Calculation of the energy levels and wave functions of electrons in nanowires by the shooting method

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In this work, the energy levels and wave functions in rectangular and cylindrical nanowires with a finite potential well are calculated. The Schrödinger equation in Cartesian and cylindrical coordinate systems was solved by the shooting method. The calculations take into account the nonparabolicity of the energy spectrum of electrons. The graphs of the dependence of the energy levels on the sizes of nanowires are obtained. When calculating the energy levels and wave functions, changes in the effective mass of electrons were taken into account. The calculations were performed for the quantum well of the InP/InAs/InP heterostructure.

Keywords: Nanowires, Quantum wells, Heterostructure, Energy levels, Wave function, Nonparabolic zone

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1. Introduction

In recent years, ongoing miniaturization of electronic circuits led to an emerging interest in nanoscaled materials. These unique properties can be attributed to the limited motion of electrons in the confined dimensions of the nanomaterial. The study of semiconducting one-dimensional structures has been an important problem in the physics of solid state. At present, the energy spectrum of electrons and holes in quantum wells of InP/InAs/InP heterostructures is being intensively calculated.

In works [1, 2], technologies for growing nanowires are given and nanowires with various sizes are obtained. In [3], the relaxation time of the electron spin in a semiconductor quantum wire was experimentally investigated. The spectrum of optical absorption in quantum wires of different radii is investigated. To determine the energy spectrum and wave function of electrons in rectangular quantum nanowires in [4–6], the Schrödinger equation was solved by various mathematical methods. For a cylindrical quantum wire with a finite potential and parabolic dispersion, the Schrödinger equations were solved analytically [7, 8]. The Schrödinger equation was solved by the shooting method for rectangular [9] and cylindrical [10, 11] quantum wires. This work is devoted to calculating the energy of electrons in a quantum wire with a finite potential using the shooting method.

2. Calculation of the energy and wave function of electrons in a quantum wire with a finite potential well by the shooting method

We will solve the Schrödinger equation for electrons with variable effective mass using the shooting method [10]. In this case, the effective mass is a function of the electron coordinate, the Schrödinger equation can be written in the following form.

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial y}\frac{1}{m^*(y)}\frac{\partial}{\partial y}\psi(y)+V(y)\psi(y)=E\psi(y) \quad (1)$$

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z}\psi(z)+V(z)\psi(z)=E\psi(z) \quad (2)$$

Equations (1) and (2) can be rewritten in the following form.

$$\frac{\partial}{\partial y}\frac{1}{m^*(y)}\frac{\partial}{\partial y}\psi(y) = \frac{2}{\hbar^2}(V(y)-E)\psi(y) \tag{3}$$

$$\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z}\psi(z) = \frac{2}{\hbar^2}(V(z)-E)\psi(z) \tag{4}$$

We divide the left sides of equations (3) and (4) into separate parts.

$$\frac{1}{m^*(y)}\frac{\partial^2}{\partial y^2}\psi(y) - \frac{1}{(m^*(y))^2}\frac{\partial}{\partial y}m^*(y)\frac{\partial}{\partial y}\psi(y) = \frac{2}{\hbar^2}(V(y)-E)\psi(y) \tag{5}$$

$$\frac{1}{m^*(z)}\frac{\partial^2}{\partial z^2}\psi(z) - \frac{1}{(m^*(z))^2}\frac{\partial}{\partial z}m^*(z)\frac{\partial}{\partial z}\psi(z) = \frac{2}{\hbar^2}(V(z)-E)\psi(z) \tag{6}$$

The derivatives of the wave function and effective mass are replaced by the following transformations.

$$\frac{d\psi}{dy} \approx \frac{\Delta\psi}{\Delta y} = \frac{\psi(y+\delta y)-\psi(y-\delta y)}{2\delta y}, \qquad \frac{d\psi}{dz} \approx \frac{\Delta\psi}{\Delta z} = \frac{\psi(z+\delta z)-\psi(z-\delta z)}{2\delta z} \tag{7a}$$

$$\frac{d^2\psi}{dy^2} \approx \frac{\psi(y+\delta y)-2\psi(y)+\psi(y-\delta y)}{(\delta y)^2}, \qquad \frac{d^2\psi}{dz^2} \approx \frac{\psi(z+\delta z)-2\psi(z)+\psi(z-\delta z)}{(\delta z)^2} \tag{7b}$$

$$\frac{dm}{dy} \approx \frac{m(y+\delta y)-m(y-\delta y)}{2\delta y}, \qquad \frac{dm}{dz} \approx \frac{m(z+\delta z)-m(z-\delta z)}{2\delta z} \tag{7c}$$

Substituting expressions (7a), (7b), and (7c) into equations (5) and (6), we obtain the following equations

$$\frac{\psi(y+\delta y)}{m^*(y+\delta y/2)} = \left[\frac{2(\delta y)^2}{\hbar^2}(V(y)-E) + \frac{1}{m^*(y+\delta y/2)} + \frac{1}{m^*(y-\delta y/2)}\right]\psi(y) - \frac{\psi(y-\delta y)}{m^*(y-\delta y/2)} \tag{8}$$

$$\frac{\psi(z+\delta z)}{m^*(z+\delta z/2)} = \left[\frac{2(\delta z)^2}{\hbar^2}(V(z)-E) + \frac{1}{m^*(z+\delta z/2)} + \frac{1}{m^*(z-\delta z/2)}\right]\psi(z) - \frac{\psi(z-\delta z)}{m^*(z-\delta z/2)} \tag{9}$$

Using these equations, one can calculate the wave functions and energy levels of electrons in a potential well from a finite depth.

3. Calculation of the energy levels of electrons of a cylindrical quantum wire with a finite depth of the potential well by the method of Shooting

The Schrödinger equation in a cylindrical coordinate system is as follows:

$$-\frac{\hbar^2}{2}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\frac{\rho}{m(\rho)}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right)f(\mathbf{r}) + U(\mathbf{r})f(\mathbf{r}) = Ef(\mathbf{r}) \tag{10}$$

We seek the solution of this equation in the following form.

$$f(\mathbf{r}) = e^{ik_z z}e^{il\varphi}\psi(\rho) \tag{11}$$

Here the parameters kx and l do not depend on coordinates. Therefore, equation (10) will be solved for the radial wave function. Taking into account the coordinate dependence of the effective mass, the Schrödinger equation takes the following form.

$$-\frac{\hbar^2}{2\rho}\frac{\partial}{\partial\rho}\frac{\rho}{m(\rho)}\frac{\partial}{\partial\rho}\psi(\rho) + V(\rho)\psi(\rho) = E\psi(\rho) \tag{12}$$

Equation (12) is solved by the finite difference method [10]. In this case, we will use expressions (7a), (7b), (7c) for the derivatives of the effective mass and wave functions of electrons. Then equation (12) takes the following form.

$$\rho m(\rho)\frac{\psi(\rho+\delta\rho)-2\psi(\rho)+\psi(\rho-\delta\rho)}{(\delta\rho)^2}- \frac{\psi(\rho+\delta\rho)-\psi(\rho-\delta\rho)}{2\delta\rho}\left(\rho\frac{m(\rho+\delta\rho)-m(\rho-\delta\rho)}{2\delta\rho}-m(\rho)\right) = \frac{2\rho(m(x))^2}{\hbar^2}[V(\rho)-E]\psi(\rho) \quad (13)$$

Hence follows the following equation.

$$\psi(\rho+\delta\rho)= \frac{8\left\{\frac{(\delta\rho m(x))^2}{\hbar^2}[V(\rho)-E]+m(\rho)\right\}}{\left\{2m(\rho)\left(2+\frac{\delta\rho}{\rho}\right)-m(\rho+\delta\rho)+m(\rho-\delta\rho)\right\}}\psi(\rho)- \frac{\left\{2m(\rho)\left(2-\frac{\delta\rho}{\rho}\right)+m(\rho+\delta\rho)-m(\rho-\delta\rho)\right\}}{\left\{2m(\rho)\left(2+\frac{\delta\rho}{\rho}\right)-m(\rho+\delta\rho)+m(\rho-\delta\rho)\right\}}\psi(\rho-\delta\rho) \quad (14)$$

If the values of $\psi(\rho-\delta\rho)$ and $\psi(\rho)$ are known for the wave functions, then using equation (14) it is possible to determine the value of $\psi(\rho-\delta\rho)$ for an arbitrary energy. To calculate the wave function and energy of electrons and holes, it is necessary to take into account the following three boundary conditions.

$$\psi(\infty)\to 0,\ \ \psi(0)=1,\ \ \psi(\delta\rho)=1$$

4. Findings and conclusions

It is known that the lattice constant for InP is 0.5869 nm and this value is close to the value of the lattice constant for InAs 0.6058 nm [12]. This makes it possible to obtain an ideal heterostructure using these materials. Figure 1 shows the band diagram of the InP / InAs heterostructure. Table 1 shows the required parameters for InAs and InP obtained by various authors. The potential well depth for the InP / InAs / InP heterostructure is 0.52 eV. When studying the energy spectrum, the radius of the nanowire was taken from 5 to 20 nm. In [13] for the relationship between the radius and length of nanowires is given. The length of the nanowire is many times greater than its radius [13]. This allows you to solve a one-dimensional problem.To take into account the nonparabolicity of the zone, we use the Kane model [14]. In [11], [15, 16] various approximations for the effective mass are given, we will use the following expression for the effective mass.

$$m_{\mathrm{InPi}}(E)=m_{0\,\mathrm{InPi}}\left(1+2\alpha_{\mathrm{InPi}}(E-V(\rho))\right)$$

$$\alpha_{\mathrm{InPi}}=\frac{1}{E_{g\,\mathrm{ln}\,P}}\left(1-\frac{m_i}{m_0}\right)^2,\quad \alpha_{\mathrm{InAsi}}=\frac{1}{E_{g\,\mathrm{ln}\,As}}\left(1-\frac{m_i}{m_0}\right)^2$$

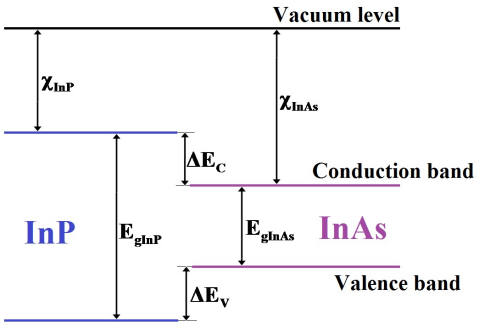

Fig. 1. InP/InAs zone diogram

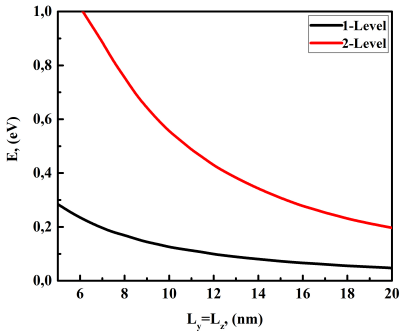

Fig. 2. Dependence of the electron energy in a rectangular nanowire with a finite potential well on the size of the well

where $i = e,\ hh,\ lh$

Usually, the electron wave function as $\rho\to\infty$ is equal to zero. If at the size of the potential well R, we choose that the wave function at a distance inside the barrier is R/2, and then the error in calculating the energy was 0,001 meV compared to $\rho\to\infty$.

Using the above equations (8) and (9) for the heterostructure of InP / InAs / InP nanowires with a rectangular cross section, we determine the energy levels and wave functions of electrons. Fig. 2 shows the energies of the first and second levels for a rectangular nanowire with a finite depth of the potential well when the side of the well changes from 5 nm to 50 nm. An increase in the size of the well leads to a decrease in the values of the energy levels.

Fig. 3 shows the wave functions of electrons corresponding to the energy levels (1; 1), (1; 2), (2; 1), and (2; 2) in a rectangular nanowire with a side of 10 nm. Solving equation (14), we find the energy levels and wave functions of electrons in a cylindrical nanowire. Fig. 4 shows the change in energy levels with an increase in the radius of a cylindrical nanonite from 5 to 20 nm. Fig. 5 shows the wave functions of electrons of the first four energy levels

Table 1. Material parameters of InAs and InP

Parameter	InAs	InP
$E_g, (eV)$	0.35[12]	1.35[12, 17]
	0.36[17]	1.424[18]
	0.417[18]	1.42[19, 20]
m_e/m_0	0.022[12]	0.077[12, 18]
	0.023[18]	0.079[19]
$\chi, (eV)$	4.92[12]	4.38[12]
	4.9[17]	4.4[17]

of a nanowire with a radius of 8 nm.

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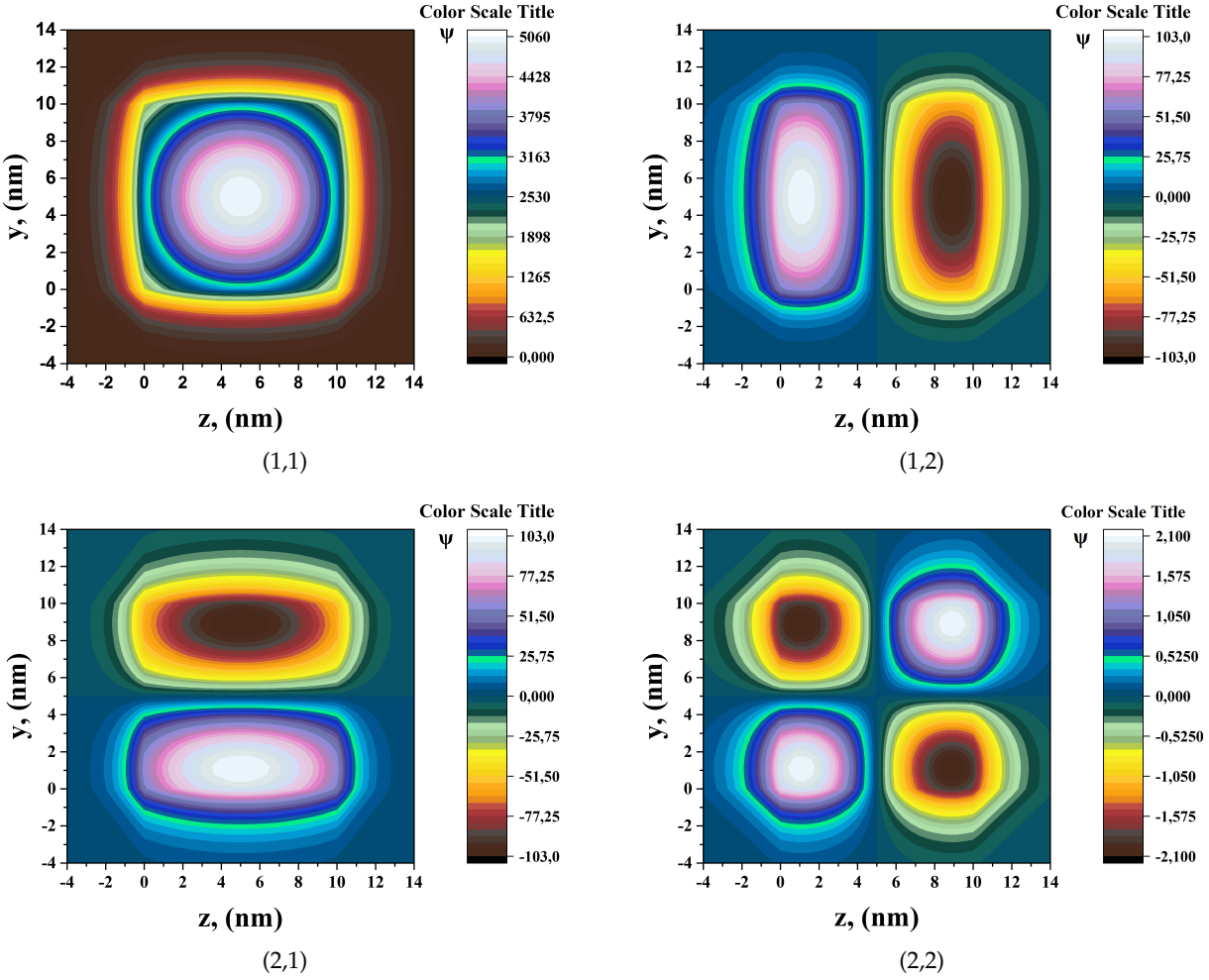

Fig. 3. Dependence of the electron energy in a rectangular nanowire with a finite potential well on the size of the well

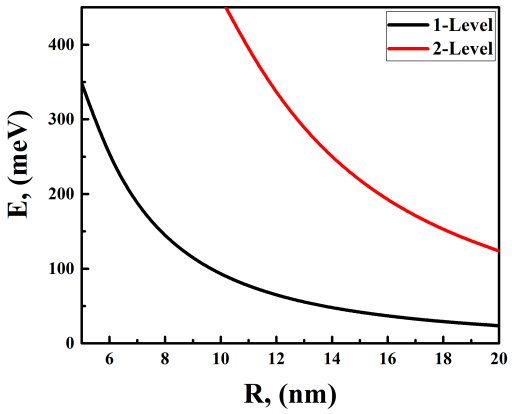

Fig. 4. Dependence of the electron energy on the radius of a cylindrical nanowire with a potential well of finite depth

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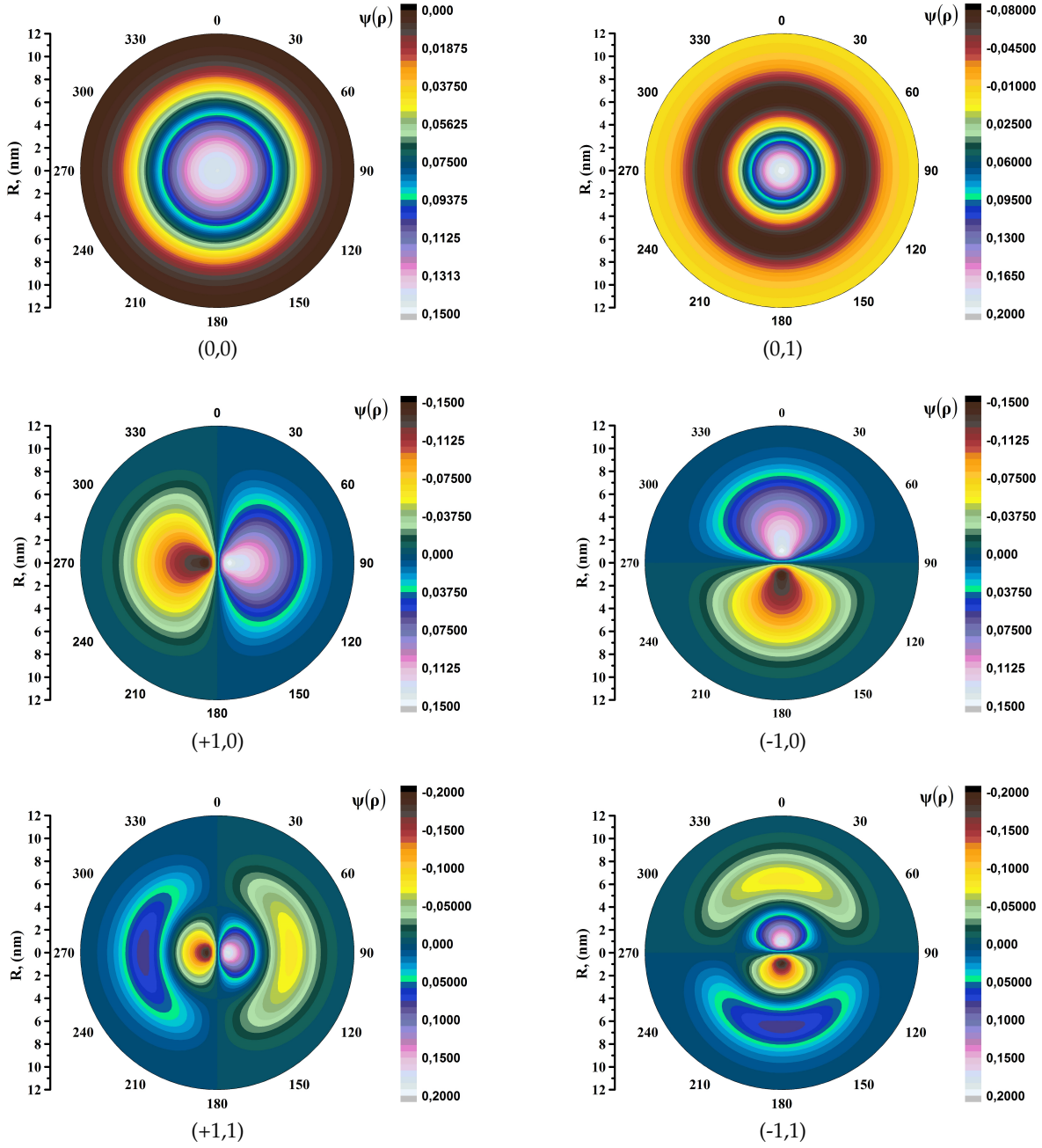

Fig. 5. Dependence of the wave function of electrons of a cylindrical nanowire with a finite potential well on the size of the well