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Model for calculating the refractive index of different materials

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Simple model based on energy gap data, has been proposed for calculating the refractive index of different semiconductors, insulators, oxides and halides. The proposed model is applicable to the whole range of energy gap materials. The calculated values of refractive index are compared with the experimental values and the values reported by other researchers. A fairly good agreement has been obtained between them.

Keywords: Refractive index, Energy gap, Semiconductors, Insulators, Oxides, Halides

1 Introduction

In the last few decades, a considerable amount of experimental and theoretical work has been done on refractive index of various semiconductors, insulators, oxides and halides. These materials, particularly semiconductors, have potential applications in the fields of light emitting diodes (LED), photo-detectors (PD), laser diodes (LD), optoelectronic devices, integrated circuits, switches, filters and modulators and now-a-days in nanotechnology and biotechnology[1-4].

Moss[5-7] has proposed that all energy levels in a solid are scaled down by a factor $1/\varepsilon_{opt}^2$ or $1/n^4$, where n is the refractive index and ε_{opt} is the optical dielectric constant, which is equal to the square root of the refractive index, i.e., $\varepsilon = \sqrt{n}$. Ravindra *et al.*[8-10] have proposed a linear relation between the energy gap and the refractive index for some semiconducting materials. Ravindra and Srivastava[11] have modified the Moss[5-7] formula for solar cells, where one has to evaluate the refraction loss inorder to improve the conversion efficiency of semiconductors. Dionne and Woolley [12] have proposed a logarithmic relation between the energy gap and refractive index for alloy semiconductors. Reddy *et al.*[3] have correlated refractive index and plasmon energy and calculated the values of various physical parameters like bond length, microhardness, bulk modulus, interatomic force constant and lattice energy for II-VI and III-V semiconductors using earlier models in which these parameters are calculated from their plasmon energy[13-15]. Recently, Reddy *et al.*[1] have proposed interesting relationships among refractive index, energy gap and optical electronegativity and calculated the refractive index of large number of semiconductors, insulators, oxides and halides. Anani *et al.*[16] have also proposed a model for calculating the refractive index of III-V semiconductors from their energy gaps.

The models proposed by earlier researchers have been successfully used for calculating the refractive index of materials with reasonable accuracy but for limited number of materials. Some models are good for low energy gap and some for high energy gap materials but none of them is precisely applicable for whole range of energy gap materials. Therefore, it has been thought of interest to develop a model, which can be used for the entire range of energy gaps. In the present paper, a simple model for the calculation of refractive index of different semiconductors, insulators, oxides and halides from their energy gaps has been proposed. The model is based on the fact that there is strong correlation between the energy gap and refractive index of materials. In Table 1, 34-different materials have been listed in increasing order of their energy gaps starting from 0.1 eV to 8.5 eV along with the experimental values of refractive indices. The proposed model is applicable to the whole range of energy gaps. The calculated values of refractive index are compared with the experimental values and the values reported by other researchers. A fairly good agreement has been obtained between them.

2 Theory

The relation between refractive index (n) and energy gap (E_g) first given by Moss[5-7] for specific class of semiconductors is as follows:

$$n^4 E_g = K \quad \ldots (1)$$

where K is the constant and equals to 95 according to Moss[7] and 108 eV according to Ravindra *et al.*[8] The above Eq. (1) does not hold good for both low and high energy gap materials which can be seen in column 5 of Table 1. Ravindra *et al.*[10,11] have proposed the following linear relation between refractive index and energy gap:

$$n = 4.084 + \beta E_g \quad \ldots (2)$$

where $\beta = -0.62$ eV^{-1}. In the Eq. (2), n = 0 if $E_g = 6.58$ eV which indicates that the materials whose $n \geq 4.1$ cannot occur. However, there exist number of materials like GeTe, InSb, PbSe and PbTe having n > 4.1 as listed in column 3 of Table 1. This model[10, 11] is also not good for low values of n (column 6, Table 1). Finkernath[17] has widely discussed the shortcomings of above equation at low and high value of n. Reddy *et al.*[18] have proposed an empirical relation between the refractive index and the band gap for a variety of compounds:

$$n = \sqrt{\frac{12.417}{E_g - 0.365}} \quad \ldots (3)$$

Eq. (3) is the modified form of original Moss[5-7] equation with a second arbitrary constant (0.365) added in order to improve the results. This gives better agreement with the experimental values than the Moss model, but cannot be used for low energy gap materials as shown in column 7 of Table 1.

Table 1 — Refractive Index of different materials

Materials	Expt. Energy Gap[23] (eV)	Refractive Index (n)							
		Exp. [23]	Authors Cal. Eq. (8)	Moss[5-7]	Ravindra *et al.*[8,10]	Reddy *et al.*[18]	Anani *et al.*[16]	Herve *et al.*[19]	Reddy *et al.*[1]
GeTe	0.10[#]	6.000[#]	7.0724	5.5518	4.0220	NA	7.9062	4.0123	
InSb	0.17,0.235*[§]	5.130	5.3697	4.7931	3.9724	NA	6.1911	3.9283	3.93
PbSe	0.278	4.590	5.0866	4.2543	3.9042	NA	5.7776	3.8189	
PbTe	0.311	5.350	4.9060	4.1509	3.8856	NA	5.6433	3.7902	
InAs	0.354,0.417*[§]	4.100	4.4634	4.0305	3.8608	NA	5.3777	3.7527	3.76
Ge	0.664	4.052	3.8419	3.3892	3.6376	4.5651	4.0955	3.4491	
GaSb	0.726,0.812*[§]	3.820	3.6006	3.2909	3.5818	4.3144	3.9185	3.3816	3.38
Si	1.124	3.4777	3.2423	3.0348	3.3896	3.7803	3.4819	3.1707	
GaAs	1.420[§], 1.519*	4.02,3.3[a§]	3.0070	2.8579	3.2011	3.4736	3.2011	2.9913	3.04
CdTe	1.56[§],1.475[+]	2.817	2.9172	2.8500	3.1912	3.4606	3.1889	2.9826	
AlSb	2.22[§], 2.386*	3.190[#]	2.6036	2.6953	2.9680	3.2196	2.9578	2.8000	2.90
AlAs	2.153[§],3.099*	2.870	2.6295	2.5752	2.7448	3.0443	2.7872	2.6426	2.65
GaP	2.78,2.26[§],2.886*	3.35,3.2[a§]	2.5886	2.5519	2.6952	3.0113	2.7550	2.6105	
ScN	2.26[#]	2.610[#]	2.5887	2.5463	2.6828	3.0034	2.7472	2.6026	
ZnTe	2.30[§],2.394[+]	2.962	2.5741	2.5463	2.6828	3.0034	2.7472	2.6026	2.61
CdS	2.40[#],2.50[+§]	2.380[#]	2.5058	2.5083	2.5960	2.9503	2.6955	2.5492	2.55
CuBr	3.00	2.117	2.3628	2.3903	2.2798	2.7899	2.5398	2.3759	
CuI	3.10	2.346	2.3379	2.3822	2.2550	2.7790	2.5293	2.3637	
AlP	3.00[#],3.63*[§]	2.750[#]	2.2220	2.3722	2.2240	2.7658	2.5165	2.3485	2.35
SiC	2.6	2.600	2.4743	2.3528	2.1620	2.7401	2.4918	2.3189	
CuCl	3.30	1.970	2.2913	2.3146	2.0318	2.6899	2.4437	2.2601	2.26
GaN	3.30,3.299*[§]	2.400[#]	2.2915	2.2825	1.9140	2.6482	2.4040	2.2102	2.28
ZnS	3.68,	2.3505	2.2122	2.2760	1.8892	2.6398	2.3960	2.2000	2.20
BN	7.5,	2.117	1.7585	2.1318	1.2320	2.4564	2.2247	2.1851	
ZnO	3.35[§],3.4[+]	2.015	2.2802	2.1092	1.1080	2.4282	2.1989	2.1373	2.16
GeO_2	5.60	1.6045	1.9322	2.0674	NA	2.3763	2.1519	1.8710	1.91
AlN	6.20[#],4.9*[§]	2.160[#]	2.0171	1.9785	NA	2.2676	2.0549	1.7341	2.14
CsI	6.20	1.7806	1.8698	1.9706	NA	2.2576	2.0465	1.7221	1.72
CsBr	6.90	1.6929	1.8064	1.8865	NA	2.1561	1.9591	1.5989	1.60
NaBr	7.5	1.640	1.7585	1.8742	NA	2.1412	1.9466	1.5815	1.58
CsCl	7.40	1.640	1.7661	1.8563	NA	2.1199	1.9287	1.5567	1.56
KBr	7.60	1.5566	1.7510	1.8449	NA	2.1062	1.9173	1.5409	1.58
KCl	8.5	1.4879	1.6890	1.8284	NA	2.0865	1.9009	1.5186	1.52
SiO_2	8.4	1.5600	1.6955	1.7907	NA	2.0416	1.8641	1.4689	

NA – Not applicable, [#] Ref [16], *Ref [4], [§] These values have been used for regression, [a]Ref [24], [+] Ref [25]

Anani *et al.*[16] have proposed the following relation for the refractive index of III-V semiconductors considering the fact that the refractive index for an infinite energy gap is equal to zero:

$$n^4 = 1 + \frac{A}{E_g^2} \quad \ldots (4)$$

where A is an empirically calculated constant equals to 40.8 eV. The calculated values of n from Eq. (4) for most of the materials (26 out of 34) have been found to be higher than the experimental values in both low and high energy gap regions (column 8, Table 1). Based on the oscillatory theory, Herve and Vandamme[19] have proposed the following relation for the refractive index:

$$n = \sqrt{1 + \left(\frac{A}{E_g + B} \right)^2} \quad \ldots (5)$$

where A = 13.6 eV and B = 3.4 eV are the constants. The above Eq. (5) gives poor agreement for high energy gap materials (column 9, Table 1). Duffy[20,21] has correlated energy gap with electronegativity ($\Delta\chi$) for various binary systems and proposed the relation:

$$E_g = 3.72\ (\Delta\chi) \quad \ldots (6)$$

where $\Delta\chi = [\chi_{anion} - \chi_{cation}]$ and χ_{anion} and χ_{cation} are the optical electronegativities of anion and cation, respectively. Using Eqs (5) and (6), Reddy *et al.*[1] have recently proposed the following relation between n with $\Delta\chi$:

$$n = \sqrt{1 + \left(\frac{A}{3.72\Delta\chi + B} \right)^2} \quad \ldots (7)$$

The validity of Eq. (7) has been tested for more than 100 compounds by Reddy *et al.*[1] For the low values of n (1-2) it gives better results but for high value of n (4-6) the deviation is very high, i.e., between 10 to 46% (column 10, Table 1).

Basically there are two approaches for modeling the refractive index of materials. The first approach is to determine the model parameters for particular group of semiconductors and then find the optimal function describing the dependence of these parameters for other semiconductors. However, in the second approach it fits simultaneously the data sets for all available materials in order to minimize the discrepancies between the calculated and the experimental data for the entire range of energy gaps consideration. The first method has been found to be less accurate and degrades the accuracy of the estimated refractive index[16].

In this paper, the second approach to model refractive index of mixed materials belonging to groups IV, II-VI and III-V semiconductors, insulators, oxides and halides listed in Table 1 in increasing order of energy gaps have been opted. Experimental values of energy gap and refractive index of these materials have been taken from different sources. Finally, the data is simulated using simulation software and obtained the following relation between n and E_g:

$$n = K\, E_g^C \quad \ldots (8)$$

where K = 3.3668 and C = –0.32234 are the constants. The values of these constants have been obtained optimizing the experimental data of refractive index and energy gap in the regression software.

3 Discussion

In the present paper, a simple model has been developed based on experimental data of energy gap to evaluate the refractive indices of various semiconductors, insulators, oxides and halides for entire range of energy gap (E_g = 0.1-8.5 eV). Using this model, i.e., Eq. (8), the values of refractive indices have been calculated for 34-different materials. The calculated values are listed in column 4 of Table 1. A fairly good agreement has been obtained between the calculated and the experimental values. The validity of Eq. (8) has also been tested for some of ternary chalcopyrites like $CuAlS_2$, $CuAlSe_2$ and $CuAlTe_2$, whose experimental values of energy gaps are 3.5, 2.70 and 2.06, respectively[22]. The calculated values of refractive index from Eq. (8) comes out to be 2.248, 2.444, 2.667, respectively, for $CuAlS_2$, $CuAlSe_2$ and $CuAlTe_2$ semiconductors, which are in good agreement with the known values 2.45, 2.60, 2.44 and 2.41 for $CuAlSe_2$ and 2.69, 3.30, 2.61 and 2.81 for $CuAlTe_2$ (Ref. 1).

4 Conclusions

The index of determination of Eq. (8) for calculating the refractive index of different materials has been found to be 0.9133, which shows that the calculated values are 91.33% close to the experimental values. Hence, it is possible to predict the value of refractive index for entire range of energy

gap materials. The proposed model gives better agreement with the experimental values than the models proposed by earlier workers, which in turn demonstrate the soundness of the present model.

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