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# A simple model for refractive index-energy gap interrelation of some compound semiconductors

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**Abstract** : In this paper, we propose simple relations connecting the high frequency refractive index and energy gap $E_g$ of some compound semiconductors. For semiconductors belonging to groups II-VI and III-V, we propose that the refractive index $n$ is given by $n = F/(E_g + B)$, where $B$ is a numerical constant and $F$ is a parameter, which takes into account the contribution of the valence electron plasmon energy. In addition, a linear relationship between the refractive index $n$ and the energy gap $E_g$, is proposed for semiconductors belonging to group I-VII. This relation reads as $n = a - b E_g$, where $a$ and $b$ are numerical constants. The examination of the present relations shows a reliable agreement between calculated and experimental values of refractive index. Comparison between present values and those given by other workers are also considered.

**Keywords** : Model, refractive index and energy gap, compound semiconductors

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## 1. Introduction

Optical constants, namely, refractive index and dielectric constant are considered to be fundamental parameters which play important roles in determining transport, lattice dynamical and optical properties of semiconductors.

Some semiconducting materials were known to crystallize in zinc-blende and wurtzite structures and consequently, to have a binding mechanism similar to that of

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germanium and silicon. Thus, the nature of the interatomic interactions, the bond energy and the consequent structural relationships determine the physical properties of simple and compound semiconductors.

The width of the forbidden gap $E_g$ is one of the most important semiconductor parameters. This width is found to be considerably larger in II-VI compounds and increases further in I-VII compounds. The materials of the II-VI compounds show also $E_g$ decreasing with increasing atomic weight. Among the III-V compounds, one can therefore expect the lightest compound BN to have the largest forbidden gap and the heaviest compound Insb, to have the smallest one. The values of the forbidden gap of the other III-V compounds will be in between them.

The semiconducting materials of II-VI, III-V and I-VII groups are found to be of great interest because of their applications in integrated optical devices such as switches, filters and modulators. Then, the correlation between the high frequency refractive index and its related properties have been studied by many researchers [1–4]. Several attempts have been carried out to obtain a relation connecting the high frequency refractive index $n$ and the energy gap $E_g$ in semiconductors [5,6].

Ravindra *et al* [7] proposed the following linear relationship between $n$ and $E_g$,

$$n = 4.08 - 0.62\, E_g. \tag{1}$$

Relation (1) follows from the Penn model [8] and also from the treatment due to Wemple [9].

Gopal [10] have shown that the Penn model for the dielectric constant of semiconductors can be modified to construct a general relation between optical refractive index and the energy band gap, which avoids the shortcoming of relation (1). His relation reads as follows :

$$n^2 = 1 + \frac{A}{\left(E_g + C\right)^2} \tag{2}$$

where $A$ and $C$ are numerical constants having the values 169 and 2.7 respectively.

More recently, Reddy and Anjaneyulu [11] proposed a linear relation between $n$ and $E_g$, which is of the form

$$n = 3.59 - \ln E_g. \tag{3}$$

Relation (3) is an empirical formula and it gives better values of refractive index compared to the relation derived by Ravindra *et al* [7].

However, our study of the above stated relations (1), (2) and (3) showed that there is a considerable deviation between calculated values of refractive index and experimental ones among the most studied compound semiconductors.

In the present work, we propose a simple model for evaluating the refractive index in some compound semiconductors belonging to II-VI and III-V groups. In this model, we

introduce a parameter, which takes into account the contribution of the valence electron plasmon energy to the refractive index. In semiconductors of I-VII group, we find that the refractive index is linearly dependent on energy gap.

## 2. Theory

The high frequency dielectric constant $\varepsilon_\infty$ as evaluated from Penn model, is given by Gupta *et al* [5] as

$$\varepsilon_\infty - 1 = (E_p / P)^2 D \tag{4}$$

with $$D = 1 - (E_p / 4E_f) + \frac{1}{3}(E_p / 4E_f)^2, \tag{5}$$

where $E_p$ is the valence electron plasmon energy, $E_f$ is the Fermi-energy and $P$ is the Penn gap. The latter can be expressed in terms of the minimum energy gap by

$$P = E_g + B, \tag{6}$$

where $B$ is constant.

In our presentation, we consider $E_p$ as a variable parameter, in contrast to other workers. Accordingly, we propose that the refractive index $n$ is related to the energy gap $E_g$ in semiconductors of groups II-VI and III-V by the following relation

$$n = \frac{F}{(E_g + B)} \tag{7}$$

The parameter $F$ is determined by applying eq. (7) to the considered groups of semiconductors having experimently known band gap $E_g$ and refractive index $n$. Then, we find a correlation between the parameter $F$ and both variables $E_g$ and $E_p$. The dependence of $F$ on $E_g$ and $E_p$ is indicated in Figure 1. Then, we have

$$F = K(E_g / E_p), \tag{8}$$

where $K$ is a numerical constant found to be dependent on the semiconductor group, whereas $B$ is found to be nearly constant.

In considering semiconductors belonging to I-VII group, we propose that the refractive index $n$ is linearly dependent on the energy gap $E_g$ according to the following equation

$$n = a - bE_g, \tag{9}$$

where $a$ and $b$ are numerical constants.

In order to evaluate the constants $B$ and $K$ in eqs. (7) and (8), we denote the given data for $E_g$, $E_p$ and $n$ in the line number $i$ by $X_i$, $Y_i$ and $Z_i$ respectively. From eqs. (7) and (8) we can write

$$Z = \frac{KU}{(X + B)}, \tag{10}$$

where $U = E_g/E_p$. We calculate now the best values for $K$ and $B$ which give the minimum error $E$

$$= \sum_{i}^{n} \left( Z_i - \frac{KU_i}{X_i + B} \right) \tag{11}$$

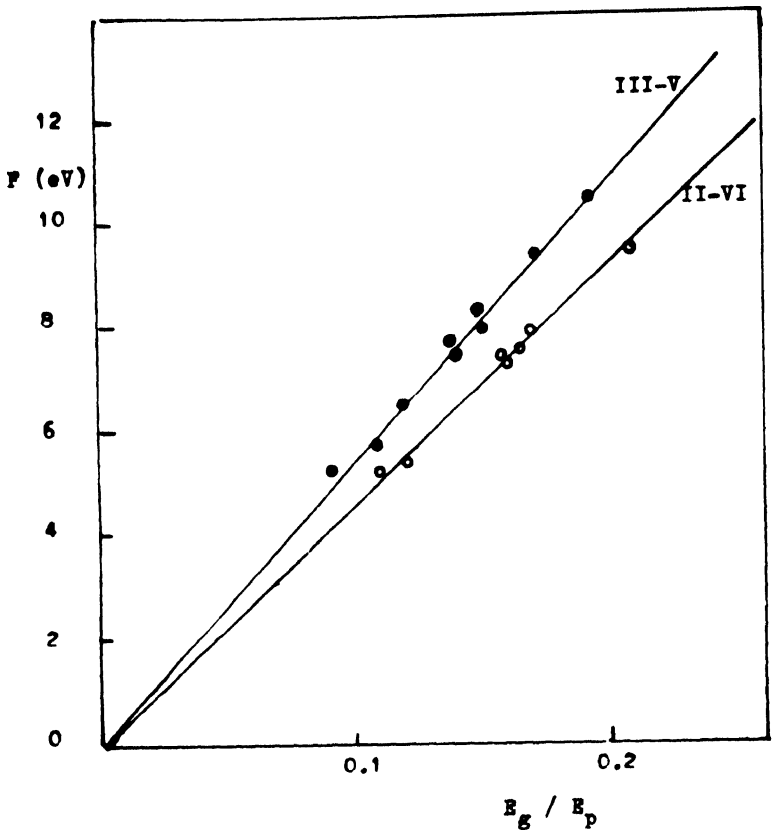


**Figure 1.** The dependence of the parameter $F$ on the ratio $E_g/E_p$

The necessary conditions for the minimum error lead to the following system of non-linear equations,

$$\sum_{i=1}^{n} \frac{Z_i U_i}{X_i + B} - K \sum_{i=1}^{n} \frac{U_i^2}{(X_i + B)} = 0$$

and $$\sum_{i=1}^{n} \left( Z_i - \frac{KU_i}{X_i + B} \right) \frac{KU_i}{(X_i + B)^2} = 0. \tag{12}$$

We have implemented the Pascal procedure for solving these equations using the so called bisection method [12].

The constants of eq. (9) have been estimated with the aid of a numerical algorithm, which is based on the method of minimal least-square errors.

The computed constants $B$, $K$, $a$ and $b$ are listed in Table 1.

**Table 1.** Values of the computed constants $B$, $K$ (eqs 6 and 7) and $a$, $b$ (eq. 8).

| Group of compound | Values of the numerical constants |
|---|---|
| II-VI | $B = 0.44$ eV |
| | $K = 45.50$ eV |
| III-V | $B = 0.40$ eV |
| | $K = 55.10$ eV |
| I-VII | $a = 3.95$ |
| | $b = 0.62$ (eV)$^{-1}$ |

## 3. Results and data analysis

The results of our calculation of high frequency refractive indices of semiconductor groups II-VI, III-V and I-VII are given in Table 2. The present evaluation of refractive indices

**Table 2.** Energy gap $E_g$ valence electron plasmon energy $E_p$ and refractive index data $n$ at 300 K

| Semi-conductor | $E_g$ (eV) [14–16] | $E_p$ (eV) [4] | $n$ known [4, 14, 15] | present | eq (1) | eq. (2) | eq. (3) |
|---|---|---|---|---|---|---|---|
| ZnO | 3.70 | 21.50 | 1.92 | 1.89 | 1.79 | 2.26 | 2.28 |
| ZnS | 3.54 | 16.70 | 2.39 | 2.42 | 1.89 | 2.31 | 2.33 |
| ZnSe | 2.58 | 15.60 | 2.47 | 2.49 | 2.48 | 2.66 | 2.64 |
| ZnTe | 2.26 | 14.40 | 2.70 | 2.64 | 2.68 | 2.81 | 2.77 |
| CdS | 2.40 | 14.88 | 2.38 | 2.58 | 2.60 | 2.74 | 2.71 |
| CdSe | 1.70 | 14.19 | 2.49 | 2.55 | 3.03 | 3.11 | 3.06 |
| CdTe | 1.50 | 13.10 | 2.68 | 2.69 | 3.19 | 3.30 | 3.23 |
| BN | 4.60 | 24.55 | 2.10 | 2.06 | 1.23 | 2.04 | 2.06 |
| AlN | 3.80 | 22.90 | 2.20 | 2.18 | 1.73 | 2.24 | 2.25 |
| AlP | 2.50 | 16.70 | 2.75 | 2.84 | 2.22 | 2.49 | 2.49 |
| AlAs | 2.16 | 15.31 | 2.92 | 3.03 | 2.74 | 2.86 | 2.82 |
| AlSb | 1.60 | 13.91 | 3.20 | 3.17 | 3.09 | 3.18 | 3.12 |
| GaN | 3.25 | 22.00 | 2.20 | 2.23 | 2.07 | 2.40 | 2.41 |
| GaP | 2.24 | 16.57 | 2.90 | 2.82 | 2.70 | 2.82 | 2.78 |
| InN | 2.00 | 18.82 | 2.35 | 2.44 | 2.84 | 2.94 | 2.90 |
| InP | 1.27 | 14.52 | 3.10 | 2.89 | 3.30 | 3.42 | 3.35 |
| CuCl | 3.31 | 16.66 | 1.93 | 1.90 | 2.03 | 2.38 | 2.39 |
| CuBr | 2.94 | 15.18 | 2.10 | 2.13 | 2.26 | 2.51 | 2.51 |
| CuI | 2.60 | 13.99 | 2.35 | 2.34 | 2.47 | 2.65 | 2.63 |
| AgCl | 3.10 | 16.04 | 2.00 | 2.03 | 2.16 | 2.45 | 2.46 |
| AgBr | 2.85 | 15.12 | 2.21 | 2.18 | 2.32 | 2.55 | 2.54 |
| AgI | 2.80 | 13.02 | 2.22 | 2.21 | 2.35 | 2.57 | 2.56 |

shows a good agreement with experimentally known ones. However, the examination of the models proposed by others [7,10,11] and indicated that these models cannot be used for accurate determination of refractive indices. This may be due to the fact that these authors assumed the valence electron plasmon energy to be constant. In contrast, the proposed eqs. (7) and (8) involve a parameter $F$, which is a function of $E_p$ and $E_g$. Then, the numerical constant $K$ is a characteristic quantity of semiconductor group. On the other hand, $B$ is found to be nearly constant (= 0.4) and it is additive to the lowest energy band $E_g$.

For semiconductors of I-VII group, we propose a linear relation governing the refractive index $n$ and the energy gap $E_g$. This equation is as follows

$$n = 3.95 - 0.62\, E_g. \tag{13}$$

Eq. (13) is similar to that previously assumed by Ravindra *et al* [7] and it differs only in the values of the constants. In this group, refractive index is nearly independent on valence electron plasmon energy $E_p$. The variation in $E_p$ is about 10% on going from CuCl to AgBr among this group. Therefore, the linearity between $n$ and $E_g$ in this group can be attributed to the systematic variation in the parameters describing the chemical binding. This is clear from the gradual increase of anion radius from 1.81 Å for $Cl^-$ to 2.20 Å for $I^-$. Whereas, Cu- and Ag-atoms exhibit nearly the same Pauling electronegativity (= 1.9) [13].

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