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Quantum computations for temperature variation of refractive indices of covalent semiconductors

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The well-established theory of ion-dependent quantum dielectrics is used to compute the temperature derivatives of optical refractive indices of II–VI and III–V covalent semiconductors. The ion characteristics of these materials vary a little from one another, due to variation in the plasma frequency of crystals and the d core effect. The computed values of the temperature derivatives of optical refractive indices are finally compared with the experimentally obtained values, and with the values predicted by some other workers. The correspondence between our theoretical predictions and the available, experimental data is shown, to be the most consistent to-date for a wide variety of crystals of interest.

Keywords: *optical refractive index; temperature dependence; d core effect*

1. Introduction

The model [1] for ion dependent quantum dielectrics, for ionic crystals, is now well established. This model produced multiple applications such as high resolution photographic lenses, optical instrumentation, and high power laser beams which are required to operate under a wide variety of temperature conditions. In this communication, we highlight a theory to study the effect of heat on the refractive indices of binary covalent semiconductors. The families under study are II–VI and III–V binary covalent semiconductors. The optical refractive properties of these dielectric compounds vary a little from one another, due to variation in plasma frequency and the d core effect. These properties depend upon the electric permittivities and optical refractive index of the crystal. Thus the study of the temperature dependence of refrac-

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tive indices for binary families is an integral part of the present study. The computed results have been thoroughly analyzed and a number of technological applications of the derivative have been presented.

It was noticed that in ionic solids, namely families of $A^N B^{8-N}$ compounds, with N increasing from 1 to 4, as we move from type I–VII to type IV–IV families a gradual transition from high ionicity to high covalency occurs [2]. The gradual change is from rock salt to wurtzite and zinc blende and finally to diamond structures.

The ionic compounds of I–VII binary crystals are purely ionic with a high percentage of heteropolar parts and a negligible homopolar part, showing pure cation dependent dielectric behaviour. However, solids belonging to the II–VI families have comparable homopolar and heteropolar parts. Thus, these solids may be considered as covalent as well ionic and hence show anion as well as cation dependent dielectric behaviour. The solids belonging to the III–V families are covalent in nature [1, 3]. Experimentally, it is also proved that the optical refractive properties of crystals vary with temperature. Therefore, after thermal treating of the solids, their optical refractive indices n and high frequency electric permittivity ε_∞ change, thereby varying their average energy gaps (E_g). Thus, we use our theory of ion-dependent dielectrics to compute the temperature derivatives of the refractive indices.

2. Theory

To study the temperature dependences of the optical refractive indices in the crystals under consideration, we will use the well established ion-dependent correlation [4, 5] between the optical refractive index and the average energy gap

$$n^2 = 1 + CE_g^k \tag{1}$$

where the parameter k is a family characteristic and the constant C is an ion characteristic for a given family. The parameter k is different for different binary families like II–VI and III–V etc., and is readily available in our base paper [3], whereas C is also found for different ions in different families.

Differentiation of Eq. (1) with respect to temperature leads to

$$\frac{1}{n}\left(\frac{dn}{dT}\right) = \frac{\left(n^2-1\right)}{2n^2}\left[\frac{k}{E_g}\left(\frac{dE_g}{dT}\right) + \frac{1}{C}\left(\frac{dC}{dT}\right)\right] \tag{2}$$

All terms in this equation are represented with unit per Kelvin and while deriving this correlation, the effect of core d electrons is neglected. In fact, the presence of core d electrons affects the number of free electrons per atom, which subsequently changes the plasma frequency by a small amount [6]. It is also noticed that the ion characteristic C varies a little from one ionic solid to another with the same cation, due to variation in the plasma frequency of the crystal [3].

3. Procedure

In order to compute the temperature derivatives of the optical refractive indices of various covalent semiconductors from the above model, we may rewrite Eq. (1) as:

$$\ln (n^2 - 1) = k \ln E_g + \ln C \tag{3}$$

Then, using the measured values of average energy gaps E_g [1] and the refractive indices n [6], a dependence of $\ln(n^2 - 1)$ on $\ln E_g$ is plotted and the parameter k, characteristic of the family, and the values of the parameter C, characteristic of the ion, are evaluated. Using these values, we have calculated the value of $(1/C)(dC/dT)$, which should remain constant for the same anion solids in the covalent families, and for the same cation solids in ionic families [7]. These data are listed in Table 1, along with the measured values of dE/dT for all representative compounds [8].

Table 1. Input parameters used for computing the temperature variation of refractive index

Family	Solid	E_g [1]	n [6]	k	$(1/C)(dC/dT)$ $\times 10^{-5}$/K	$-(dE_g/dT)$ $\times 10^{-5}$/K [8]
II–VI	ZnS	8.1	2.28	–1.000	2.012	5.00
	ZnSe	7.6	2.43	–1.000	2.012	5.40
	ZnTe	6.1	2.70	–1.000	2.012	6.30
III–V	GaP	5.3	2.92	–0.652	4.389	3.25
	InP	5.1	3.09	–0.652	4.389	4.00
	GaAs	5.0	3.30	–0.652	7.693	3.76
	InAs	4.7	3.51	–0.652	7.693	3.55
	GaSb	4.2	3.79	–0.652	11.726	3.80
	InSb	4.1	3.96	–0.652	11.726	3.46

Table 2. The computed values of $(1/n)(dn/dT)$, for various semiconductors along with the available experimental values and those computed through other theories

Family	Solid	Present model	Experimental value [10]	Other theories	
				[8]	[9]
II–VI	ZnS	3.3	3.3	4.3	–
	ZnSe	3.7	3.6	5.1	–
	ZnTe	5.3	5.2	8.3	–
III–V	GaP	3.7	3.7	4.2	2.2
	InP	4.2	4.0	6.2	3.6
	GaAs	5.8	5.6	5.8	5.4
	InAs	5.7	5.7	6.3	6.7
	GaSb	8.2	8.2	7.7	9.3
	InSb	12.7	12.9	8.0	15.0

These reference values are used to compute the values of $(1/n)(dn/dT)$ for the crystals, using Eq. (2). The computed values of $1/n)(dn/dT)$, namely the temperature derivatives of refractive indices, for various semiconductors in respective groups are given in Table 2, along with the available experimental values and those computed from other theories [8, 9], for comparison.

4. Conclusion

The computed values of $(1/n)(dn/dT)$ being the temperature derivatives of refractive indices, obtained through the present theoretical model are in better agreement with the available experimental values [10] than those predicted by Tsay et al. [8] and Yu et al. [9]. The predicted values of the temperature dependence of the refractive index may have a wide range of applications. Therefore, through this study we can obtain more data on behaviour of such crystals under application of heat. This property may be relevant to the field of photoelasticity, photoconductivity and solar cell technology [11]. Other applications of interest in this field are semiconductor electronics and high-power laser technology etc.

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