been a subject of great interest in the field of electronic world.

In the most recent proposal, Ravindra et al. (1981) calculated the temperature derivatives of refractive indices and compared them with the measured values of (dn/dt) and with those of Moss for Si, Ge and III-V solids. Both these predictions by Ravindra and Moss gave errors by 1.5 : 1 but for indium compounds the errors are of the order of 3 : 1. The calculated values from Moss equation are quite over estimated than observed values. In case of PbS the experimental value of dn/dT is equal to -6×10^{-4} per K while Moss and Ravindra's predictions give -9.8×10^{-4} per K and -2.3×10^{-4} per K respectively which are both not in good agreement. Thus, the validity of Moss and Ravindra's proposals are quite inadequate for all simple and binary complex families.

Thus, in the next section, we will use our own quantum ion dependent dielectric theory to formulate the temperature dependences, which should be applicable to all ionic, covalent and complex binary families simultaneously.

Calculations for Temperature variation of Refractive Indices for Mixed Binary Crystals

To study the temperature variation of refractive indices for I-VII, II-VI and III-V binary crystals, we use our ion dependent correlation between refractive index (n) and the average energy gap (E_g) as given by the following equation:

$$n^2 = 1 + CE_g^k \quad \dots(1)$$

Here, K is different for different family and C is different for different ions. Thus, differentiation of above equation with respect to temperature at constant pressure we get

$$\left(\frac{dn^2}{dT}\right)_p = CK E_g^{K-1} \left(\frac{dE_g}{dT}\right)_p + E_g^k \left(\frac{dC}{dT}\right)_p$$

Or
$$\left(\frac{dn^2}{dT}\right)_p = K.C \frac{E_g^K}{E_g} \left(\frac{dE_g}{dT}\right)_p + C E_g^k \frac{1}{C} \left(\frac{dC}{dT}\right)_p$$

Or
$$\left(\frac{dn^2}{dT}\right)_p = K \frac{(n^2 - 1)}{E_g} \left(\frac{dE_g}{dT}\right)_p + (n^2 - 1) \frac{1}{C} \left(\frac{dC}{dT}\right)_p$$

Or
$$2\left(\frac{dn}{dT}\right)_p = \frac{(n^2 - 1)}{E_g} \left(\frac{dE_g}{dT}\right)_p + (n^2 - 1) \frac{1}{C} \left(\frac{dC}{dT}\right)_p$$

Or
$$\frac{1}{n} \left(\frac{dn}{dT}\right)_p = \frac{(n^2 - 1)}{2n^2} \left[\frac{K}{E_g} \left(\frac{dE_g}{dT}\right)_p + \frac{1}{C} \left(\frac{dC}{dT}\right)_p \right] \quad \dots(2)$$

Similarly, we can derive temperature derivative of n at constant volume to get a similar result as

$$\frac{1}{n} \left(\frac{dn}{dT}\right)_v = \frac{(n^2 - 1)}{2n^2} \left[\frac{K}{E_g} \left(\frac{dE_g}{dT}\right)_v + \frac{1}{C} \left(\frac{dC}{dT}\right)_v \right] \quad \dots(3)$$

The calculated values of $\frac{1}{n} \left(\frac{dn}{dT}\right)$ at constant pressure and constant volume for I-VII family are enlisted in tables 1 and 2 respectively. The calculated values of $\frac{1}{n} \left(\frac{dn}{dT}\right)$ at constant pressure for II-VI and III – V families are enlisted in Table - 3

Table – 1 : Calculated values of $\frac{1}{n} \left(\frac{dn}{dT} \right)$ at constant pressure for I – VII mixed binary crystals (K = - 1.00)

Cations	Crystals 50%-50%	Refractive Index (n)	$\frac{1}{E_g} \left(\frac{dE_g}{dT} \right)_p$ X10 ⁻⁵ / K	$\frac{1}{C} \left(\frac{dC}{dT} \right)_p$ X10 ⁻⁵ / K	$\frac{1}{n} \left(\frac{dn}{dT} \right)_p$ X10 ⁻⁵ / K <i>Calculated</i>
Li	LiF-LiCl	1.52	-0.388	+5.92	1.785
	LiF-LiBr	1.60	-1.596	+5.92	2.292
	LiCl-LiBr	1.72	-2.977	+5.92	2.944
Na	NaF-NaCl	1.41	-3.000	+2.20	1.290
	NaF-NaBr	1.47	-5.365	+2.20	2.035
	NaF-NaI	1.55	-7.728	+2.20	2.899
	NaCl-NaBr	1.56	-4.972	+2.20	2.108
	NaCl-NaI	1.64	-6.976	+2.20	2.881
	NaBr-NaI	1.69	-8.124	+2.20	3.355
K	KF-KCl	1.41	-2.990	+3.96	1.724
	KF-KBr	1.45	-2.358	+3.96	1.655
	KF-KI	1.50	-1.600	+3.96	1.540
	KCl-KBr	1.52	-4.040	+3.96	2.264
	KCl-KI	1.56	-3.212	+3.96	2.116
	KBr-KI	1.60	-2.750	+3.96	2.046
Rb	RbF-RbCl	1.43	-2.232	+2.72	1.263
	RbF-RbBr	1.47	-1.802	+2.72	1.216
	RbF-RbI	1.52	-2.626	+2.72	1.513
	RbCl-RbBr	1.52	-2.588	+2.72	1.502
	RbCl-RbI	1.56	-3.245	+2.72	1.760
	RbBr-RbI	1.60	-2.861	+2.72	1.702

Table – 2 : Calculated values of $\frac{1}{n} \left(\frac{dn}{dT} \right)$ at constant volume for I – VII mixed binary crystals (K = -1.00)

Cations	Crystals 50%-50%	Refractive Index (n)	$\frac{1}{E_g} \left(\frac{dE_g}{dT} \right)_v$ X10 ⁻⁵ / K	$\frac{1}{C} \left(\frac{dC}{dT} \right)_v$ X10 ⁻⁵ / K	$\frac{1}{n} \left(\frac{dn}{dT} \right)_v$ X10 ⁻⁵ / K
Li	LiF-LiCl	1.52	+0.420	-1.58	-0.566
	LiF-LiBr	1.60	+1.581	-1.58	-0.964
	LiCl-LiBr	1.72	+2.881	-1.58	-1.476
Na	NaF-NaCl	1.41	-0.680	+1.52	+0.546
	NaF-NaBr	1.47	+1.650	+1.52	-0.035
	NaF-NaI	1.55	+3.520	+1.52	-0.584
	NaCl-NaBr	1.56	+0.934	+1.52	+0.173
	NaCl-NaI	1.64	+2.579	+1.52	-0.332
	NaBr-NaI	1.69	+3.763	+1.52	-0.729
K	KF-KCl	1.41	-0.360	+0.44	+0.200
	KF-KBr	1.45	-1.378	+0.44	+0.476
	KF-KI	1.50	-3.200	+0.44	+1.012
	KCl-KBr	1.52	-0.406	+0.44	+0.239
	KCl-KI	1.56	-2.077	+0.44	+0.745
	KBr-KI	1.60	-2.689	+0.44	+0.951
Rb	RbF-RbCl	1.43	-1.029	+1.59	+0.668
	RbF-RbBr	1.47	-1.888	+1.59	+0.935
	RbF-RbI	1.52	-1.871	+1.59	+0.979
	RbCl-RbBr	1.52	-2.218	+1.59	+1.078
	RbCl-RbI	1.56	-2.169	+1.59	+1.109
	RbBr-RbI	1.60	-2.732	+1.59	+1.318

Table – 3 : Calculated values of $\frac{1}{n} \left(\frac{dn}{dT} \right)$ at constant pressure for mixed binary crystals of II – VI and III – V families

Family	Crystals 50%-50%	K	Refractive Index (n)	$\frac{1}{E_g} \left(\frac{dE_g}{dT} \right)_p$ X10 ⁻⁵ / K	$\frac{1}{C} \left(\frac{dC}{dT} \right)_p$ X10 ⁻⁵ / K	$\frac{1}{n} \left(\frac{dn}{dT} \right)_p$ X10 ⁻⁵ / K
		(a)		(b)		
II-VI	ZnS-ZnSe	-1.000	2.355	-6.639	2.012	3.547
	ZnS-ZnTe		2.490	-8.250	2.012	4.300
	ZnSe-ZnTe		2.565	-8.716	2.012	4.549
III-V	GaP-InP	0.652	3.005	-6.987	4.389	3.980
	GaAs-InAs		3.405	-7.536	7.693	5.761
	GaSb-InSb		3.875	-8.743	11.726	8.138

(a) Singh R.P. et al. (1986)

(b) Obtained for 50%-50% mixtures of compounds from measured values of individuals (Tsay et al., 1973 and Sarkar et al., 1980)

Analysis of the Result

The temperature dependences of refractive index and electronic dielectric constant play a important roles in the thermal distortion of high power laser beams, transversing various optical elements and windows. This concept was originally initiated by sparks (1971) for pure crystals which can be extended now for mixed crystals. The associated aberration under most conditions in proportional to temperature derivative of refractive index and both the magnitude of (dn/dT) as well as its frequency dependence are important in this direction.

The temperature dependence of optical dielectric constant and refractive index (n) of crystals may lead to the field of optical instrumentation (Smakula, 1962) such as high resolution photographic lenses. This was initially proposed by Smakula (1962) for pure crystals but he could not ultimately get any proper results. Our ion dependent formulation is well applicable to such fields.

We can derive efficient solar cells from the mixed crystals by applying proper amount of heat or vary average energy gap to any required extent.

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