Energy Gap–Refractive Index Relations in Semiconductors – An Overview

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Introduction

The refractive index and energy gap of semiconductors represent two fundamental physical aspects that characterize their optical and electronic properties. The applications of semiconductors as electronic, optical and optoelectronic devices are very much determined by the nature and magnitude of these two elementary material properties. These properties also aid in the performance assessment of band gap engineered structures for continuous and optimal absorption of broad band spectral sources. In addition, devices such as photonic crystals, wave guides, solar cells and detectors require a pre-knowledge of the refractive index and energy gap. Application specific coating technologies (ASPECTTM) [1] including antireflection coatings and optical filters [2] rely on the spectral properties of materials. The energy gap determines the threshold for absorption of photons in semiconductors. The refractive index in the semiconductor is a measure of its transparency to incident spectral radiation. A correlation between these two fundamental properties has significant bearing on the band structure of semiconductors. In 1950, Moss [3] proposed a basic relationship between these two properties using the general theory of photoconductivity which was based on the photo effect studies of Mott and Gurney [4], Smekal [5], Zwicky [6], Gudden and Pohl [7] and Pearson and Bardeen [8]. According to this theory, the absorption of an optical quantum will raise an electron in alkali halides to an excited state rather than freeing it from the center. Thermal energy then moves this electron to the conduction band from the lattice. Such a photo effect takes place in imperfections at certain lattice points, and thus, the electron behaves similar to an electron in an isolated atom with a dielectric constant of the bulk material. As a result of this effective dielectric constant, e_{Eff}, the energy levels of the electron are scaled down by a factor of $1=e^2_{Eff}$ which approximately corresponds to the square of the refractive index, n. This factor, thus, should be proportional to the energy required to raise an electron in the lattice to an excited state as given by the Bohr formula for the ionization energy, E, of the hydrogen atom, $E = 2p^2 m^*e^4 /e^2 h^2$, where, m^* is the electron effective mass, e is the electronic charge, e is the relative permittivity and h is the Plank constant. This minimum energy determines the threshold wavelength, k_e, which then varies as the fourth power of the refractive index. Experimental data on different photoconductive compounds show that the values of n^4 /k_e were close to 77 throughout a range of refractive indices.

The similarities in the quotient show that the photoelectrons stem from the same type of lattice imperfections, or alternatively, the binding energies to the different types of hydrogen-like centers are similar. Thus the Moss relation was formulated as [3]: n4 ke ¼ 77=lm ð1Þ where n is the refractive index and ke is the wavelength corresponding to the absorption edge. In terms of energy gap, this is [9]: n4 Eg ¼ 95 eV ð2Þ According to this relation, the refractive index of a semiconductor can be determined with a known energy gap, Eg. This relation, again, was based on the general assumption that all energy levels in a solid are scaled down by a factor of 1=e2 eff.
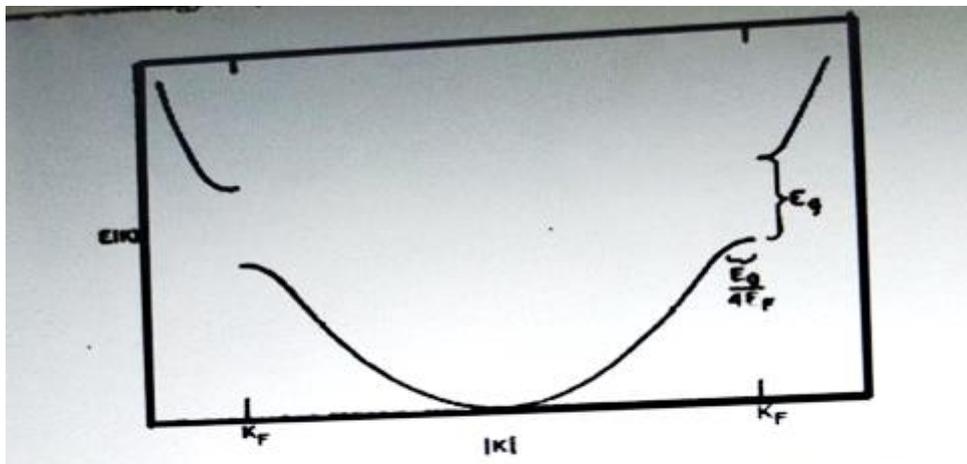
Fig. 1. Electron energy as a function of k for isotropic three-dimensional nearly free electron model [10].
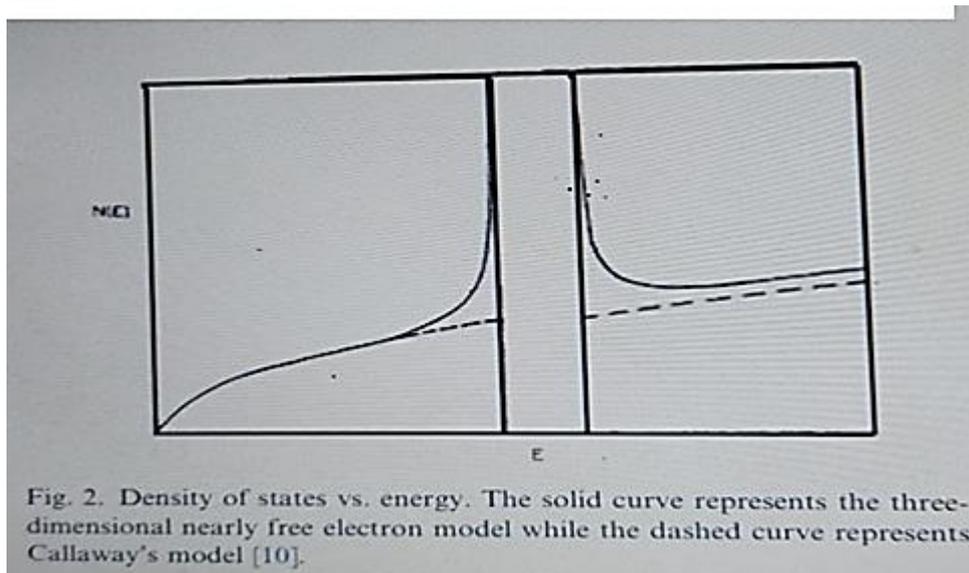
Fig. 2. Density of states vs. energy. The solid curve represents the three-dimensional nearly free electron model while the dashed curve represents Callaway's model [10].

Penn model

In 1962, Penn [10] proposed a simple model for an isotropic semiconductor with electrons in a sphere of momentum space and are characterized by an isotropic energy gap. In his investigation of a nearly free electron model for a semiconductor, Penn showed that two common assumptions were flawed in Callaway's approximation of the static dielectric constant [11]. Previous semiconductor models did not allow for the formation of standing waves in the Brillouin zone. The Umklapp process was neglected. The energy, E, and wave function, w, with respect to the state k for this model are given by, E k ¼ 1 2 fE0 k þ E0 k0 ½ðE0 k E0 k0Þ 2 þ E2 g 1=2 g wk ¼ ðeikr þ a k eik0 r Þ=½1 þ ða k Þ 2 1=2 where a k 1 2 Eg=ðE k E0 k0Þ E0 k ðh2 =2mÞk2 ; k0 k 2KF^k ð3Þ Here, E is the electron energy, k is the wave vector, KF is the Fermi wave vector and a represents

an averaged Jones boundary [12]. The electron energy E as a function of wave vector k for an isotropic three-dimensional free electron model is plotted in Fig. 1. This model of placing the energy gap above the Fermi surface was first suggested by Callaway [11] in his investigation of the correlation energy of electrons. Fig. 2 shows the density of states vs. the energy and describes the treatment of the Penn model. The dashed line represents Callaway's model and the solid line represents the Penn model. According to the Penn model, the states from the energy gap are removed and piled up at the top of the valence band and the bottom of the conduction band [10]. The resulting graph is thus asymptotic.

Ravindra relation

The Ravindra relation, which was initially proposed empirically [13] was shown to be an approximation [14] of the Penn model [10]. One feature common to all the semiconductor band structures is that the valence and conduction bands are more or less parallel to each other at least along the symmetry directions. This formed the basis for Gupta and Ravindra [14] to define: Ep ¼ Eg þ K ð9Þ Using Eq. (9) in the Penn model in Eq. (8) and considering the situation for which Eg/K < 1, Gupta and Ravindra arrived at an expression for the refractive index: n ¼ K1 K2Eg þ K3E2 g K4E3 g ð10Þ where the values of K are calculated by Gupta and Ravindra [14] and the higher values are neglected since they are too small to be considered. Eq. (10) then reduces to a form: n ¼ 4:16 1:12Eg þ 0:31E2 g 0:08E3 g ð11Þ The oscillator model from Wemple [15] defines the dielectric constant as: e =1+ Ed/E0 where e is the real part of the complex dielectric constant, Ed is the oscillator strength and E0 is the average energy gap which is approximately equal to the Penn energy gap, Ep. Performing a similar treatment with the dielectric function in the optical region, they [14] show a similar equation for the refractive index with the constants evaluated.

Moss relation and its implications

It is perhaps noteworthy to mention that other optical properties of semiconductors are merely integral relations to the energy gap and refractive index. Moss [9] pointed out that the absorption edge can be calculated using the refractive index. Moss [9] showed that the refractive index and absorption edge are related by:

which for long wavelengths at zero frequency becomes, n 1 ¼ 1 2p2 Z K dk

Here, K is the absorption coefficient and ke is the wavelength corresponding to the absorption edge. This function is integrated over the wavelength rather than energy. This expression shows that the long wavelength refractive index is determined simply by the total area under the curve of absorption coefficient vs. wavelength – it is independent of the absorption spectrum [18]. As a result, if a certain level of absorption persists over a given energy interval – as it occurs where absorption is due to transitions between two allowed energy bands – then, the smaller the width of the forbidden zone, the greater will be the spread of absorption in wavelength, resulting in a greater value of the integral and larger n [9].

In conducting this study, Herve and Vandamme [22] found two particular temperature dependences. Generally, the energy gap and temperature are inversely proportional for most semiconductors, that is, as T increases, the energy gap decreases, and, as a result, the refractive index increases. This occurs in diamond and similar structures. On the other hand, infrared detector materials including the lead sulphide, lead selenide and lead telluride exhibit a positive temperature coefficient of energy gap and negative refractive index temperature

dependence. Herve and Vandamme [22] found that the Moss relation showed the strongest deviation at lower energy gaps.

The pressure derivative of the refractive index is another significant parameter which explains pressure induced distortion. The first pressure derivative calculated through the Ravindra relation indicates a greater effect of applied hydrostatic pressure to the refractive index. Results of calculations show that the pressure derivative is negative and this appears to be the trend among the III–V group. However, a study by Johanssen et al. [29] shows a direct linear relation between refractive index and increase in pressure. Thus, it is believed that ionicity of the material plays a significant role in determining the magnitude and sign of the pressure coefficient of refractive index.

Conclusion

The various energy gap–refractive index relations and their applications to semiconductors have been summarized in the above study. The analysis examines the contributions of Moss, Penn, Finkenrath, Wemple and Ravindra. Applications of these relations to IR detector materials such as Pb1xSrxSe and Hg1xZnxTe and UV detector material such as GaN have been discussed.

N.M. Ravindra is indebted to Dr. T.S. Moss for his enormous appreciation of the fundamental physics of semiconductors and beyond. He appreciates very much his interactions with Dr. Moss for over 15 years which continued without any impediment from physical or geographical boundaries. Dr. Moss will be dearly missed but his contributions to fundamental semiconductor physics will go a long way. The work reported in this paper is dedicated to Dr. T.S. Moss.

References :

1. N.M. Ravindra, NJIT Internal Memorandum, Applications Specific Coating Technology, July 2005.
2. N.F. Mott, R.W. Gurney, Electronic Processes and Ionic Crystals, Oxford University Press, London, 1940.
3. B. Gudden, R.W. Pohl, Z. Phys. 37 (1926) 881.
4. T.S. Moss, Phys. Stat. Sol. (B) 131 (1985) 415.
5. N.M. Ravindra, Sushil Auluck, V.K. Srivastava, Phys. Stat. Sol. (B) 93 (1979) K155.
6. G. Yu, H. Ishikawa, M. Umeno, T. Egawa, J. Watanabe, T. Soga, T. Jimbo, Appl. Phys. Lett. 73 (1998) 1472.
7.] R. Zheng, T. Taguchi, M. Matssura, J. Appl. Phys. 87 (2000) 2526.