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Original research article

A theoretical evaluation of optical properties of InAs/InP quantum wire with a dome cross-section

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A B S T R A C T

In the present work, we have theoretically studied the optical properties of a InAs quantum wire with dome cross section. We have used a numerical method which is based on a combination of coordinate transformation and the finite difference method. For this purpose, we have used analytical expressions for optical properties obtained by the compact-density matrix formalism. We have evaluated the linear, non-linear and the total absorption coefficients between the ground state for electron and heavy hole as a function of photon energy. The linear, non-linear and total refractive index changes are also investigated. These optical properties are determined with varying the incident optical intensity and the height of the wire.

1. Introduction

In recent years, there has been considerable interest in the physics of low-dimensional semiconductor structures. These structures confine charge carriers in one, two, and three dimensions, notably when this quantum confinement leads to formation of discrete energy levels, the enhancement of the density of states at specific energies and the change of electronic and optical properties [1,2]. For example, these structures are superlattices, quantum wires, single and multiple quantum wells, and quantum dots [2–5]. The most important classes of semiconductor heterostructures is the class of quantum wires. Among them, quantum wires with rectangular [6], triangular [7], T-shaped [8], V-groove [9,10], dome [11,12] and other cross sections have received a particular interest due to the progress in semiconductor growth techniques like chemical lithography [13,14], molecular-beam epitaxy [15,16], etc.

In an earlier paper [11], we have studied the electronic properties of quantum wire with different shapes using a numerical method based on the combination of coordinate transformation and the finite difference method (FDM). We have investigated the influence of the quantum wire shape and height; first on the electron and hole energy levels and second on the transition energies.

Recently, the linear and nonlinear optical properties of lowdimensional semiconductor structures have been widely studied by several workers [17–23] due to their potential applications in optoelectronic and photonic devices. Accordingly, in the present paper, we intend to study the optical properties of InAs/InP quantum wire with dome cross-section. We use the density matrix formulation to obtain the linear and third-order nonlinear absorption coefficient and refractive index changes. For example, Khordad et al. [24–26] investigated the non-linear and total intersubband absorption coefficients and refractive index change by using the density matrix formalism.

We evaluate interband optical absorption coefficients and refractive index changes of the wire as a function of photon energy. The evaluation has been performed in two ways: (1) Keeping height of the wire fixed and varying the incident optical intensity (2) keeping incident optical intensity fixed and varying the height of the wire.

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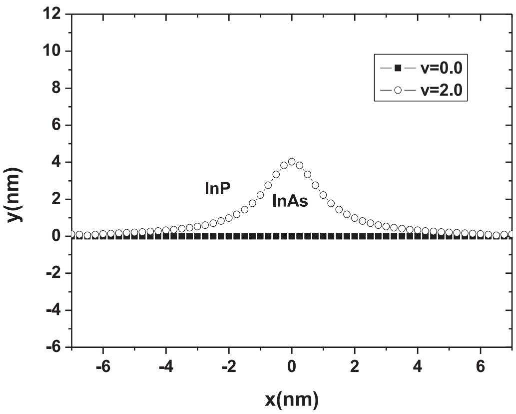

Fig. 1. The cross-section profile of quantum wire in the real x–y space.

We outlined this work as follows: In Section 2, we will present the total Hamiltonian of the system and relevant eigenvalues. In addition, some details of the theoretical method and the appropriate choice of coordinate transformation will be also exposed. In Section 3, using the density matrix, we will obtain the linear and nonlinear interband optical absorption coefficients and refractive index changes. Section 4 will be confined to the results and discussion whereas Section 5 will be presenting the conclusions.

2. The Hamiltonian

The quantized energy levels E for electrons (holes) in conduction (valence) band and their corresponding wave functions $\psi(x, y)$allows us to study the linear, nonlinear and total absorption coefficients and refractive index changes of the system. Therefore, in this part, we solve the Schrodinger equation for a charge carrier in a quantum wire which have a dome-like shape (Fig. 1).

Electrons (holes) in a quantum wire are described by the effective mass Hamiltonian which is given by

$$H = -\frac{\hbar^2}{2}\left(\nabla\frac{1}{m^*(x, y)}\nabla\right) + V(x, y) \tag{1}$$

We obtain the electron (hole) energy levels E and their corresponding wave function by solving the Schrodinger equation,

$$-\frac{\hbar^2}{2}\left(\nabla\frac{1}{m^*(x, y)}\nabla\right)\psi(x, y) + V(x, y)\psi(x, y) = E\psi(x, y) \tag{2}$$

m^* is the electron or hole effective mass, E is the confinement energy and $V(x, y)$ is the total potential which is given by:

$$V(x, y) = \frac{\hbar^2 k_z^2}{2m^*} + V_p(x, y)$$

$V_p(x, y)$ is the $2D$ potential profile determined by the conduction or valence band offset, we can write Eq. (2) as:

$$-\frac{\hbar^2}{2}\left(\frac{\partial}{\partial x}\frac{1}{m^*_{x,y}}\frac{\partial\psi(x, y)}{\partial x} + \frac{\partial}{\partial y}\frac{1}{m^*_{x,y}}\frac{\partial\psi(x, y)}{\partial y}\right) + \left[\frac{\hbar^2 k_z^2}{2m^*} + V_p(x, y)\right]\psi(x, y) = E\psi(x, y) \tag{3}$$

Once the coordinate transformation $x = x(u, v)$ and $y = y(u, v)$ is chosen, the Schrodinger equation Eq. (3) becomes:

$$-\frac{\hbar^2}{2}\left[u_x\frac{\partial}{\partial u}\left(\frac{u_x}{m^*}\frac{\partial\psi}{\partial u} + \frac{v_x}{m^*}\frac{\partial\psi}{\partial v}\right) + v_x\frac{\partial}{\partial v}\left(\frac{u_x}{m^*}\frac{\partial\psi}{\partial u} + \frac{v_x}{m^*}\frac{\partial\psi}{\partial v}\right) + u_y\frac{\partial}{\partial u}\left(\frac{u_y}{m^*}\frac{\partial\psi}{\partial u} + \frac{v_y}{m^*}\frac{\partial\psi}{\partial v}\right) + v_y\frac{\partial}{\partial v}\left(\frac{u_y}{m^*}\frac{\partial\psi}{\partial u} + \frac{v_y}{m^*}\frac{\partial\psi}{\partial v}\right)\right] + V_p\psi = E\psi \tag{4}$$

Where $\psi[x(u, v), y(u, v)] = \psi(u, v)$, $V_p[x(u, v), y(u, v)] = V_p(u, v)$, $u_{x,y} = u_{x,y}(u, v)$ and $v_{x,y} = v_{x,y}(u, v)$.

As seen in an earlier paper [11], we took advantage of numerical method of FDM to solve the Schrodinger equation throughout our complex geometry. Therefore, we can discretize Eq. (4) as follows:

$$-\frac{\hbar^2}{2K^2}\left[\begin{array}{l} M^1_{uu}\left(\frac{1}{m^*}\right)_{i+1/2,j} - M^2_{uu}\left(\frac{1}{m^*}\right)_{i-1/2,j} + M^1_{uv}\left(\frac{\mu}{m^*}\right)_{i+1/2,j} - M^2_{uv}\left(\frac{\mu}{m^*}\right)_{i-1/2,j} + \\ \mu_{i,j}\left[M^1_{vu}\left(\frac{1}{m^*}\right)_{i,j+1/2} - M^2_{vu}\left(\frac{1}{m^*}\right)_{i,j-1/2} + M^1_{vv}\left(\frac{\mu}{m^*}\right)_{i,j+1/2} - M^2_{vv}\left(\frac{\mu}{m^*}\right)_{i,j-1/2}\right] + \\ \rho_{i,j,k}\left[M^1_{vv}\left(\frac{\rho}{m^*}\right)_{i,j+1/2} - M^2_{vv}\left(\frac{\rho}{m^*}\right)_{i,j-1/2}\right] \end{array}\right] + V_{pi,j}\psi_{i,j} = E_{i,j}\psi_{i,j} \tag{5}$$

where