

Calculations of Optical Properties for Quaternary III-V Semiconductor Alloys in the Transparent Region and Above (0.2-4.0eV)

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Abstract

The modeling of the spectral behavior of the refractive indices of the binary, ternary and quaternary III-V semiconductor alloys in the energy range from 0.2 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 AlGaAsSb, AlGaInAs, AlGaInP, GaInAsSb, and GaInPAs alloys is presented. These calculations have been applied to the design of Bragg mirrors with the highest refractive index contrast for heterostructure lasers.

Keywords: dielectric constant, compound semiconductors, optical properties, interband transition contributions.

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. The refractive indices have been reported for many III-V binary, as well as for limited number of ternary compounds. However, this data is limited and does not extend to many compounds of present interest. It is therefore important to develop a theoretical model, which is both extensive and accurate.

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 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 harmonic oscillator model does not incorporate the concept of the optical energy band gap. Thus, the optical energy band gap of semiconductors cannot be directly determined from this approach [4]. 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.

When the photon energy is smaller than the band gap energy, the quasi-classical Boltzmann equation or Drude theory based on a simple harmonic oscillator model can be applied [1]. However, the Drude theory ignores the carrier related effects around the band gap and the results are valid only in the low optical frequency region. An extension of the Drude theory through the quantum density matrix method has been presented by Jensen *et al.*[5]. The experimentally observed dispersion of the refractive index near the fundamental absorption edge can be accounted for by a quantum mechanical calculation, which modifies the wavelength dependence predicted by the classical Drude theory. This approach differs from the usual method of the refraction index calculation, which involves the initial calculation of the imaginary part of the dielectric constant and integrating it using the Kramers-Kronig relation to obtain the real part of the dielectric constant. The advantage of this method is that an expression for the index of refraction, n , can be obtained in terms of band structure parameters, such as the energy band gap, E_g , the spin-orbit splitting energy, Δ , and the effective masses.

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 [6] and Cardona *et al.*[7], and then developed by Adachi [8], and Lin *et al.*[9]. 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 [9].

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_i 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 the Appendix. We note that a parameter fit is required for the present extended ITC model, which is similar to the SCP model parameter fitting. However, after the above listed changes are introduced into the SCP model, the resulted extended ITC theoretical model shows better agreement with available experimental results. The index of refraction for the following alloys has been calculated: AlP, AlAs, AlSb, GaP, GaAs, GaSb, InP, InAs, InSb, AlGaAsSb, AlGaInAs, AlGaInP, GaInAsSb, and GaInPAs. The comparison between the available experimental and calculated data is presented for the above mentioned quaternary semiconductor alloys. Finally, we have used the results of these calculations in the design of Bragg mirrors for Vertical Cavity Surface Emitting Lasers.

The Extended ITC Model

The dielectric constant $\epsilon(E) = \epsilon_1(E) + i\epsilon_2(E)$ describes the optical response of the medium as a function of photon energy E . The imaginary part of the dielectric function $\epsilon_2(E)$ 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 $\epsilon_1(E)$ was calculated through the knowledge of the imaginary part, $\epsilon_2(E)$, 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 ternary, $A_xB_{1-x}C$, and quaternary, $A_xB_{1-x}C_yD_{1-y}$, semiconductor alloys each of the terms become a function of the alloy mole fraction, x and y . There are several absorption mechanisms [11] that contribute to the imaginary part of the dielectric constant, therefore $\epsilon_2(E)$ can be written as:

$$\begin{aligned} \epsilon_2(E, x, y) = & \epsilon_2^{E_0}(E, x, y) + \epsilon_2^{exE_0}(E, x, y) + \epsilon_2^{E_0+\Delta}(E, x, y) + \\ & + \epsilon_2^{E_1}(E, x, y) + \epsilon_2^{E_2}(E, x, y) + \epsilon_2^{E_i}(E, x, y) \end{aligned} \quad (1)$$

where $\epsilon_2^{E_0}$ and $\epsilon_2^{E_0+\Delta}$ are contributions due to the absorption by direct interband optical transitions near the fundamental absorption edge and spin-orbit transitions, $\epsilon_2^{exE_0}$ is due to the absorption by the discrete series of excitons near the E_0 energy gap, $\epsilon_2^{E_1}$ and $\epsilon_2^{E_2}$ are contributions of the higher energy interband transitions, and $\epsilon_2^{E_i}$ is due to the indirect interband absorption effects.

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 E_1 peak arises from the transitions occurring over a large portion of the BZ around the L critical point (CP), between the upper valence band (VB) and the lowest conduction band (CB) along the $\langle 111 \rangle$ direction in the Brillouin zone. The higher interband transitions in the X region, along the $\langle 100 \rangle$ direction, usually do not correspond to a single well defined critical point (CP). The peak is assumed as a combination of several transitions resulting in a peak in the joint density of states. These transitions can occur between the upper VB and the lower components of the second CB around the Γ CP, between the upper VB and the second lowest CB plus spin-orbit splitting component, between the upper VB and lower CB along the $\langle 100 \rangle$ X direction. Because the investigated model is concerned primarily with the lower energy transitions, the higher interband transition contributions from the X region were modeled as a constant M contribution. Similarly, the real part of the dielectric function can be presented as the following sum:

$$\begin{aligned} \varepsilon_1(E, x, y) = & \varepsilon_1^{E_0}(E, x, y) + \varepsilon_1^{exE_0}(E, x, y) + \varepsilon_1^{E_0+\Delta}(E, x, y) + \\ & + \varepsilon_1^{E_1}(E, x, y) + \varepsilon_1^{E_2}(E, x, y) + \varepsilon_1^{E_i}(E, x, y) \end{aligned} \quad (2)$$

The detailed description of the individual contributions to the real and imaginary parts of the dielectric constant is given in the Appendix. The presented model is applicable in the photon energy range from 0.2eV to about 4eV. The crystal parameters such as energy band gap values, effective electron and hole masses, and static dielectric constant employed in the calculations are given in the Table 1 [1,12]. Also, the values of the bowing parameters used for the energy band gap calculations for the ternary alloys are listed in the Table 2 [12-16]. The complex dielectric constant and refractive index of binary alloys were first calculated and the results were then used in the calculations for quaternary alloys.

It is noted that the dielectric constant of the semiconductor also depends on the impurities or lattice defects as well as on the alloy disorder and lattice thermal vibrations. These effects reduce lifetime of the free electron-hole pair states through the lifetime broadening effects included in the present model [17]. The intensity of the exciton spectrum is also known to be strongly affected by damping or lifetime broadening [17].

When the incident photon energy is insufficient to cause band-to-band transition or formation of excitons, the nonlinear optical absorption process in a semiconductor can still occur through the excitation of lattice vibrations, and through the two photon absorption or free-carrier absorption which involves the emission or absorption of phonon [7]. The effect of intraband transitions on the optical properties of

semiconductors is known to be observed at energies well below the fundamental band edge and to become increasingly pronounced towards longer wavelengths. Their contribution to the refractive index can be obtained from the classical Drude dispersion theory. Since the present extended ITC model primarily deals with the transition energies around and above the fundamental absorption edge of the semiconductor under consideration, the effect of free carrier absorption at very low energies was not included in the calculations. As a result, the presented model has the lower limit of the applicable energies set at approximately 0.2eV.

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:

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

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

where ω denotes the photon frequency and c denotes the speed of light in vacuum.

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. These parameters are obtained through minimization of the total error function, F , over all available experimental points for each semiconductor alloy of interest, and is given below as:

$$F = \sum_{i=1}^N \left((n_{th}(E_i) - n_{exp}(E_i))^2 + (k_{th}(E_i) - k_{exp}(E_i))^2 \right) \quad (75)$$

Tables 3-6 provide the values of the fitted parameters used in the calculations of the refraction index of the quaternary semiconductor alloys.

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 as well as the comparison with the available experimental data for several quaternary III-V semiconductor alloys is shown in Figures 1-12. Excellent agreement between calculations and experiments is shown, although for two compositions, $Al_{0.3}Ga_{0.16}In_{0.54}As$ and $Al_{0.22}Ga_{0.29}In_{0.49}P$, the difference between the theory and experiment is about 0.1 in the units of the index of refraction. The strongest resonance peak of the index of refraction occurs at the E_1 transition energy for all alloys. 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 bowing constants of the E_0 transition for the quaternary damping parameters were found positive for all alloys investigated. The increase in the broadening parameter 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 $y=1$ [18]. Therefore, the high atomic disorder in the triple-cation sublattice of $Al_{0.3}Ga_{0.16}In_{0.54}As$ and $Al_{0.22}Ga_{0.29}In_{0.49}P$ alloys with compositions x, y, z close to the middle point may be responsible for the 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 strength parameters of the indirect band gap transitions, described by D_L and D_X , show a splitting behavior for most of the alloys. The strength of these transitions is usually divided unequally, with one of the parameters being higher than the other one. This behavior arises from the unequal contribution of indirect optical transitions over different regions of the Brillouin zone. Our calculations do not show that transitions from the L CP prevail as has been assumed in other models [12,19].

The valley contributions to the real part of the dielectric constant are separated according to the partition of the Brillouin zone. For all materials, the L region with corresponding direct E_1 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.

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 continuum exciton transitions at the E_0 CP are very similar to noninteracting electron hole pair characteristics, and therefore their contribution is similar to regular $\epsilon(E)$ expressions at the E_0 energy [20]. Exciton transitions usually are not observed when either the thermal energy exceeds the exciton binding energy, or when screening effects push the exciton levels into the continuum of CB [21]. Therefore, room temperature excitonic effects are not as important as those at low temperatures. At low temperatures, the optical spectra may not be explained within the framework of the one-electron approximation used for RT model, since the excitonic effects may profoundly modify the CP singularity structure [20].

The results of the $\text{Ga}_x\text{In}_{1-x}\text{P}_y\text{As}_{1-y}$, $\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$, $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$, $\text{Ga}_x\text{In}_{1-x}\text{P}_y\text{As}_{1-y}$, $\text{Al}_x\text{Ga}_y\text{In}_z\text{As}$ and $\text{Al}_x\text{Ga}_y\text{In}_z\text{P}$ alloys 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 highest index of refraction difference can be found in GaInAsSb, AlGaInAs, GaInPAs, GaSb, InAs and InSb alloys. The $\text{Al}_{0.05}\text{Ga}_{0.42}\text{In}_{0.53}\text{As}/\text{InP}$ 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 the quaternary III-V semiconductor alloys 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 for all alloys is due to the direct and indirect optical transitions along $\langle 111 \rangle$ and $\langle 100 \rangle$ 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 materials, 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. The strength of the excitonic transitions is weak and contributes only 0.1% to the dielectric constant. The continuum exciton states at the E_0 and E_1 CPs are believed to have a one-electron like characteristics. This ensures that the continuum exciton contributions to the dielectric constant can be approximated using the expression for the regular E_0 or E_1 transitions. 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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Appendix

E_0 and $E_0+\Delta$ Transitions: $\epsilon_2^{E_0}(E)$ and $\epsilon_1^{E_0}(E)$, $\epsilon_2^{E_0+\Delta}(E)$ and $\epsilon_1^{E_0+\Delta}(E)$ contributions

The direct band gap E_0 and the spin-orbit level $E_0+\Delta$ transitions in the diamond and zinc-blende type semiconductors occur at the center of the Brillouin zone, at the Γ point. These transitions are the three-dimensional M_0 critical points. The relation between the band structure and $\epsilon_2(E)$ is given as:

$$\epsilon_2(E) = \frac{e^2 \hbar^2}{\pi m E^2} \int dk^3 M_{cv}(k)^2 \delta [E_c(k) - E_v(k) - E] \quad (6)$$

where the Dirac δ function represents the joint spectral density of states between the valence (VB) and conduction band (CB) states differing by the energy $E=\hbar\omega$ of the incident light, and $M_{cv}(k)$ is the momentum matrix element between the VB and CB states. In order to evaluate the contribution of the E_0 critical point (CP) to ϵ_2 , we considered the momentum matrix element $M_{cv}(k)$ to be constant with respect to the photon energy. Therefore, the expression in Eq.(6) for ϵ_2 then becomes:

$$\epsilon_2^{E_0}(E) = \frac{A}{E^2} \int dk^3 \delta [E_c(k) - E_v(k) - E] \quad (7)$$

where A is the fitting parameter which contains all of the constants and the momentum matrix element. The integral in Eq.(7) is the joint density of states which is proportional to the square root of energy, resulting in [17]:

$$\epsilon_2^{E_0}(E) = \sum_{i=1}^2 \frac{2A_i}{3E^2} \sqrt{E - E_0} \Theta(E - E_0) \quad (8)$$

where $i=1$ denotes heavy hole and $i=2$ denotes light hole. The fitting parameters A_i are given by:

$$A_1 = \frac{\sqrt{2}e^2 M_{cv}^2 u_{hh}^{1.5}}{4\pi\epsilon_0 m_0 \hbar} = \frac{\alpha}{4} u_{hh}^{1.5} \quad \text{and} \quad A_2 = \frac{\sqrt{2}e^2 M_{cv}^2 u_{lh}^{1.5}}{12\pi\epsilon_0 m_0 \hbar} = \frac{\alpha}{12} u_{lh}^{1.5} \quad (9)$$

where $\alpha = \frac{\sqrt{2}e^2 M_{cv}^2}{\pi\epsilon_0 m_0 \hbar}$

where ϵ_0 is a permittivity of vacuum, and m_0 is a free electron mass. The reduced effective mass (Eq.(10)) of the electron/heavy hole (light hole), is given as $u_{hh}(u_{lh})$, where m_e^* is the effective electron mass and m_{hh}^* is the effective heavy hole mass:

$$\frac{1}{u_{hh}} = \frac{1}{m_e^*} + \frac{1}{m_{hh}^*} \quad (10)$$

Solving Kramers-Kronig relation for the E_0 contribution to ϵ_2 , we obtain:

$$\epsilon_1^{E_0}(E) = \sum_{i=1}^2 \frac{A_i}{E^2} \left[2\sqrt{E_0} - \sqrt{E_0 + E} - \sqrt{E_0 - E} \Theta(E_0 - E) \right] \quad (11)$$

where $\theta(x)$ is the Heaviside step function,

$$\Theta(x) = \begin{cases} 1, & \text{for } x \geq 0 \\ 0, & \text{for } x < 0 \end{cases} \quad (12)$$

The model includes two types of interband transition contributions to the dielectric function at the lowest direct band gap: free electron-hole pair transition (band-to-band transition) and the Wannier exciton transitions or discrete series excitons. The free exciton transitions in the vicinity of the E_0 CP are introduced through a weakly bounded exciton, having a ground state Rydberg energy given by:

$$R_{ex} = \frac{u_{hh}e^4}{8h^2\epsilon_s^2\epsilon_0^2} \quad (13)$$

where ϵ_s is the static dielectric constant.

The $\epsilon_2^{ex}(E)$ part of the imaginary dielectric function given in Eq.(14) is due to the E_0 ground state exciton transitions, and may be described by a Lorentzian line shape [20]. The lifetime broadening effects caused by phonon and defect scattering are included as a complex part of the photon energy $E = \hbar\omega + i\Gamma$, where Γ is the half-width at half-maximum (HWHM) of the Lorentzian function for the transitions investigated. Hence, the following expression is obtained for the imaginary part of the dielectric function for the E_0 transition [9]:

$$\begin{aligned} \epsilon_2^{E_0}(E) = & \epsilon_2^{ex}(E) + \\ & + \sum_{i=1}^2 \left[\frac{2\pi\sqrt{R_i^{ex}} A_i \left(0.5 + a \tan\left(\frac{(E - E_0)}{\pi\Gamma_0}\right) \right)}{\left(E^2 + \Gamma_0^2\right) \left[1 - 2\exp(a_i)\cos(b_i) + \exp(2a_i)\right]} \times \right. \\ & \left. \times \left[\left(E^2 - \Gamma_0^2\right) \left[1 - \exp(a_i)\cos(b_i)\right] + 2E\Gamma_0 \exp(a_i)\sin(b_i) \right] \right] \end{aligned} \quad (14)$$

$$\text{where } A_{ex} = \frac{e^2\hbar^2 M_{cv}^2}{2\epsilon_0 m_0}, \quad a_i = -\pi\sqrt{2R_i^{ex}} \sqrt{\frac{\sqrt{\Gamma_0^2 + (E - E_0)^2} + E - E_0}{\Gamma_0^2 + (E - E_0)^2}}$$

$$\text{and } b_i = \pi\sqrt{2R_i^{ex}} \sqrt{\frac{\sqrt{\Gamma_0^2 + (E - E_0)^2} - E + E_0}{\Gamma_0^2 + (E - E_0)^2}}$$

$$\epsilon_2^{ex}(E) = \frac{A_{ex}}{\pi E^2} \left(\frac{\Gamma_{ex}^{hh}}{a_{hh}^3 \left[(E - E_{hh}^{ex})^2 + \Gamma_{hh,ex}^2 \right]} + \frac{\Gamma_{ex}^{lh}}{3a_{lh}^3 \left[(E - E_{lh}^{ex})^2 + \Gamma_{lh,ex}^2 \right]} \right) \quad (15)$$

where E_{hh}^{ex} (E_{lh}^{ex}) is the heavy hole (light hole) exciton transition energy given by: $E_0 - R_{hh}^{ex}$ ($E_0 - R_{lh}^{ex}$), and a_{hh} (a_{lh}) is the radius (in Å) of the ground state heavy hole (light hole) exciton given as $(0.529 \epsilon_s m_0)/u_{hh}$. The HWHM of the Lorentzian line-shape function is given as Γ_0 for the E_0 transition, and the HWHM of the

Lorentzian function for the heavy hole or light hole transitions is given as Γ_{ex} . To simplify the model, $\Gamma_{\text{hh}}^{\text{ex}}$ and $\Gamma_{\text{lh}}^{\text{ex}}$ are considered to be equal.

The same broadening and excitonic effects are introduced into the expression of the real part of the dielectric function from Eqs.(14) and (15), and we obtain:

$$\begin{aligned} \varepsilon_1^{E_0}(E) = & \varepsilon_1^{\text{ex}}(E) + \\ & + \left(\frac{A_{\text{hh}} + A_{\text{lh}}}{(E^2 - \Gamma_0^2)^2 + (2E\Gamma_0)^2} \right) \left[(E^2 - \Gamma_0^2)(2\sqrt{E_0} - r_1 - r_2) - 2E\Gamma_0(r_3 + r_4) \right] \end{aligned} \quad (16)$$

$$\text{where } r_1 = \sqrt{\frac{E_0 + E + \sqrt{\Gamma_0^2 + (E_0 + E)^2}}{2}}$$

$$r_2 = \sqrt{\frac{E_0 - E + \sqrt{\Gamma_0^2 + (E_0 - E)^2}}{2}}$$

$$r_3 = \sqrt{\frac{-E_0 - E + \sqrt{\Gamma_0^2 + (E_0 + E)^2}}{2}}$$

$$r_4 = \sqrt{\frac{-E_0 + E + \sqrt{\Gamma_0^2 + (E_0 - E)^2}}{2}}$$

and

$$\varepsilon_1^{\text{ex}}(E) = \frac{2A_{\text{ex}}}{\pi} \left(\frac{\frac{E_{\text{ex,hh}}^2 - E^2 + \Gamma_{\text{ex}}}{a_{\text{hh}}^3 E_{\text{hh}}^{\text{ex}} \left((E_{\text{ex,hh}}^2 - E^2 + \Gamma_{\text{ex}}^2)^2 + 4E^2 \Gamma_{\text{ex}}^2 \right)} +}{\frac{E_{\text{ex,lh}}^2 - E^2 + \Gamma_{\text{ex}}}{3a_{\text{lh}}^3 E_{\text{lh}}^{\text{ex}} \left((E_{\text{ex,lh}}^2 - E^2 + \Gamma_{\text{ex}}^2)^2 + 4E^2 \Gamma_{\text{ex}}^2 \right)}} \right) \quad (17)$$

The contributions from $E_0 + \Delta$ transitions to dielectric function are presented in the simplified form without broadening effects:

$$\varepsilon_2^{E_0+\Delta}(E) = \frac{A_{\text{so}}}{E^2} \sqrt{E - E_0 - \Delta} \Theta(E - E_0 - \Delta_0) \quad (18)$$

and

$$\varepsilon_1^{E_0+\Delta}(E) = \frac{A_{\text{so}}}{E^2} \left[2\sqrt{E_0 + \Delta} - \sqrt{E + E_0 + \Delta} - \sqrt{E_0 + \Delta - E} \Theta(E_0 + \Delta - E) \right] \quad (19)$$

where $A_{\text{so}} = \frac{\sqrt{2}e^2 M_{\text{cv}}^2 u_{\text{so}}^{1.5}}{6\pi\varepsilon_0 m_0 \hbar} = \frac{\alpha}{6} u_{\text{so}}^{1.5}$, and u_{so} denotes the reduced effective mass of electron/hole in the

spin-orbit split-off valence band.

E₁ Transitions: $\epsilon_2^{E1}(\mathbf{E})$ and $\epsilon_1^{E1}(\mathbf{E})$ contributions

The E₁ and E₁+Δ transitions occur along the <111> direction or at L point in the BZ. The longitudinal effective mass is much higher than its transverse counterpart, thus, one can treat these CP as the 2D minimum. Neglecting lifetime broadening effect, the contribution of the E₁ transition to $\epsilon_2(\mathbf{E})$ is given as [9]:

$$\epsilon_2^{E1}(E) = \frac{\pi E_1^2}{E^2} \left(B_1 - B_2 \sqrt{E_1 - E} \Theta(E_1 - E) \right) \Theta(E - E_{11}) \quad (20)$$

where B₁ and B₂ are the strength parameters of the E₁ transition, and E₁₁ is given as

$$E_{11} = E_1 - \left(\frac{B_1}{B_2} \right)^2 \quad (21)$$

From Eqs.(20) and (21), the real part of the dielectric function for E₁ transition consists of the two parts, ϵ_1^{B1} and ϵ_1^{B2} , or the contributions from B₁ term and B₂ term, respectively:

$$\epsilon_1^{B1}(E) = -\frac{B_1 E_1^2}{E^2} \ln \left(\frac{|E^2 - E_{11}^2|}{E_{11}^2} \right) \quad (22)$$

$$\epsilon_1^{B2}(E) = \begin{cases} \frac{B_2 E_1^2}{E^2} \left(P + \sqrt{E_1 - E} \ln \left(\frac{\left(\sqrt{E_1 - E} - \sqrt{E_1 - E_{11}} \right)}{|E - E_{11}|} \right) \right) & \text{for } E < E_1 \\ \frac{B_2 E_1^2}{E^2} \left(P - \sqrt{E - E_1} a \tan \left(\sqrt{\frac{E_1 - E_{11}}{E - E_1}} \right) \right) & \text{for } E \geq E_1 \end{cases} \quad (23)$$

$$\text{where } P = \sqrt{E + E_1} \ln \left(\frac{\left(\sqrt{E + E_1} - \sqrt{E_1 - E_{11}} \right)}{E + E_{11}} \right) - 2\sqrt{E_1} \ln \left(\frac{\left(\sqrt{E_1} - \sqrt{E_1 - E_{11}} \right)}{E_{11}} \right)$$

Introducing a broadening effect, Γ_1 , into the E₁ transitions the contribution of the B₁ term to $\epsilon_2(\mathbf{E})$ is given by:

$$\epsilon_2^{B1}(E) = \frac{E_1^2 B_1}{(E^2 + \Gamma_1^2)^2} \left(\begin{aligned} & \left(E^2 - \Gamma_1^2 \right) \left(\frac{\pi}{2} - a \tan \left(\frac{E_{11} - E}{\Gamma_1} \right) \right) + \\ & + E \Gamma_1 \ln \left(\frac{(E_{11} - E)^2 + \Gamma_1^2}{E_{11}^2} \right) + \frac{\Gamma_1 (E^2 + \Gamma_1^2)}{E_{11}} \end{aligned} \right) \quad (24)$$

and the contribution of the B₂ term to $\epsilon_2(\mathbf{E})$ is given by:

$$\begin{aligned}
\varepsilon_2^{B_2}(E) &= \\
&= \frac{E_1^2 B_2}{(E^2 + \Gamma_1^2)^2} \left(\begin{aligned} &(E^2 - \Gamma_1^2) \left(\frac{b_1 b_3}{2} - b_2 b_4 \right) + \\ &\left(b_1 b_4 + 2b_2 b_3 + \right. \\ &\left. + 2\sqrt{E_1} \ln \left(\frac{(\sqrt{E_1} - \sqrt{E_1 - E_{11}})}{E_{11}} \right) \right) - \\ &\left. - \Gamma_1 (E^2 + \Gamma_1^2) \left(\frac{\sqrt{E_1 - E_{11}}}{E_{11}} + \frac{0.5}{\sqrt{E_1}} \ln \left(\frac{(\sqrt{E_1} - \sqrt{E_1 - E_{11}})}{E_{11}} \right) \right) \right) \end{aligned} \right) \quad (25)
\end{aligned}$$

where b_1 , b_2 , b_3 , and b_4 and given by:

$$b_1 = \ln \left(\frac{E_1 - E_{11} + \sqrt{2} \sqrt{\sqrt{(E_1 - E)^2 + \Gamma_1^2} + E_1 - E} \sqrt{E_1 - E_{11}} + \sqrt{(E_1 - E)^2 + \Gamma_1^2}}{E_1 - E_{11} - \sqrt{2} \sqrt{\sqrt{(E_1 - E)^2 + \Gamma_1^2} + E_1 - E} \sqrt{E_1 - E_{11}} + \sqrt{(E_1 - E)^2 + \Gamma_1^2}} \right)$$

$$\begin{aligned}
b_2 &= a \tan \left(\frac{\sqrt{2} \sqrt{E_1 - E} + \sqrt{\sqrt{(E_1 - E)^2 + \Gamma_1^2} + E_1 - E}}{\sqrt{\sqrt{(E_1 - E)^2 + \Gamma_1^2} - E_1 + E}} \right) + \\
&+ a \tan \left(\frac{\sqrt{2} \sqrt{E_1 - E} - \sqrt{\sqrt{(E_1 - E)^2 + \Gamma_1^2} + E_1 - E}}{\sqrt{\sqrt{(E_1 - E)^2 + \Gamma_1^2} - E_1 + E}} \right)
\end{aligned}$$

$$b_3 = \sqrt{\frac{\sqrt{\sqrt{(E_1 - E)^2 + \Gamma_1^2} - E_1 + E}}{2}}$$

$$b_4 = \sqrt{\frac{\sqrt{\sqrt{(E_1 - E)^2 + \Gamma_1^2} + E_1 - E}}{2}}$$

The real part of the dielectric constant for the E_1 transition with introduced broadening effect is shown in Eqs.(26) and (27):

$$\varepsilon_1^{B1}(E) = \frac{-B_1 E_1^2}{(E^2 + \Gamma_1^2)^2} \times \left((E^2 - \Gamma_1^2) \left(\ln \left(\frac{\sqrt{(E + E_{11})^2 + \Gamma_1^2}}{E_{11}^2} \right) + \ln \left(\sqrt{(E - E_{11})^2 + \Gamma_1^2} \right) \right) - \right. \quad (26)$$

$$\left. - 2E\Gamma_1 \left(\frac{\pi}{2} - a \tan \left(\frac{E_{11} - E}{\Gamma_1} \right) \right) \right)$$

$$\varepsilon_1^{B2}(E) = \frac{B_2 E_1^2}{(E^2 + \Gamma_1^2)^2} \left((E^2 - \Gamma_1^2) \left(\begin{aligned} & \left(\sqrt{E_1 + E} \ln \left(\frac{\left(\sqrt{E_1 + E} - \sqrt{E_1 - E_{11}} \right)}{E_{11} + E} \right) - \right. \\ & \left. - 2\sqrt{E_1} \ln \left(\frac{\left(\sqrt{E_1} - \sqrt{E_1 - E_{11}} \right)}{E_{11}} \right) - \right. \\ & \left. - \frac{b_1 b_4}{2} - b_2 b_3 \right) - \right. \quad (27) \\ & \left. + E\Gamma_1 (b_1 b_3 - 2b_2 b_4) \right) \end{aligned} \right) +$$

The total contribution of the real and imaginary part of the dielectric function for the E_1 transition is calculated as a sum of the B_1 and B_2 terms presented above:

$$\varepsilon_2^{E1}(E) = \varepsilon_2^{B1}(E) + \varepsilon_2^{B2}(E) \quad (28)$$

$$\varepsilon_1^{E1}(E) = \varepsilon_1^{B1}(E) + \varepsilon_1^{B2}(E) \quad (29)$$

E_2 and Higher Transitions: $\varepsilon_2^{E2}(E)$ and $\varepsilon_1^{E2}(E)$ contributions

The contributions to the dielectric function from the transitions at energies higher than E_1 are usually labeled as E_2 and are modeled as a single damped harmonic oscillator with energy E_2 as presented in Eqs.(30) and (31):

$$\varepsilon_2^{E2}(E) = \frac{C\beta}{E_2 \left(\left(1 - \left(\frac{E}{E_2} \right)^2 \right)^2 + \left(\frac{E\beta}{E_2} \right)^2 \right)} \quad (30)$$

$$\varepsilon_1^{E_2}(E) = \frac{C \left(1 - \left(\frac{E}{E_2} \right)^2 \right)}{\left(\left(1 - \left(\frac{E}{E_2} \right)^2 \right)^2 + \left(\frac{E\beta}{E_2} \right)^2 \right)} \quad (31)$$

where C is the strength parameter of the E_2 transition, and β is the damping factor.

Since E_2 transitions in X region of the BZ do not correspond to a single, well defined CP, its characteristics is more complicated for analysis [17]. Higher energy transitions also contribute to the dielectric function. However, these contributions vary weakly with photon energy. Therefore, we have modeled the effects of these transitions as a single real additive constant, M, to the real part of the dielectric function.

Indirect Transitions: $\varepsilon_2^{Ei}(E)$ and $\varepsilon_1^{Ei}(E)$ contributions

Indirect transitions from Γ point states at the VB edge to the X and L point states at the CB edges are appreciable at room temperature. The transition requires a phonon to conserve both energy and momentum. The solution for $\varepsilon_2(E)$ using a second order time-dependent perturbation theory without introducing a broadening effect is given as [9]:

$$\varepsilon_2^{Ei}(E) = \frac{D}{E^2} \left(E - E_g^{id} \pm \hbar\omega_q \right) \Theta \left(E - E_g^{id} \pm \hbar\omega_q \right) \Theta(E_c - E) \quad (32)$$

where D is the indirect transition strength parameter, and E_c is a cutoff energy which accounts for the finite width of the energy bands. The phonon energy, $\hbar\omega_q$, taking part in the indirect transition was ignored in the final calculations. The energies of the indirect band gaps at X and L points are always different, and hence our model treats these transitions separately. Therefore, the dielectric function for the indirect transitions is presented as a sum of two terms corresponding to E_X and E_L indirect band gap energies with D_X and D_L as a strength parameters of these transitions:

$$\varepsilon_2^{Ei}(E) = \sum_{i=X}^L \left(\frac{D_i}{E^2} (E - E_i)^2 \Theta(E - E_L) \Theta(E_c - E) \right) \quad (33)$$

By applying Kramers-Kronig relation to $\varepsilon_2^{Ei}(E)$ the real part of the dielectric function due to indirect band gap transitions is obtained [9] and is given in Eq.(34):

$$\begin{aligned} \varepsilon_1^{Ei}(E) &= \\ &= \sum_{i=X}^L \left(\frac{2D_i}{\pi} \left(\frac{-E_i^2}{E^2} \ln \left(\frac{E_c}{E_i} \right) + \frac{(E + E_i)^2}{2E^2} \ln \left(\frac{E + E_c}{E + E_i} \right) + \frac{(E - E_i)^2}{2E^2} \ln \left| \frac{E - E_c}{E - E_i} \right| \right) \right) \end{aligned} \quad (34)$$

Introducing the lifetime broadening effects, Γ_X and Γ_L , to the E_X and E_L indirect band gap transitions, the dielectric function is described as:

$$\varepsilon_2^{Ei}(E) = \sum_{i=X}^L \left(\frac{D_i}{\pi(E^2 + \Gamma_i^2)^2} \left[d_1 E_i \Gamma_i (E^2 + \Gamma_i^2 - EE_i) + \frac{E_i \Gamma_i (E^2 + \Gamma_i^2)(E_c - E_i)}{E_c} + d_2 d_3 \right] \right) \quad (35)$$

$$\varepsilon_1^{Ei}(E) = \sum_{i=X}^L \left(\frac{D_i}{\pi(E^2 + \Gamma_i^2)} \left[-2E_i^2 (E^2 - \Gamma_i^2) \ln\left(\frac{E_c}{E_i}\right) + \frac{d_4}{2} \ln\left(\frac{(E + E_c)^2 + \Gamma_i^2}{(E + E_i)^2 + \Gamma_i^2}\right) + d_5 \right] \right) \quad (36)$$

where

$$d_1 = \ln\left(\frac{\left[\frac{(E_c - E)^2 + \Gamma_i^2}{(E_i - E)^2 + \Gamma_i^2}\right] \frac{E_i^2}{E_c^2}}{\left[\frac{(E_c - E)^2 + \Gamma_i^2}{(E_i - E)^2 + \Gamma_i^2}\right] \frac{E_i^2}{E_c^2}}\right)$$

$$d_2 = a \tan\left(\frac{E_c - E}{\Gamma_i}\right) - a \tan\left(\frac{E_i - E}{\Gamma_i}\right)$$

$$d = (E^2 + \Gamma_i^2)^2 - 2EE_i(E^2 + \Gamma_i^2) + E_i^2(E^2 - \Gamma_i^2)$$

$$d_4 = (E^2 + \Gamma_i^2)^2 + 2EE_i(E^2 + \Gamma_i^2) + E_i^2(E^2 - \Gamma_i^2)$$

$$d_5 = \frac{d_3}{2} \ln\left(\frac{(E - E_c)^2 + \Gamma_i^2}{(E - E_c)^2 + \Gamma_i^2}\right) + 2d_2 E_i \Gamma_i (EE_i - E^2 - \Gamma_i^2)$$

Composition Dependent Terms

For ternary and quaternary alloys, the composition dependence of the interband transition energies, the lattice constants, electron and hole effective masses and the fitting parameters has to be considered. The nonlinear dependence of the transition energies on the composition of the alloy is described through the corresponding binary alloy energies and ternary bowing parameters. The interpolation scheme is used to calculate the quaternary alloy energy band gap as a function of alloy composition (0...x...1, 0...y...1). For $A_xB_{1-x}C_yD_{1-y}$ quaternary alloy type the energy band gap is obtained as following [12-16]:

$$E_g(x, y) = \left(\begin{aligned} &x(1-x)[(1-y)E_{ABD}(x) + yE_{ABC}(x)] + y(1-y)[(1-x)E_{BCD}(y) + \\ &+ xE_{ACD}(y)] \end{aligned} \right) \times (x(1-x) + y(1-y))^{-1} \quad (37)$$

where E_{ABC} , E_{ABD} , E_{BCD} , and E_{ACD} are the ternary alloy energy band gaps containing the corresponding bowing parameters. For $A_xB_yC_zD$ ($AB_xC_yD_z$) type quaternary alloys (where $0 \dots x \dots 1$, $0 \dots y \dots 1$, $0 \dots z \dots 1$, $x+y+z=1$) the energy band gap is given by Eq.(38) below:

$$E_g(x, y) = \frac{xyE_{ABC}(u) + y(1-x-y)E_{ACD}(v) + x(1-x-y)E_{ABD}(w)}{xy + y(1-x-y) + x(1-x-y)} \quad (38)$$

$$\text{where } u = \frac{1-x+y}{2}; \quad v = \frac{2-x-2y}{2}; \quad w = \frac{2-2x-y}{2}.$$

The dependence of the energy band gap of the $A_xB_{1-x}C$ ternary alloy on its composition is given as:

$$E_g(x) = xE_{AC} + (1-x)E_{BC} - bp_{ABC}x(1-x) \quad (39)$$

where bp_{ABC} is a bowing parameter and, in general is a positive number. The bowing parameters used in the calculations are given in the Table 2 [12-16].

The composition dependence of the lattice constants, effective electron and hole masses of the ternary or quaternary alloys is given by the linear Vegard's law interpolation scheme. Application of the Vegard's law based on the linear behavior of the ternary or quaternary parameters allows one to find an unknown alloy parameter using the available binary alloy or end point constants. Hence, the composition dependence of $A_xB_{1-x}C$ ternary alloy parameter $P_{ABC}(x)$ is given as:

$$P_{ABC}(x) = xP_{AC} + (1-x)P_{BC} \quad (40)$$

where P_{AC} and P_{BC} are constant parameter values of the corresponding binary alloys. For the $A_xB_{1-x}C_yD_{1-y}$ quaternary alloy type, the parameter $P_{ABCD}(x,y)$ is expressed as:

$$P_{ABCD}(x, y) = x \cdot y \cdot P_{AC} + x \cdot (1-y) \cdot P_{AD} + (1-x) \cdot y \cdot P_{BC} + (1-x) \cdot (1-y) \cdot P_{BD} \quad (41)$$

Likewise, the expression for composition dependence of parameter $P_{ABCD}(x,y)$ for $A_xB_yC_zD$ ($AB_xC_yD_z$) quaternary alloy type is:

$$P_{ABCD}(x, y) = xP_{AB} + yP_{AC} + (1-x-y)P_{AD} \quad (42)$$

Each quaternary fitting parameter of the $A_xB_{1-x}C_yD_{1-y}$ alloy is modeled as a nonlinear function of the composition z and y , in the following form:

$$P(x, y) = x(1-x)P_{AC} + y(1-x)P_{BC} + x(1-y)P_{AD} + (1-x)(1-y)P_{BD} + BP_1x(1-x) + BP_2y(1-y) \quad (43)$$

where P_{AC} , P_{BC} , P_{AD} , P_{BD} are the binary constants corresponding to one of the fitting parameters (α , Γ_0 , B_1 , B_2 , E_1 , D_X , D_L , Γ_X , Γ_L , E_c , M), BP_1 and BP_2 are the corresponding bowing parameters. In the case of the $A_xB_yC_zD$ type alloy, the quaternary parameter is given as:

$$P(x, y) = xP_{AD} + yP_{BD} + zP_{CD} + BP_1x(1-x) + BP_2y(1-y) \quad (44)$$

Tables 5 and 6 present the values of the bowing parameter determined by fitting the theoretical dielectric function to the available experimental data for $\text{Ga}_x\text{In}_{1-x}\text{P}_y\text{As}_{1-y}$, $\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$, $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$, $\text{Ga}_x\text{In}_{1-x}\text{P}_y\text{As}_{1-y}$, $\text{Al}_x\text{Ga}_y\text{In}_z\text{As}$ and $\text{Al}_x\text{Ga}_y\text{In}_z\text{P}$ alloys.

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Figure Captions

- Figure 1. Refractive index of $\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ for $x=0.8$, $y=1$.
- Figure 2. Refractive index of $\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ for $x=0.4$, $y=1$.
- Figure 3. Refractive index of $\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ for $x=0.2$, $y=1$.
- Figure 4. Refractive index of $\text{Al}_x\text{Ga}_y\text{In}_z\text{As}$ for $x=0.3$, $y=0.16$, $z=0.54$.
- Figure 5. Refractive index of $\text{Al}_x\text{Ga}_y\text{In}_z\text{As}$ for $x=0.48$, $y=0$, $z=0.52$.
- Figure 6. Refractive index of $\text{Al}_x\text{Ga}_y\text{In}_z\text{As}$ for $x=0$, $y=0.47$, $z=0.53$.
- Figure 7. Refractive index of $\text{Al}_x\text{Ga}_y\text{In}_z\text{P}$ for $x=0.5$, $y=0$, $z=0.5$.
- Figure 8. Refractive index of $\text{Al}_x\text{Ga}_y\text{In}_z\text{P}$ for $x=0.22$, $y=0.29$, $z=0.49$.
- Figure 9. Refractive index of $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ for $x=0.85$, $y=0.14$.
- Figure 10. Refractive index of $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ for $x=0.47$, $y=1$.
- Figure 11. Refractive index of $\text{Ga}_x\text{In}_{1-x}\text{P}_y\text{As}_{1-y}$ for $x=0.24$, $y=0.49$.
- Figure 12. Refractive index of $\text{Ga}_x\text{In}_{1-x}\text{P}_y\text{As}_{1-y}$ for $x=0.47$, $y=0$.

Tables

Table 1. Material parameters of the binary III-V semiconductor alloys used in the calculations [1,12].

	AIP	AlAs	AlSb	GaP	GaAs	GaSb	InP	InAs	InSb
a, Å	5.464	5.661	6.136	5.451	5.653	6.096	5.869	6.058	6.479
E₀, eV	3.62	3.03	2.3	2.78	1.424	0.75	1.344	0.354	0.172
E_X, eV	2.41	2.153	1.615	2.272	1.804	1.25	2.74	2.28	1.71
E_L, eV	4.0	2.363	2.211	2.637	1.81	0.81	1.74	1.53	1.03
Δ, eV	0.0	0.3	0.673	0.08	0.341	0.819	0.07	0.38	0.85
M_{e lng}^{eff}	3.67	1.1	1.64	7.25	0.063	0.041	0.077	0.022	0.014
M_{e tr}^{eff}	0.212	0.19	0.23	0.313	-	-	-	-	-
M_{hh}^{eff}	0.513	0.409	0.94	0.56	0.5	0.28	0.56	0.35	0.34
M_{ln}^{eff}	0.211	0.153	0.14	0.16	0.076	0.05	0.12	0.026	0.016
ε_s	9.8	10.06	12.04	11.11	12.9	15.7	12.61	12.25	17.76

Table 2. Bowing parameters of the ternary semiconductor alloys used for the calculations of the energy band gap values [12-16].

	C₀, eV	C_X, eV	C_L, eV		C₀, eV	C_X, eV	C_L, eV
AIPsB	1.2	0.0	0.0	AlGaP	0.0	0.0	0.0
AIPAs	0.22	0.0	0.0	AlInP	0.0	0.0	0.0
AlAsSb	0.72	0.0	0.0	GaInP	0.758	0.15	0.68
GaPSb	1.2	0.0	0.0	AlGaAs	0.438	0.16	0.0
GaPAs	0.186	0.211	0.25	AlInAs	0.74	0.0	0.0
GaAsSb	1.2	1.09	0.09	GaInAs	0.4	0.15	0.5
InPSb	1.2	1.56	1.6	AlGaSb	0.47	0.0	0.21
InPAs	0.36	0.27	0.26	AlInSb	0.42	0.0	0.0
InAsSb	0.596	0.6	0.55	GaInSb	0.413	0.24	0.33

Table 3. Values of the fitted parameters obtained from the index of refraction simulations for the binary III-V semiconductor alloys, AlP, AlAs, AlSb, GaP, GaAs, GaSb.

	AlP	AlAs	AlSb	GaP	GaAs	GaSb
α	499.99	281.4	59.62	111.44	1238.17	5137.22
M	0.602	-2.247	1.499	1.116	2.087	25.04
Γ_0	0.01	0.001	0.001	0.01	0.0161	0.01
B₁	1.883	6.416	3.759	5.452	4.624	5.328
B₂	9.973	12.25	7.126	11.549	7.724	9.491
E₁	4.2	3.886	2.809	3.63	2.906	2.02
D_x	2.166	0.0	16.93	-13.48	13.81	-27.59
D₁	0.0	11.29	60.81	-5.581	5.03	9.548
Γ_x	0.01	0.001	0.001	0.01	0.001	-2.0
Γ_1	0.01	0.001	0.001	0.01	0.001	0.7783
E_c	6.01	8.077	4.268	3.238	5.771	35.1

Table 4. Values of the fitted parameters obtained from the index of refraction simulations for the binary III-V semiconductor alloys, InP, InAs, InSb.

	InP	InAs	InSb
α	873.09	4035.03	1289.11
M	3.163	6.91	3.298
Γ_0	0.01	0.28	0.0001
B₁	4.586	2.062	1.529
B₂	6.913	5.262	4.429
E₁	3.1	2.45	1.81
D_x	-42.51	-10.0	-42.88
D₁	14.077	48.31	51.89
Γ_x	0.01	0.01	0.01
Γ_1	0.01	0.01	0.01
E_c	3.325	3.145	3.907

Table 5. Bowing constants of the fitting parameters for the quaternary alloys, AlGaAsSb, GaInAsSb, GaInPAs.

	GaInPAs		GaInAsSb		AlGaAsSb	
	BP ₁	BP ₂	BP ₁	BP ₂	BP ₁	BP ₂
α	-1491.11	-1036.45	-1.92×10^{-3}	-0.65×10^{-3}	50.72	41.56
M	11.67	-138.59	5.26	-15.14	15.84	-8.13
Γ_0	-0.22	2.69	0.65	1.14	2.83	5.28
B₁	-7.79	108.05	-2.18	2.88	-1.71	-20.02
B₂	32.43	-6.08	-4.31	-12.28	-12.01	4.39
E₁	-0.75	163.55	-0.90	0.79	-0.13	15.16
D_x	-57.13	72.05	-8.89	-5.81	-72.98	-7.38
D₁	45.49	-121.09	-18.06	-19.73	0.49	1.97
Γ_x	5.57	-2.80	-7.01	-9.66	-0.52	-12.16
Γ_1	-0.14	1.35	-2.32×10^{-2}	4.83	-77.70	-64.30
E_c	-2.19	-0.49	-2.60	3.26	-2.61	12.33

Table 6. Bowing constants of the fitting parameters for the quaternary alloys, AlGaInAs and AlGaInP.

	AlGaInAs		AlGaInP	
	BP ₁	BP ₂	BP ₁	BP ₂
α	-24.67	-20.58	-0.21	-1.36
M	23.49	-4.44	4.33	-5.81
Γ_0	9.02	-1.02	-0.79	1.99
B₁	-13.31	12.81	-5.17	-8.29
B₂	-31.46	16.16	-5.72	1.66
E₁	-7.41×10^{-3}	7.66×10^{-2}	-6.78	0.55
D_x	-17.43	-43.29	-0.37	0.51
D₁	-26.72	-37.51	0.16	-0.35
Γ_x	-4.07	-9.60	6.18×10^{-2}	-4.01×10^{-2}
Γ_1	93.25	-2.32×10^{-2}	0.16	1.41
E_c	21.78	-7.74	-11.15	4.22























