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Optical and electronic properties of some semiconductors from energy gaps

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ABSTRACT

II-VI and III-V tetrahedral semiconductors have significant potential for novel optoelectronic applications. In the present work, some of the optical and electronic properties of these groups of semiconductors have been studied using a recently proposed empirical relationship for refractive index from energy gap. The calculated values of these properties are also compared with those calculated from some well known relationships. From an analysis of the calculated electronic polarisability of these tetrahedral binary semiconductors from different formulations, we have proposed an empirical relation for its calculation. The predicted values of electronic polarisability of these semiconductors agree fairly well with the known values over a wide range of energy gap. The proposed empirical relation has also been used to calculate the electronic polarisability of some ternary compounds.

1. Introduction

Semiconductors rich in optoelectronic properties have generated a lot of research and technological interest in recent times because of their novel applications in different 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]. Among different novel materials fabricated, II-VI and III-V group semiconductors and alloys find wide range of interesting applications. These materials exhibit Wurzite and Zinc blende tetrahedral crystal structures. Wide band gap II-VI semiconductors are used in optoelectronic devices such as LEDs and LDs operating in blue-green spectral range [3]. These materials are characterized by different degree of ionicity which make them suitable for high electro-optical and electromechanical coupling. II-VI binary semiconductors such as ZnS, ZnSe and ZnTe find applications as blue lasing materials and can be used in the fabrication of optical wave guides and modulated heterostructure [4–6]. Oxides like ZnO are used in nano medicines [7]. Recently there have been a lot of studies on the elastic, electronic and optical properties of some II-VI group semiconductors [4,10,11,19,12–17,8,9,18]. III-V group of semiconductors also exhibit tetrahedral structures and have interesting applications in optoelectronics and photovoltaics because of their direct band gaps and high refractive indices. They are used in the fabrications of high efficiency solar cells. Large breakdown fields, high thermal conductivities and electron transport properties of III-V nitrides such as GaN, InN, AlN make them suitable for novel optoelectronic applications in visible and ultra violet spectral range [3]. In recent times there have been a lot of interest in the calculation of the electronic and optical properties of III-V binary semiconductors and their alloys [20,21,29,22–28,30].

In semiconductors, two basic properties namely energy gap and refractive index mostly decide their optical and electronic behaviour. Refractive index of a material usually decreases with an increase in energy gap fostering an underlying relationship between these two fundamental quantities. There have been many attempts to correlate these two quantities with a suitable empirical or semi-empirical relation [31–48]. Recently, an empirical relation, based on some experimental refractive index data of some elemental and binary semiconductors has been proposed by Tripathy, which can be equally applied to all regions of energy gap and can also be applied to ternary semiconductors [49]. In the present work, we have used this recently proposed relation to investigate some of the optical and electronic properties of some II-VI and III-V group semiconductors and some electronic properties of ternary compounds. The organisation of the work is as follows. In Section 2, we have calculated different optical properties of II-VI and III-V group semiconductors such as dielectric constant, optical susceptibility and reflectivity using the relation proposed in Ref. [49]. The calculated values are also compared with the values

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predicted using some well known relations. In Section 3, different electronic properties such as ionicity and electronic polarisability of III-V and II-VI group semiconductors have been calculated and compared with the predicted values of other calculations. From an analysis of the electronic polarisability of the semiconductors, we have proposed an empirical relation for its calculation. The proposed empirical relation is then applied to calculate the electronic polarisability of some ternary semiconductors. At the end, conclusions and summary of the work are presented in Section 4.

2. Optical properties

2.1. Refractive index

Refractive index n of a material is a measure of its transparency to the incident photons. For semiconductor materials, it is considered as an important physical parameter. A proper design of optoelectronic device needs an accurate knowledge of refractive indices of materials. Refractive index is closely related to the electronic properties and band structure of the material. Theoretically, two different approaches are adopted to calculate the refractive index. In the first approach, it is calculated from the electronic behaviour concerning the local fields and the molar volume of the material. In the second approach, a more involved quantum mechanical calculation is performed to calculate the band structure which in turn is related to the refractive index of the material. Since the band structure of a semiconductor is intimately related to its optical behaviour, there have been attempts to calculate refractive index from energy gaps. In this context, so many empirical relations between refractive index and energy gap E_g have been proposed earlier [31,35,34,42,43,39,40,45]. These relations have been widely used in literature to calculate different opto-electronic properties of different groups of semiconductors. Recently, Tripathy has proposed an empirical relation to calculate refractive index of semiconductors from their energy gaps [49]. In that work, it has been shown that, the relation (hereafter termed as Tripathy relation) can be successfully used for different group of semiconductors for a wide range of energy gaps. According to the Tripathy relation, the refractive index of a semiconductor with energy gap E_g is given by

$$n = n_0[1 + \alpha e^{-\beta E_g}], \tag{1}$$

where $n_0 = 1.73$, $\alpha = 1.9017$ and $\beta = 0.539\ \text{eV}^{-1}$ are the constant parameters for a given temperature and pressure. The temperature and pressure dependence of these parameters is again a subject of intensive future investigations. Even though the above relation can be applied to semiconductors with a wide range of energy gaps, the prominent region in which this relation works well is within the range $0 < E_g < 5$ eV. Besides the Tripathy relation, some other popular empirical relations available in literature are

Moss relation [31]:

$$n^4 E_g = 95\ \text{eV}, \tag{2}$$

Ravindra relation [35]:

$$n = 4.084 - 0.62E_g, \tag{3}$$

Herve-Vandamme (HV) relation [39,40]:

$$n^2 = 1 + \left(\frac{A}{E_g + B}\right)^2, \tag{4}$$

where A is the hydrogen ionization energy 13.6 eV and $B = 3.47$ eV is a constant assumed to be the difference between UV resonance energy and band gap energy. Since II-VI and III-V groups of semiconductors have enough potential for optoelectronic device applications, we are interested in the present work to use the values of refractive indices calculated from these formulations to investigate some of their optical and electronic properties. For the purpose of calculation, we have considered those semiconductors belonging to these specific groups with energy gap lying in the range $0 < E_g < 5$ eV. The calculated values of refractive indices of these semiconductors can be obtained from Ref. [49].

2.2. Dielectric constant and linear optical susceptibility

The dielectric properties of a material is usually measured through a frequency dependent complex dielectric function having its real and imaginary parts, $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$. The dielectric function describes the response of the semiconductor to the electromagnetic radiation mediated through the interaction of photons and the electrons. It depends upon the electronic band structure and explains the combined excitations of Fermi sea. The real part of the dielectric constant determines the refractive index of a material and the imaginary part determines the absorption coefficient. The static limit dielectric constant ϵ_∞ is related to the refractive index n through a simplified expression $\epsilon_\infty = n^2$, where the magnetic permeability of the medium is close to 1. In the present work, we have used the Tripathy relation in Eq. (1) to calculate the static limit of the dielectric constants of some II-VI and III-V semiconductors spanning over a wide range of energy gaps. In this context, we have considered semiconductors both from the narrow as well as wide band gap region. Once the dielectric constant is calculated, the linear optical susceptibility can then be obtained in a straightforward manner using the relation $\chi = \epsilon_\infty - 1$. In the II-VI group semiconductors, the dielectric constants are calculated for CdS, CdSe, ZnS, ZnTe, ZnSe, ZnO, MgS, MgTe, MgSe, SrS, SrTe, SrSe and are plotted as function of energy gaps in Fig. 1. These semiconductors have energy gaps lying in the range $1.5 < E_g < 5$ eV. In the figure, the known values of dielectric constants have also been shown for comparison. Our results are compared with the values calculated from the well known expressions of refractive index as proposed by Moss in Eq. (2), Ravindra in Eq. (3) and Herve and Vandamme in Eq. (4). It can be observed from the figure that, dielectric constant decreases with the increase in energy gap. The theoretical trends of the calculated dielectric constants fairly match with the experimental trend. However, in the lower energy gap region i.e. $E_g < 2$ eV, the calculated values remain above the known ones and in the higher band gap region i.e $E_g > 3.5$ eV, the predicted values remain below the known dielectric constants. It is interesting to note from the figure that, the calculated values from Tripathy relation agree fairly well with the known values at more number of data points as compared to that of HV relation particularly for ZnTe, ZnSe, ZnO, ZnS, MgTe and SrS. For BaSe and MgSe the calculated dielectric constants from Tripathy relation exactly match with the known values. Tripathy relation and HV relation behave alike for higher energy gap region whereas in the lower energy gap region, Tripathy relation predicts a bit higher value of dielectric constant. The over prediction in the low energy gap region can be attributed to the exponential decay nature of the refractive index with energy gap in Tripathy relation. However, refractive index from Tripathy relation becomes softer in the wide band gap region and compares well with that of the HV relation. It is worth to mention here that, for the specific group of semiconductors considered here, HV relation predicts reasonably good values of refractive indices compared to those of Moss' and Ravindra relation [49]. Calculations from Ravindra relation do not have good agreement with the known values and therefore, for II-VI group of semiconductors in the energy gap range $1.5 < E_g < 5$ eV one must be careful while using this relation. It can be emphasized that, Moss relation and Tripathy relation predict the dielectric constants reasonably well over the range of band gap considered in the present work and they can be used to a satisfactory extent for this group of semiconductors.