Calculations of Dielectric Constant for AlGaInAs Quaternary Semiconductor Alloy in the Transparent Region and Above (0.4-4.0eV)

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ABSTRACT

The modeling of the spectral behavior of the refractive index of AlGaInAs quaternary III-V semiconductor alloy in the energy range from 0.4 to 4eV, including the transparent region, is presented. The extended model of interband transition contributions incorporates not only the fundamental absorption edge contribution to the dielectric function, but also contributions from higher energy and indirect transitions. It is demonstrated that indirect energy transitions must be included in the calculations of the complex dielectric function of the material in the transparent region. Indirect transitions from different critical points in the Brillouin zone are treated separately. The comparison between the theoretical refractive indices and the experimental data for AlGaInAs alloy is presented. These calculations have been applied to the design of Bragg mirrors with the highest refractive index contrast for heterostructure lasers.

INTRODUCTION

The design and analysis of such devices as injection lasers, photodiodes, detectors, solar cells, multilayer structures, and microcavities requires the exact knowledge of the optical constants of III-V compound semiconductors in the region near the fundamental absorption edge as well as at the higher photon energies. In modeling of the optical constants of semiconductors in the fundamental optical region, several approaches are typically used: (1) empirical formulas, (2) damped harmonic oscillator (DHO) models, (3) standard critical point (SCP) models. Optical constants determined from empirical formulas (such as the Sellmeier dispersion equations for the refractive index and Urbach's rule for the absorption coefficient [1], or the expression for n based on interpolation of a dielectric quantity using Vegard's rule by Burkhard *et al*.[2]) are not related through the Kramers-Kronig dispersion relation and are valid only over a very limited energy range.

A semi-empirical single effective oscillator model based on quasi-classical Boltzmann equation or Drude theory proposed by Wemple *et al*.[3] does provide an analytical expression for the dispersion of the semiconductor refractive index at photon energies significantly below the direct band edge. The Drude theory ignores the carrier related effects around the band gap, and thus the results are valid only in the low optical frequency region. This model also lacks the agreement with experimental data at the band edge, which is the energy range of the most interest for semiconductor laser devices.

The standard critical point (SCP) model can determine the position of critical points of the semiconductor band structure, but cannot accurately predict the dielectric function [4]. The modified SCP model was initially proposed by Korovin [5] and Cardona *et al.*[6], and then developed by Adachi [7], and Lin *et al*.[8]. The model of interband transition contributions (ITC model) was introduced as a method to analyze the refractive index of III-V compounds at energies below and above the direct band gap by including the electron-hole pair transitions, and by adding the excitonic terms at the two lowest energy gap transitions. The comparison between

available experimental results of the spectral behavior of III-V compound semiconductors and the theoretical data calculated using the above mentioned models often reveals a lack of agreement, which is pronounced for the photon energies around the fundamental absorption edge. These differences may arise from the excitonic effects, which are largely ignored in the calculations of the real part of the dielectric constant [8].

In the present work, an extended model of interband transition contributions (EITC) is developed for the calculations of real and imaginary parts of the dielectric constant of compound semiconductors. The model introduces (1) the broadening effects, caused by phonon and defect scattering in direct and indirect transitions; (2) the strength of direct band gap transitions as a function of the effective electron, heavy hole and light hole masses of the semiconductor; (3) the exciton contributions; (4) the separate contributions of E_x and E_l indirect band gap transitions to the real and imaginary part of the dielectric constant. The importance of indirect and higher direct energy transitions is demonstrated through these calculations and through the comparison with experimental results. The detailed description of our extended ITC model is given in Reference [9], where the index of refraction for the following alloys has also been calculated and compared with the available experimental results: AlP, AlAs, AlSb, GaP, GaAs, GaSb, InP, InAs, InSb, AlGaAsSb, AlGaInAs, AlGaInP, GaInAsSb, and GaInPAs. In this work we apply the extended ITC model for the calculation of the dielectric constant of AlGaInAs alloy, which is then used for the Bragg mirror design.

THE EXTENDED ITC MODEL

The dielectric constant $\varepsilon(E) = \varepsilon_1(E)+i\varepsilon_2(E)$ describes the optical response of the medium as a function of photon energy E. The imaginary part of the dielectric function $\varepsilon_2(E)$ is calculated based on a simplified model of the band structure using the joint density of states for each Critical Point (CP) considered. The real part of the dielectric function $\varepsilon_1(E)$ was calculated through the knowledge of the imaginary part, $\varepsilon_2(E)$, by employing the Kramers-Kronig relation [10]. Thus, the total imaginary and real parts of the dielectric function are presented as a sum of several terms that represent the contribution of different energy CPs. These points are associated with electronic transitions in the band structure at the energies designated as E_0, $E_0+\Delta$, E_0^{ex}, E_1, E_2, and E_i. In case of quaternary, $A_xB_yC_zD$, semiconductor alloy each of the terms become a function of the alloy mole fraction, x, y and z=1-x-y. There are several absorption mechanisms [11] that contribute to the imaginary part of the dielectric constant, therefore $\varepsilon_2(E)$ can be written as:

$$\varepsilon_2(E,x,y) = \varepsilon_2^{Eo}(E,x,y) + \varepsilon_2^{exEo}(E,x,y) + \varepsilon_2^{Eo+\Delta}(E,x,y) + \\ + \varepsilon_2^{E1}(E,x,y) + \varepsilon_2^{E2}(E,x,y) + \varepsilon_2^{Ei}(E,x,y) \quad (1)$$

where ε_2^{Eo} and $\varepsilon_2^{Eo+\Delta}$ are contributions due to the absorption by direct interband optical transitions near the fundamental absorption edge and spin-orbit transitions, ε_2^{exEo} is due to the absorption by the discrete series of excitons near the E_0 energy gap, ε_2^{E1} and ε_2^{E2} are contributions of the higher energy interband transitions, and ε_2^{Ei} is due to the indirect interband absorption effects. Similarly, the real part of the dielectric function can be presented as the following sum:

$$\varepsilon_1(E,x,y) = \varepsilon_1^{Eo}(E,x,y) + \varepsilon_1^{exEo}(E,x,y) + \varepsilon_1^{Eo+\Delta}(E,x,y) + \\ + \varepsilon_1^{E1}(E,x,y) + \varepsilon_1^{E2}(E,x,y) + \varepsilon_1^{Ei}(E,x,y) \quad (2)$$

The absorption spectrum for photon energies greater than the band gap energy is composed of many peaks correlated with Van-Hove singularities of the joint density of states [11]. For III-V zinc-blende type semiconductors, the contributions of two main peaks (E_1 and E_2) must also be included. These peaks correspond to the direct optical transitions at the L and X points of the BZ, respectively. The E_1 peak is treated as a two-dimensional M_0 type critical point, while the structure of the E_2 peak is characteristic of a damped harmonic oscillator.

The detailed description of the individual contributions to the real and imaginary parts of the dielectric constant is given in the Reference [9]. The presented model is applicable in the photon energy range from 0.4eV to about 4eV. The initial crystal parameters required for the calculations include energy band gap values, effective electron and hole masses, static dielectric constant, and the values of the bowing parameters used for the energy band gap calculations for the ternary alloys. The complex dielectric constant and refractive index of binary alloys (AlAs, GaAs, InAs) were first calculated and the results were then used in the calculation for AlGaInAs quaternary alloy. The reported model also incorporates the lifetime broadening effects of the free electron-hole pair states through the damping parameters [12].

The refractive index of a semiconductor, n(E), and the extinction coefficient, k(E), were calculated in terms of the complex dielectric function as follows:

$$n(E) = \left[\frac{\varepsilon_1(E)}{2} + \frac{\sqrt{\varepsilon_1(E)^2 + \varepsilon_2(E)^2}}{2} \right]^{1/2} \tag{3}$$

$$k(E) = \left[\frac{\sqrt{\varepsilon_1(E)^2 + \varepsilon_2(E)^2}}{2} - \frac{\varepsilon_1(E)}{2} \right]^{1/2} \tag{4}$$

There are a total of 12 unknown parameters required by the model in Eqs.(1) and (2) for the real and imaginary part of the dielectric constant of a binary alloy, which include strength and damping parameters for various transitions. These parameters are obtained by fitting through minimization of the total error function, F, over all available experimental points for each semiconductor alloy of interest, which is given below as:

$$F = \sum_{i=1}^{N} \left((n_{th}(E_i) - n_{exp}(E_i))^2 + (k_{th}(E_i) - k_{exp}(E_i))^2 \right) \tag{5}$$

CALCULATION RESULTS AND DISCUSSION

The present investigation of the optical properties of the III-V semiconductor alloys is centered on describing the behavior of the refractive index for the photon energies in the transparent region as well as for the higher energies. The calculated index of refraction from our extended ITC model and the available experimental data for AlGaInAs quaternary semiconductor alloy are shown in Figures 1 and 2 demonstrating excellent agreement between the two. The strongest resonance peak of the index of refraction occurs at the E_1 transition energy. The E_1 peaks in this calculation appear to be generally sharper than the experimental values, which can be explained by the absence of the lifetime broadening effects in the current model for the E_1 optical transition.

It is believed that by adding the broadening constant as well as including the exciton effects for the E_1 transition energy, better agreement for this peak can be obtained. The increase in the broadening parameter of AlGaInAs alloy is reported, which may be attributed to the

potential fluctuations resulting from random atomic placement in the quaternary alloys as compared with binary alloys. Maximum anion disorder occurs at y=0.5, while that for the cation occurs at x=0.5 and y=1 [13]. Therefore, the high atomic disorder in the triple-cation sublattice of $Al_{0.3}Ga_{0.16}In_{0.54}As$ alloy with compositions x, y, z close to the middle point may be responsible for the slight deviations of the calculated refractive index from the one determined experimentally. In this case the bowing parameters can no longer be represented as a quadratic function of the alloy composition. The atomic disorder and composition fluctuations are expected to broaden the optical spectra.

The valley contributions to the real part of the dielectric constant are separated according to the partition of the Brillouin zone. The L region with corresponding direct E_l and indirect E_L optical transition energy contributes approximately 65 –75% to the total value of the dielectric constant while the Γ region corresponding to the E_0 transition accounts to about 5-10%, the X region, which is represented by indirect E_X energy and constant M, contributes about 15 to 30% of the total. Thus, the index of refraction is essentially determined by the band structure away from the center of the BZ, and modifications of the electronic structure at L and X points rather than Γ CPs, produce the observed variations in the index of refraction.

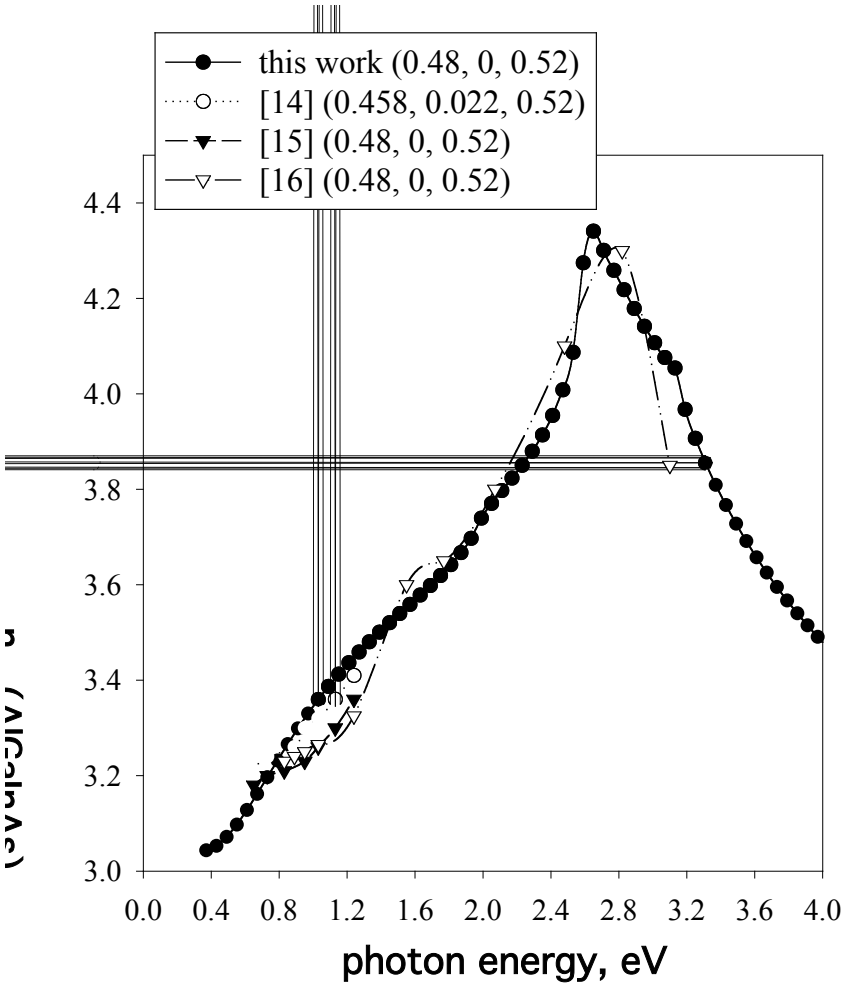

Figure 1. Refractive index of $Al_xGa_yIn_zAs$ for x=0.48, y=0, z=0.52.

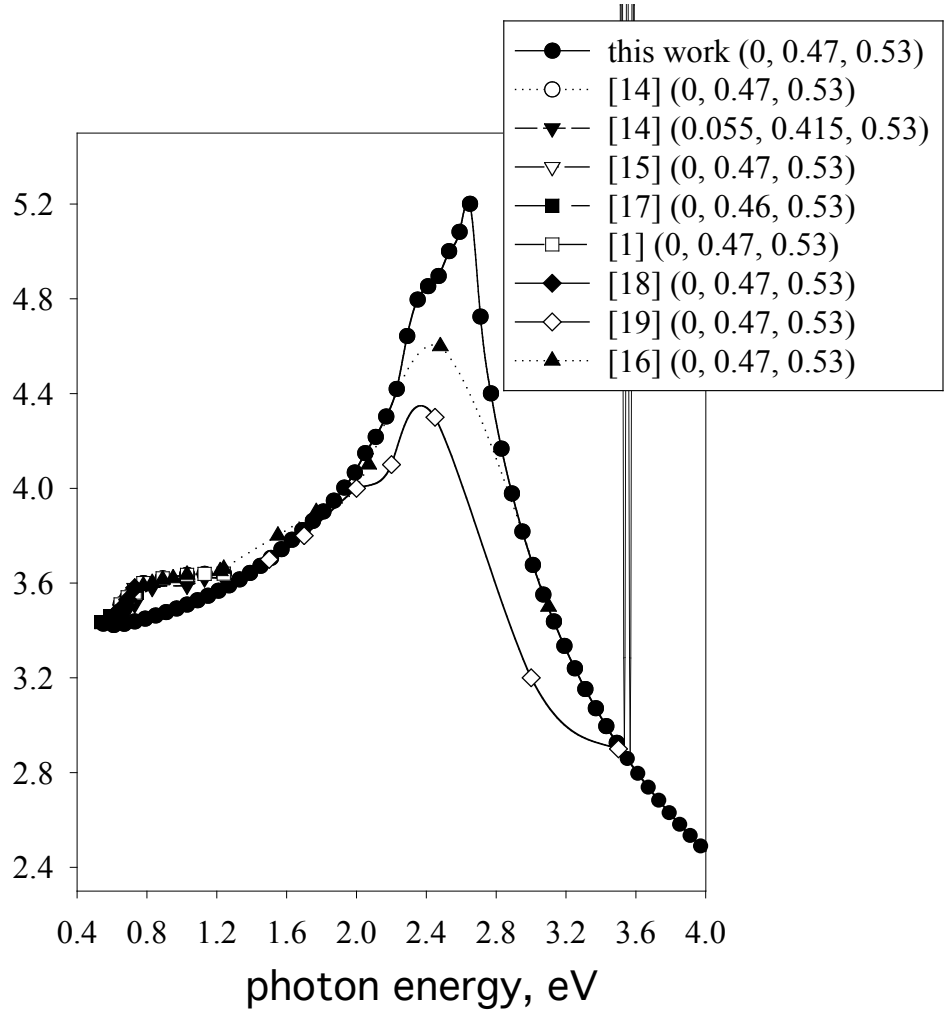

Figure 2. Refractive index of $Al_xGa_yIn_zAs$ for x=0, y=0.47, z=0.53.

The contribution to the total dielectric function of 3D discrete exciton transitions close to the E_0 transition energy are found to be negligible, about 0.1%, due to the very narrow spectral range of such transitions.

The results of the $Al_xGa_yIn_zAs$ alloy investigation were extrapolated to the different compositions of interest to photonic devices. In order to select the optimal materials for the semiconductor Distributed Bragg Reflectors (DBRs) for application in long wavelength Vertical Cavity Surface Emitting Lasers (VCSELs), the maximum and minimum refractive indices were calculated for response to the incident photon energy of 0.8eV for the alloys lattice matched to the InP substrate under the direct band gap conditions. The $Al_{0.05}Ga_{0.42}In_{0.53}As$/InP material system with index of refraction difference of 0.46 is therefore recommended for the Bragg mirror applications.

SUMMARY

An extended ITC model and calculations of optical properties for AlGaInAs quaternary III-V semiconductor alloy are presented and the results are compared with the experimental data. The successful fit of the refractive indices in the transparent optical region as well as for the

higher photon energies was attained by combining several interband transition contributions. The largest contribution to the dielectric function is due to the direct and indirect optical transitions along <111> and <100> directions in the BZ, which accounts for 85-90% of the total contributions. Therefore, except for the optical absorption in the vicinity of the Γ gap, most of the optical properties of the material, especially the index of refraction, are determined by the electronic structure around L point, rather than at the center of the BZ. Since our model is more sensitive to the indirect band gap transitions, the nature of the indirect band gap contributions to the total dielectric function of the alloy may be better understood. The influence of the discrete exciton states around the E_0 edge at room temperature was found negligible. We have applied the results of these calculations to the AlGaInAs/InP material system for applications as semiconductor distributed Bragg reflectors.

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