Optical Materials 46 (2015) 240–246

Contents lists available at ScienceDirect

Optical Materials

journal homepage: www.elsevier.com/locate/optmat

Refractive indices of semiconductors from energy gaps

S.K. Tripathy

Department of Physics, Indira Gandhi Institute of Technology, Sarang, Dhenkanal, Odisha 759146, India

ARTICLE INFO

Article history:
Received 20 February 2015
Received in revised form 10 April 2015
Accepted 17 April 2015
Available online 29 April 2015

Keywords:
Refractive index
Energy gap
Binary and ternary semiconductors
Temperature variation of refractive index

ABSTRACT

An empirical relation based on energy gap and refractive index data has been proposed in the present study to calculate the refractive index of semiconductors. The proposed model is then applied to binary as well as ternary semiconductors for a wide range of energy gap. Using the relation, dielectric constants of some III–V group semiconductors are calculated. The calculated values for different group of binary semiconductors, alkali halides and ternary semiconductors fairly agree with other calculations and known values over a wide range of energy gap. The temperature variation of refractive index for some binary semiconductors have been calculated.

1. Introduction

With the advent of recent technologies, novel semiconductors rich in their optoelectronic properties find wide range of applications in optical, electronic and optoelectronic devices such as light emitting diodes (LED), laser diodes (LD), integrated circuits (IC), photo detectors (PD), nanotechnology, heterostructure lasers and optical modulators operating in mid infra-red regions (2–5 μm) [1,2]. The optical and electronic behaviour of semiconductors are decided by two fundamental properties namely energy gap and refractive index. In general, the threshold of photon absorption of a semiconductor determines the energy gap whereas refractive index is a measure of transparency to the incident photon. The correlation between these two optoelectronic parameters of semiconductors has remained a subject of intensive research in recent times because of its role in semiconductor band structures. Moreover, electronic properties such as atomic polarizability and dielectric constant depend on the refractive index of the materials which ultimately can be calculated from the knowledge of energy gap.

Refractive index of a material is known to decrease with energy gap and therefore, these two fundamental quantities of a material are believed to have certain correlation. Over a period of time there have been many attempts to find a suitable relationship, both empirical and semi empirical, between the energy gap and refractive index of semiconductors [3–21]. Many of the empirical relations relate the refractive index n to the energy gap E_g directly whereas some relations are proposed to calculate E_g from electronegativity first and then from the calculated E_g, n is determined. Moss [3–5] on the basis of photoconductivity showed that the electron energy levels are scaled down by a factor of $\frac{1}{\epsilon_{eff}^2}$, where ϵ_{eff} is the effective dielectric constant as felt by the electron in the material. The effective dielectric constant is approximately equal to the square of the refractive index of the material. Penn proposed a simple model for isotropic systems with reasonable applications to a liquid or amorphous semiconductors [6]. Ravindra and his collaborators have proposed an empirical relation for refractive index for semiconductors which is linear in energy gap by assuming that the valence and conduction bands are more or less parallel to each other along the symmetry directions [7,8]. The Ravindra relation was conceived to be an approximation of the Penn model. Several other modifications of the Ravindra relations were also proposed to get different properties of many infrared materials [9,10]. Based on the oscillatory theory and assuming the UV resonance energy has a constant difference with energy gap, Herve and Vandamme proposed a theoretical relation for refractive index which they claimed to provide good results with lowest deviation for III–V, I–VII group semiconductors and chalcopyrites [11,12]. Reviews on the energy gap and refractive index of semiconductors based on these models can be found at [5,22,23]. Gopal in attempt to modify the Penn model for high frequency dielectric constant obtained a relation between these two fundamental properties of semiconductors [13]. Later, Reddy and his collaborators investigated about the correlation among various properties of semiconductors and proposed some empirical relations for different compounds [14–16]. Anani et al. have proposed a formulation for refractive index of III–V semiconductors [17]. Recently, Kumar and Singh proposed an empirical relation for refractive index

E-mail address: tripathy_sunil@rediffmail.com

http://dx.doi.org/10.1016/j.optmat.2015.04.026
0925-3467/

described through a power law behaviour on the energy gap by fitting the model parameters to a number of experimental energy gap and refractive index data [18]. In that work, they have claimed that, the proposed model can be equally applied for the determination of optoelectronic properties for different semiconductors including ternary chalcopyrites.

It is needless to emphasize that, a proper design of optoelectronic device requires a detailed knowledge of the refractive indices of materials and hence an accurate and reliable energy gap–refractive index relation is indispensable. From experimental point of view, energy gap of semiconductors are available for a wide range of materials. However, refractive index data for different group of semiconductors including narrow band gap region are not available to a satisfactory extent [1]. This necessitates the formulation of both theoretical and empirical relationship between these two fundamental parameters.

The purpose of the present work is to study some of the well known energy gap–refractive index relations in the context of elemental and binary semiconductors. The choice of the empirical relations is very much personal one and is on the basis of their frequent use and discussion in literature. It is obvious that, the already proposed relations are region specific. From a set of tabulated experimental values of energy gap and refractive index of semiconductors and alkali halides, we propose a relation which can be applied equally well to all possible regions of energy gap. The organisation of the present work is as follows. In Section 2, we have reviewed the energy gap–refractive index relations and on the basis of a fit to the experimental data spanning a wide region of energy gap, we propose a new relation for the refractive index. In Section 3, we have compared our results with the known values for different group of semiconductors and alkali halides. Also, we have applied the empirical model for the calculation of dielectric constants of some III–V group semiconductors. The temperature variation of refractive index for different semiconductors are also discussed. In Section 4, we have extrapolated our results to ternary compounds. At the end, we summarize our results.

2. Basic formulations

The correlation of refractive index and energy gap in semiconductors has been a subject of intensive research interest for a long time and started with the semi empirical relation of Moss as early as in 1950. Following Moss relation, there have been many similar relations have been proposed for the calculation of refractive index of materials. In the present section, we review and analyse some of the well known energy gap–refractive index relations as available in literature. These relations are widely used to calculate the refractive index of different group of semiconductors and alkali halides.

Moss relation:

$$n^4 E_g = 95 \text{ eV}, \tag{1}$$

where n and E_g are respectively the refractive index and energy gap.

Ravindra relation:

$$n = 4.084 - 0.62E_g. \tag{2}$$

Herve–Vandamme relation:

$$n^2 = 1 + \left(\frac{A}{E_g + B}\right)^2, \tag{3}$$

where A is the hydrogen ionization energy 13.6 eV and B = 3.47 eV is a constant assumed to be the difference between the UV resonance energy and band gap energy.

Reddy relation:

$$n^4(E_g - 0.365) = 154. \tag{4}$$

Kumar and Singh relation:

$$n = KE_g^C, \tag{5}$$

where $K = 3.3668$ and $C = -0.32234$.

The above mentioned relations have been proposed with claims to have good agreement with experimental values. In Fig. 1, we have plotted these relations for refractive index as function of energy gap. Also, in the figure, the known or experimental values of refractive index of some elemental and binary semiconductors including alkali halides are shown against their experimental energy gap. The experimental values have been collected from different sources [18,24–26]. One can note from the figure that, except the Ravindra relation all other relations show a common trend. Ravindra relation being a linear one has its own shortcomings. Eventhough this relation works well in a fairly low and medium values of energy gap, it fails in the very low and high energy gap region. Further, the refractive index becomes negative for Ravindra relation for semiconductors having energy gap greater than 6.587 eV and hence cannot be used for materials with refractive index greater than 4.1. In other words for materials like GeTe, InSb, PbSe, PbSnTe and PbTe with larger energy gap ($E_g > 6.587$ eV) this equation may not be valid.

Herve–Vandamme relation has been derived from the oscillatory theory assuming a constant difference of energy between band gap and UV resonance energy which can be thought of as a modified version of Moss relation. The behaviour of Herve–Vandamme and Moss relation are similar from a low value of energy gap i.e $E_g \simeq 1$ eV to large values. In their work, Herve and Vandamme claimed that, their model provides a good fit for III–V, I–VII group semiconductors and chalcopyrites. For materials with high band gap energy, this model is somewhat accurate. However, at low values of energy gap ($E_g < 1.4$ eV) this relation fails to predict the experimental refractive index.

Moss relation fairly follows the trend of the experimentally determined refractive index. Moss relation is restricted by the structure of materials and at very low values and at large values of energy gap Moss relation is not a good one to rely upon for the calculation of refractive index of materials. It can be observed from the figure that, Moss relation is reliable in the range 0.5 eV $< E_g <$ 3.68 eV of the energy gap.

Reddy relation is a modification of Moss relation with a constant term subtracted from the energy gap and has the same behaviour as that of Moss relation. It is certainly a bit improved than Moss'. This relation gives a better agreement to the experimental

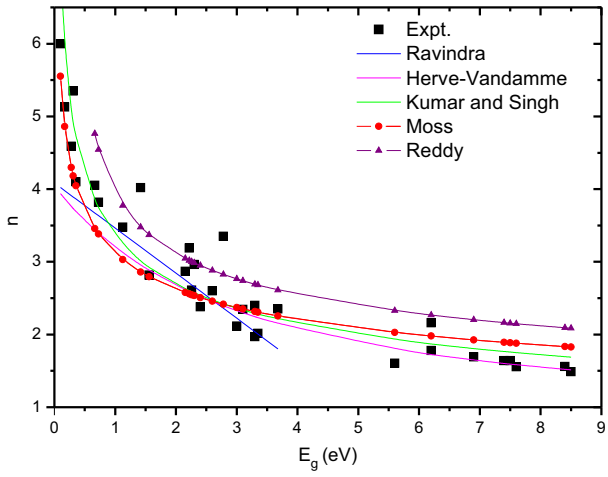

Fig. 1. (Color online) Refractive index of semiconductors as function of energy gap. The experimental values are shown as unconnected solid black squares. Calculated refractive indices from some well known relations are also shown in the plot.