Effect of subband nonparabolicity on optical properties of InSbAs/AlSb deep quantum well heterostructures

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Abstract. Optical properties of heterostructures with deep quantum wells have been studied in the framework of four-band Kane mode permitting a nonparabolic energy spectrum of charge carriers to be taken into account. The system AlSb/InAs$_{0.84}$Sb$_{0.16}$/AlSb was used as an example. It is established that the nonparabolicity weakly influences the overlap integral between $s$- and $p$-states, but notably increase the state density and optical absorption coefficient in the conduction band.

1. Introduction

Heterostructures with deep quantum wells that use InAsSb solid solutions as the active region can be considered as promising materials for infrared optoelectronics [1, 2]. These compounds are characterized by the bandgap width $E_g$ and effective electron mass $m_e$ that are minimum among $A_3B_5$ semiconductors [3, 4]. There is here a significant nonparabolicity in the energy spectrum of charge carriers. This necessarily leads to adjusting substantial corrections to the energies of dimensional quantization levels as compared to those observed under the parabolic dispersion law, even for the ground state of conduction band. The purpose of present investigation is to calculate the optical absorption coefficient and radiation recombination rate for intraband optical transitions between various subbands of dimensional quantization with and without nonparabolicity in the energy spectrum of AlSb/InAs$_{0.84}$Sb$_{0.16}$/AlSb heterostructure with deep quantum wells. The nonparabolicity in the energy spectrum is described with a four-band Kane model.

2. Basic Equations

For the charge carriers, we used the wave functions of the type $\psi = \Psi_s |s\rangle + \Psi_p |p\rangle$, where $|s\rangle$ and $|p\rangle$ are the Bloch functions of $s$- and $p$-type, and $\Psi_s$ and $\Psi_p$ are the spinors. Near the $\Gamma$-point, the spherical approximation Kane equations are given by the following expressions:

$$(E_c - E)\Psi_s - iP\nabla\Psi = 0,$$

$$(E_v - \delta - E)\Psi_p - iP\nabla\Psi_s + \frac{\hbar^2}{2m_0} (\gamma_1 + 4\gamma_2)\nabla(\nabla\Psi)$$

$$- \frac{\hbar^2}{2m_0} (\gamma_1 - 2\gamma_2) [\nabla \times [\nabla \times \Psi]] + i\delta[\sigma \times \Psi] = 0. \quad (1)$$

Here $E_c$ and $E_v$ are the energies of conduction and valence band edges, $P$ is the Kane matrix element, $\delta = \Delta_{so}/3$ is the spin-orbit splitting constant, $m_0$ is the free electron mass, $\gamma_1$ and $\gamma_2$ are generalized Lattinger parameters, and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices.
The nonparabolicity in the energy spectra are described by the following expressions:

\[ E_c = \frac{\hbar^2 (k_c^2 + q^2)}{2m_c}, \]

\[ E_{bh} = -E_g - \frac{\hbar^2 (k_{bh}^2 + q^2)}{2m_{bh}}, \]

\[ E_{lh} = -E_g - \frac{\hbar^2 (k_{lh}^2 + q^2)}{2m_{lh}}, \]

where \( E_c, E_{bh} \) and \( E_{lh} \) are the energies of electrons, heavy and light holes, \( k_c, k_{bh} \) and \( k_{lh} \) are the quantized wave vector components of electrons, heavy and light holes, \( m_h \) and \( m_l \) are effective masses of heavy and light holes.

The energy spectra with regard to their nonparabolic features are written for electrons and light holes as:

\[ P^2 (k^2_e + q^2) = \frac{E_c (E_c + E_g) (E_e + E_g + 3\delta)}{E_c + E_g + 2\delta}, \]

\[ E_{lh} = -E_g - \frac{3}{2} \delta - \frac{\hbar^2 (k_{lh}^2 + q^2)}{4} (m_l^{-1} + m_h^{-1}) \]

\[ + \sqrt{2\delta^2 + \left(\frac{\delta^2}{2} - \frac{\hbar^2 (k_{lh}^2 + q^2)}{4} (m_l^{-1} - m_h^{-1})^2 \right)^2}, \]

where \( m_i^{-1} = -\frac{2P^2}{\hbar^2 E_{lh}} + m_0^{-1}(\gamma_1 + 4\gamma_2) \) and \( m_0^{-1} = m_0^{-1}(\gamma_1 - 2\gamma_2) \).

The optical absorption coefficient \( \alpha \) as a function of transition frequency \( \omega \) is given by the following expression [6]:

\[ \alpha(\omega) = \sum_{i,j} \frac{4\pi}{\sqrt{\kappa_0}} \frac{e^2}{\hbar c a \hbar \omega} \int q d\mathbf{p} P_{ij}^2 \delta(E_i - E_j - \hbar \omega), \]

where the indices \( i \) and \( j \) refer to various subbands in the conduction and valence bands, \( \kappa_0 \) is a static dielectric permittivity, \( P_{ij}^2 = \left| P_{ij} \right|^2 + \left| P_{ji} \right|^2 \), and \( P_{ij} \) is the matrix element of optical transition in the four-band Kane model which is defined as \( P_{ij} = i \int \left< \Psi_i \right| \left< \Psi_j \right| \psi \right>, \)

The radiative recombination rate of quantum wells for non-degenerated electrons can be calculated using the following formula [7]:

\[ R_{ph} = \frac{4\kappa_\infty}{\sqrt{\kappa_0}} \frac{e^2}{\hbar c} \sum_{i,j} \left| P_{ij} \right|^2 \left( E_i(q_T) - E_j(q_T) \right) \frac{n_p}{N_j} \exp\left( -\frac{\varepsilon_j}{k_B T} \right), \]

where \( \kappa_\infty \) is a high frequency permittivity, \( q_T = \frac{\sqrt{2k_B m}\varepsilon}{\hbar} \) is the wave vector of thermal motion, \( T \) is absolute temperature, \( N_j = \frac{m_j k_B T}{\pi \hbar^2} \) is an effective density of states in the valence band, \( n \) and \( p \) are the carrier concentrations, and \( \varepsilon_j \) is the distance between the subband \( j \) and ground level in the valence band.

The radiative recombination time is presented by the following equation [7]:
\[ \tau_{phij} = \frac{\sqrt{k_0} \ h c}{4 \pi \kappa_e e^2} \left( \frac{\hbar c^2 m \ k_B T}{p_0 (q_f) \left( E_i(q_f) - E_j(q_f) \right)} \right) \exp\left( \frac{-e_j}{k_B T} \right). \]  

(6)

In the case of strong degeneracy, we should use \( q_F \) instead of \( q_T \) in formulas (5) and (6).

3. Results

The energies and quantized wave vector components calculated with and without nonparabolicity of energy spectrum with the quantum well width of \( a=10 \text{ nm} \) are presented in Table 1.

**Table 1.** Energies and quantized wave vector components for various levels of dimensional quantization in AlSb/InAs\(_{0.84}\)Sb\(_{0.16}\)/AlSb heterostructure with the quantum well width of \( a=10 \text{ nm} \) as calculated with and without allowance for the energy spectrum nonparabolicity.

| Dimensional quantization level | Without nonparabolicity | With nonparabolicity |
|-------------------------------|-------------------------|----------------------|
|                              | Quantized wave vector component \( k, 10^6 \text{ cm}^{-1} \) | Energy level \( E, \text{ meV} \) | Quantized wave vector component \( k, 10^6 \text{ cm}^{-1} \) | Energy level \( E, \text{ meV} \) |
| c1                            | 2.78                    | 163                  | 2.456                  | 95 |
| c2                            | 5.481                   | 632                  | 5.206                  | 294 |
| c3                            | 7.458                   | 1170                 | 8.051                  | 501 |
| hh1                           | 5.3                     | 26                   | 5.3                    | 26 |
| hh2                           | 6.66                    | 46                   | 2.66                   | 6 |
| lh1                           | 1.606                   | 46                   | 1.377                  | 20 |

The effective masses of charge carriers related to the dimensional quantization level and calculated with the four-band Kane model, are presented in Table 2.

**Table 2.** Charge carrier effective masses of various dimensional quantization levels in the AlSb/InAs\(_{0.84}\)Sb\(_{0.16}\)/AlSb heterostructure with the quantum well width of \( a=5 \text{ and } 10 \text{ nm} \) as calculated with and without regard to the nonparabolicity in the energy spectrum.

| Dimensional quantization level | \( a=5 \text{ nm} \) | \( a=10 \text{ nm} \) |
|-------------------------------|---------------------|---------------------|
|                              | Energy level \( E, \text{ meV} \) | \( m_\parallel / m_{0} \) | Energy level \( E, \text{ meV} \) | \( m_\parallel / m_{0} \) |
| c1                            | 220                 | 1.78                | 95                  | 1.341 |
| c2                            | 612                 | 3.104               | 294                 | 2 |
| c3                            | 1010                | 4.4                 | 501                 | 2.728 |
| c4                            |                     | 720                 | 3.46                |       |
| c5                            |                     | 938                 | 4.181               |       |
| c6                            |                     | 1150                | 4.784               |       |
| lh1                           | 114                 | 2.267               | 20                  | 1.339 |

As can be seen, the allowance for the nonparabolicity in the energy spectrum significantly influences the results of calculation for the positions of dimensional quantization levels and the carrier effective mass and, therefore, the density of states function.

The frequency dependences of a total optical absorption coefficient as calculated with and without allowance for nonparabolicity in the energy spectrum are presented in Fig. 1.
Fig. 1. Dependence of total optical absorption coefficient $\alpha$ on the optical transition frequency $\omega$ in the AlSb/InAs$_{0.84}$Sb$_{0.16}$/AlSb heterostructure with the quantum well width of $a=10$ nm as calculated in the framework of the parabolic spectrum model (dashed curve) and with allowance for the nonparabolicity in this spectrum, in the framework of four-band Kane model (solid curve).

The radiation recombination time for various optical transitions as calculated in cases of non-degenerated and strongly degenerate electrons, is given in Table 3.

Table 3. Radiative recombination time $\tau_{phi}$ for various optical transitions in AlSb/InAs$_{0.84}$Sb$_{0.16}$/AlSb heterostructure with quantum well width of $a=10$ nm, $T=300$ K, and $p=10^{12}$ cm$^{-2}$ as calculated with and without nonparabolicity in the energy spectrum in the cases of non-degenerated and strongly degenerate electrons ($n=5\times10^{12}$ cm$^{-2}$).

| Transition | Without nonparabolicity | With nonparabolicity |
|------------|-------------------------|----------------------|
|            | Non-degenerate electron case | Strongly degenerate case | Non-degenerate electron case | Strongly degenerate case |
|            | $\tau_{phi}$ s          | $\tau_{phi}$ s       | $\tau_{phi}$ s          | $\tau_{phi}$ s          |
| c1-hh1     | 8.1·10$^{-9}$          | 7.1·10$^{-9}$        | 1.2·10$^{-8}$          | 1.5·10$^{-8}$          |
| c2-hh1     | 2.5·10$^{-8}$          |                      | 2.2·10$^{-8}$          |                      |
| c3-hh1     | 4.3·10$^{-7}$          |                      | 9.6·10$^{-5}$          |                      |
| c1-hh2     | 4.5·10$^{-7}$          | 2.7·10$^{-8}$        | 2.9·10$^{-7}$          | 7.6·10$^{-8}$          |
| c2-hh2     | 3.6·10$^{-7}$          |                      | 1.1·10$^{-7}$          |                      |
| c1-lh1     | 1.02·10$^{-7}$         | 1.8·10$^{-7}$        | 1.1·10$^{-7}$          | 2·10$^{-7}$           |
| c2-lh1     | 5.8·10$^{-7}$          |                      | 4.6·10$^{-7}$          |                      |

As can be seen, the allowance for the nonparabolicity in the spectrum for non-degenerate electrons leads to the radiative recombination time that increases for the transitions with coinciding parity of the initial and final states and to this time decreasing for the transitions between the states of different parity.
4. Conclusions
It has been thus calculated that the nonparabolicity in the energy spectrum in heterostructures with deep quantum wells significantly influences the energy levels of dimensional quantization, leading to a significant increase in the radiation absorption coefficient, especially for the optical transitions with participation of high-energy electrons.

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