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Electron Energy in Rectangular and Cylindrical Quantum Wires

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The influence of the cross-sectional shape of a quantum filament on the energy spectrum of electrons is studied. The calculation of energy levels of electrons in a quantum wire is performed. For the $Al_xGa_{1-x}As$ quantum wire with infinite and finite depths, energy level spectra were obtained. The dispersion dependence with a parabolic law in a quantum wire with finite and infinite height of the potential barrier based on $Al_{0.25}Ga_{0.75}As$ and $Al_{0.75}Ga_{0.25}As$ was calculated, and graphs of dispersion dependences were obtained. The results are obtained for the linear sizes of a quantum wire from 5 nm to 15 nm. The transverse dimensions of cylindrical and rectangular quantum wires with close energy levels are found. The analysis of energy levels in cylindrical and rectangular quantum wires is carried out, and their similarities are revealed. It is shown that the energy levels are close to each other when the cross-sectional areas of rectangular and cylindrical quantum wires become equal. The solutions of the Schrödinger equation are presented, when the solution for a cylindrical wire can be replaced by the solution for a rectangular wire.

Keywords: Quantum wire, Potential well, Energy levels.

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1. INTRODUCTION

Modern development of microelectronics is characterized by the fact that the dimensions of semiconductor devices are close to the de Broglie wavelength. Quantum wires are one-dimensional electron systems whose transverse dimensions are of the order of the de Broglie wavelength, and the wire length is many orders of magnitude greater than the de Broglie wavelength. In this case, the energy spectrum of electrons differs significantly from the energy spectrum of electrons in massive samples. In this case, the energy spectrum is divided into sub zones [1-3].

In [4-8], the effect of an external magnetic field on the electron gas energy was studied. In [9-14, 18-20], the energies of electrons in a cylindrical quantum wire were calculated.

In the present work, the energy levels of electrons in rectangular and cylindrical $Al_xGa_{1-x}As$ quantum wires are calculated; the spinning of the shape of a quantum wire on the energy spectrum of electrons is investigated.

2. THEORY

2.1 The Energy Spectrum of an Electron in a Quantum Wire in the One-electron Approximation

To determine the energy spectrum of electrons, we solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y)+U(x,y)\psi(x,y)=E\psi(x,y). \quad (1)$$

In the Cartesian system for a quantum wire of rectangular cross-section, the potential energy has the following form:

$$U(x,y)=\begin{cases}U(x)=\begin{cases}0, & 0\le x\le L_x,\\ \infty, & x<0,\quad L_x<x\end{cases}\\ U(y)=\begin{cases}0, & 0\le y\le L_y,\\ \infty, & y<0,\quad L_y<y\end{cases}\end{cases} \quad (2)$$

Here L_x and L_y are the transverse dimensions of the quantum wire, m is the effective electron mass. The solution of equation (1) with boundary conditions (2) gives the following expression for the electron energy in a rectangular quantum wire:

$$E=E_k+E_n+E_l=\frac{\hbar^2k_z^2}{2m}+\frac{\hbar^2\pi^2n^2}{2mL_x^2}+\frac{\hbar^2\pi^2l^2}{2mL_y^2}, \quad (3)$$

$$E_k=\frac{\hbar^2k_z^2}{2m},\quad E_n=\frac{\hbar^2\pi^2n^2}{2mL_x^2},\quad E_l=\frac{\hbar^2\pi^2l^2}{2mL_y^2}$$

$$n=1,2,3...,\qquad l=1,2,3... .$$

Here n and l are the integers, k_z is the wave vector along the z-axis.

2.2 The Energy Spectrum of an Electron in a Quantum Wire with a Rectangular Cross-section of a Potential Well with Finite Depth

In this case, the coordinate dependence of the potential energy has the following form:

$$U(x,y)=\begin{cases}U(x)=\begin{cases}0, & 0\le x\le L_x,\\ U_0, & x<0,\quad L_x<x\end{cases}\\ U(y)=\begin{cases}0, & 0\le y\le L_y,\\ U_0, & y<0,\quad L_y<y\end{cases}\end{cases} \quad (4)$$

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The solution of equation (1) for potential energy (4) is as follows [15, 18]

$$E_n = \frac{\hbar^2\pi^2 n^2}{2m_A L_x^2}\left(1-\frac{2}{\pi n}Arcsin\sqrt{\frac{m_B E_n}{(m_B-m_A)E_n+m_A U_0}}\right)^2, \quad n=1,2,3, \tag{5}$$

$$E_l = \frac{\hbar^2\pi^2 l^2}{2m_A L_y^2}\left(1-\frac{2}{\pi l}Arcsin\sqrt{\frac{m_B E_l}{(m_B-m_A)E_l+m_A U_0}}\right)^2, \quad l=1,2,3, \tag{6}$$

$$E = \frac{\hbar^2 k_z^2}{2m}+E_n+E_l\,. \tag{7}$$

Here m_A and m_B are the effective masses of electrons in the A and B regions.

2.3 The Energy Spectrum of an Electron in a Cylindrical Quantum Wire with Infinite Height of the Potential Barrier

In this case, the expression for the potential energy of an electron has the following form:

$$U(\mathbf{r}) = U(\rho) = \begin{cases} 0, & 0<\rho\le R \\ \infty, & R\le\rho \end{cases} \tag{8}$$

Here R is the radius of the cylinder, ρ is the distance from the center of the axis of the cylinder to the point in question. Using expressions of the operator in a cylindrical coordinate system, the Schrödinger equation for a cylindrical coordinate system (quantum wire) can be expressed as follows:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2}\right)f(\mathbf{r})+ +U(\mathbf{r})f(\mathbf{r}) = Ef(\mathbf{r}) \tag{9}$$

The solution of this equation can be written as

$$f(\mathbf{r}) = e^{ik_z z}e^{il\phi}\psi(\rho)\,. \tag{10}$$

In this case, the Schrödinger equation takes the following form:

$$\rho^2\frac{\partial^2\psi(\rho)}{\partial\rho^2}+\rho\frac{\partial\psi(\rho)}{\partial\rho}+\left(\left(k^2-k_z^2\right)\rho^2-l^2\right)\psi(\rho)=0\,. \tag{11}$$

Here, $k^2 = 2mE/\hbar^2$. The solutions to this equation are

$$f(\mathbf{r}) = C_{n,l}e^{-il\phi}J_l\left(\frac{\beta_{n,l}}{R}\rho\right)e^{ik_z z}. \tag{12}$$

Here $J_l(x)$ is the Bessel function. For a cylindrical quantum wire with infinite depth of the well, the electron energy has the following form:

$$E_{n,l,k_z} = \frac{\hbar^2\beta_{n,l}^2}{2mR^2}+\frac{\hbar^2 k_z^2}{2m}\,. \tag{13}$$

Here, $\beta_{n,l}$ are the zeros of the Bessel function.

2.4 Electron Energy of a Cylindrical Quantum Wire with Finite Depth of the Potential Well

The potential energy of an electron of a cylindrical quantum wire with finite depth is:

$$U(\mathbf{r}) = U(\rho) = \begin{cases} 0, & 0\le\rho\le R \\ W, & \rho>R \end{cases} \tag{14}$$

The solution of equation (9) with boundary conditions (14) is sought in the form (10). The Schrödinger equation for the radial distribution function in the region takes the form

$$\frac{\partial^2\psi(\rho)}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial\psi(\rho)}{\partial\rho}+\left(k_A^2-\frac{l^2}{\rho^2}\right)\psi(\rho)=0, \quad 0\le\rho\le R \tag{15}$$

We introduce a new variable

$$\xi = k_A\rho, \quad k_A = \sqrt{\frac{2m_A}{\hbar^2}E-k_z^2}\,. \tag{16}$$

Then equation (15) takes the form

$$\xi^2\frac{\partial^2\psi(\rho)}{\partial\xi^2}+\xi\frac{\partial\psi(\rho)}{\partial\xi}+\left(\xi^2-l^2\right)\psi(\rho)=0\,. \tag{17}$$

The solutions of this equation are a linear combination of the Bessel $J_l(\xi)$ and Neumann $N_l(\xi)$ functions of order l

$$\psi_1(\rho) = A_1J_l(k_A\rho)+B_1N_l(k_A\rho), \quad 0\le\rho\le R\,. \tag{18}$$

The Schrödinger equation for a radial function $\psi(\rho)$ outside the potential well takes the following form:

$$\zeta^2\frac{\partial^2\psi}{\partial\zeta^2}+\zeta\frac{\partial\psi}{\partial\zeta}+\left(-\zeta^2-M^2\right)\psi=0, \quad \rho>R\,. \tag{19}$$

Here

$$\zeta = \gamma_B\rho, \quad \gamma_B = \sqrt{\frac{2m_B}{\hbar^2}(W-E)+k_x^2}\,. \tag{20}$$

The general solution of equation (19) is a linear by the combination of the Bessel function with an imaginary argument $I_l(\xi)$ and the Macdonald function $K_l(\xi)$

$$\psi_2(\rho) = A_2K_l(\gamma_B\rho)+B_2I_l(\gamma_B\rho), \quad \rho>R\,. \tag{21}$$

Thus, for the radial wave function, we obtain the following expression:

$$\psi(\rho)=\begin{cases}A_1J_l(k_A\rho)+B_1N_l(k_A\rho), & 0\le\rho\le R\\ A_2K_l(\gamma_B\rho)+B_2I_l(\gamma_B\rho), & \rho>R\end{cases} \tag{22}$$

If we consider that the wave function is finite inside the cylinder and is zero at infinity, then the solution of the equation for the radial component of the wave function takes the following form:

$$\psi(\rho)=\begin{cases}A_1J_l(k_A\rho), & 0\le\rho\le R\\ A_2K_l(\gamma_B\rho), & \rho>R\end{cases} \tag{23}$$

Here A_1 and A_2 are constant values, the ratio A_1/A_2 is selected in such a way that the following boundary conditions for the radial wave function take place:

$$\begin{cases}\psi_1(\rho)\big|_{\rho=R}=\psi_2(\rho)\big|_{\rho=R}\\ \dfrac{1}{m_A}\dfrac{d\psi_1(\rho)}{d\rho}\bigg|_{\rho=R}=\dfrac{1}{m_B}\dfrac{d\psi_1(\rho)}{d\rho}\bigg|_{\rho=R}\end{cases} \tag{24}$$

Substituting (23) into (24) we obtain the following transcendental equation:

$$\frac{J_l'(k_AR)K_l(\gamma_BR)}{J_l(k_AR)K_l'(\gamma_BR)}=\frac{m_A}{m_B}. \tag{25}$$

Here $J'_l(\xi)$, $K'_l(\xi)$ are the derivatives with respect to ρ of the Bessel and Macdonald functions. If we consider that the solution of equation (9) satisfies the condition $f(z,\phi,\rho)=f(z,\phi+2\pi,\rho)$, $\exp(i2\pi l)=1$ then it follows that $l=0,\pm1,\pm2,\dots$.

3. DISCUSSION OF THE RESULTS

Using expressions (3) and (7) for a quantum wire with a rectangular cross-section, we compare the energy spectra for $Al_{0.25}Ga_{0.75}As$ and $Al_{0.75}Ga_{0.25}As$ samples [16, 17]. The dependences of the electron energy on the wave vector k for a rectangular potential well with infinite and finite depth are shown in Fig. 1.

Graphs in Fig. 1 are obtained for a rectangular quantum wire with a side of 10 nm. In a cylindrical quantum wire, the radius is defined as follows

$$L_xL_y=\pi R^2,\quad L_x=L_y=L,\quad \Rightarrow R=\frac{L}{\sqrt{\pi}}.$$

In this case, the cross-sectional areas of the wires are equal. In the second curve, the radius of a cylindrical quantum wire is equal to half the side of the square $R = L/2$. In this case, the cross-sectional side of a square quantum filament is equal to the diameter of the cross-section of a cylindrical quantum filament. From Fig. 1 it can be seen that the value of the energies in a cylindrical quantum wire is closer to the energies of a rectangular wire compared to the energy levels of the second cylindrical quantum wire.

The first and second energy levels of rectangular quantum filaments ($Al_{0.25}Ga_{0.75}As$) in the finite depth of the potential well differ from cylindrical quantum filaments for level 1 by 2.5 % and for level 2 by 2 %. Energy levels of a cylindrical quantum wire for the first level differ by 15 % and for the second level – by 10 %. For $Al_{0.25}Ga_{0.75}As$ samples, the difference in the values of energy levels is the same value. Fig. 1 compares the electron energy values of a rectangular quantum wire with infinite height of the potential well. The energies of the first level for the first sample differ by 7 % and of the second level – by 6 %. The energies of the second cylindrical quantum wire for the first level differ by 16 % and for the second level – by 19 %.

Fig. 2 shows the dependence of energy levels on the size of a quantum wire. Fig. 2 ($Al_{0.25}Ga_{0.75}As$) presents energy levels of a rectangular quantum well for the first level. The ratio of the energies of a rectangular wire at $L = 8$ nm from the ratio of the energies of a cylindrical wire for the first level differs by 7 %, for the second level – by 6 %. For a cylindrical quantum wire, the first level differs by 14 %, the second level – by 18 %.

For a quantum wire with a potential well of the finite depth of $Al_{0.25}Ga_{0.75}As$ at $L = 8$ nm, the dependence on the cross-sectional dimensions of a rectangular wire and a cylindrical wire for the first level differs by 1.2 %, for the second level – by 8 %; in the second sample, for the first level – by 14 %, for the second level – by 18 %. In Fig. 2, deviations of energy levels are of the same magnitude as in the previous case.

At $L = 14$ nm, the energy levels for the $Al_{0.25}Ga_{0.75}As$ sample for the first and second levels of electrons in a rectangular wire differ from those of a cylindrical wire, both for the first level and for the second level by 6 %.

In a cylindrical quantum wire of the second sample, the first and second levels differ by 18 %. Fig. 2b obtained for $Al_{0.25}Ga_{0.75}As$ shows the level difference of about the same magnitude. In Fig. 2 with electron energies for a cylindrical quantum filament $Al_{0.25}Ga_{0.75}As$ with a finite well depth for levels 1 and 2 differ by 13 % for the first and 18 % for the second levels of a rectangular quantum filament with finite depth of the potential well. For a cylindrical quantum wire 2, the first level distinguishes by 22 % the second level – by 1 %; the difference in Fig. 2d for $Al_{0.25}Ga_{0.75}As$ remains at about the same level.

4. CONCLUSIONS

To study the influence of the size and shape of a quantum wire on the energy spectrum of electrons, the Schrödinger equation was solved for rectangular and cylindrical samples. The solution of the Schrödinger equation in the Cartesian coordinate system for rectangular quantum wires is much simpler than for cylindrical quantum wires.

The calculations of the energy levels of $Al_{0.25}Ga_{0.75}As$ and $Al_{0.75}Ga_{0.25}As$ quantum wires show that the relative difference of the energies of rectangular wires from cylindrical ones does not exceed 10 %. From this it follows that the values of electron energies of a rectangular filament can be used to estimate the energy of electrons in a cylindrical quantum wire. In this case, the allowable error of calculations will be less than 10 %. When the radius of the section of the circle R and the side of the square L of cylindrical and rectangular filaments are related by the following relation, the levels of electron energy in these samples are almost the same. In this case, with a small error, instead of the energies of the cylindrical wire, it is possible to use the energies of

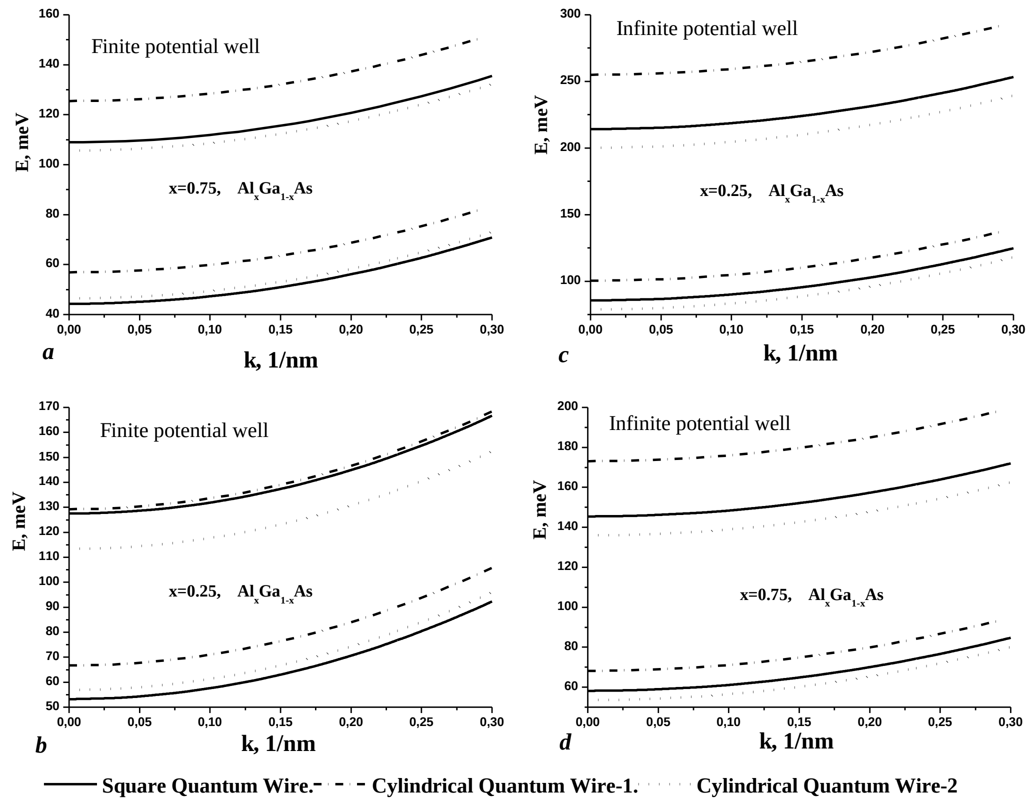

Fig. 1 – The electron energy dispersion for $Al_xGa_{1-x}As$: a) a quantum wire with a finite barrier height ($x = 0.75$-$Al_xGa_{1-x}As$), b) a quantum wire with a finite barrier height ($x = 0.25$-$Al_xGa_{1-x}As$), c) a quantum wire with an infinite barrier height ($x = 0.25$-$Al_xGa_{1-x}As$), d) a quantum wire with an infinite potential ($x = 0.75$-$Al_xGa_{1-x}As$)

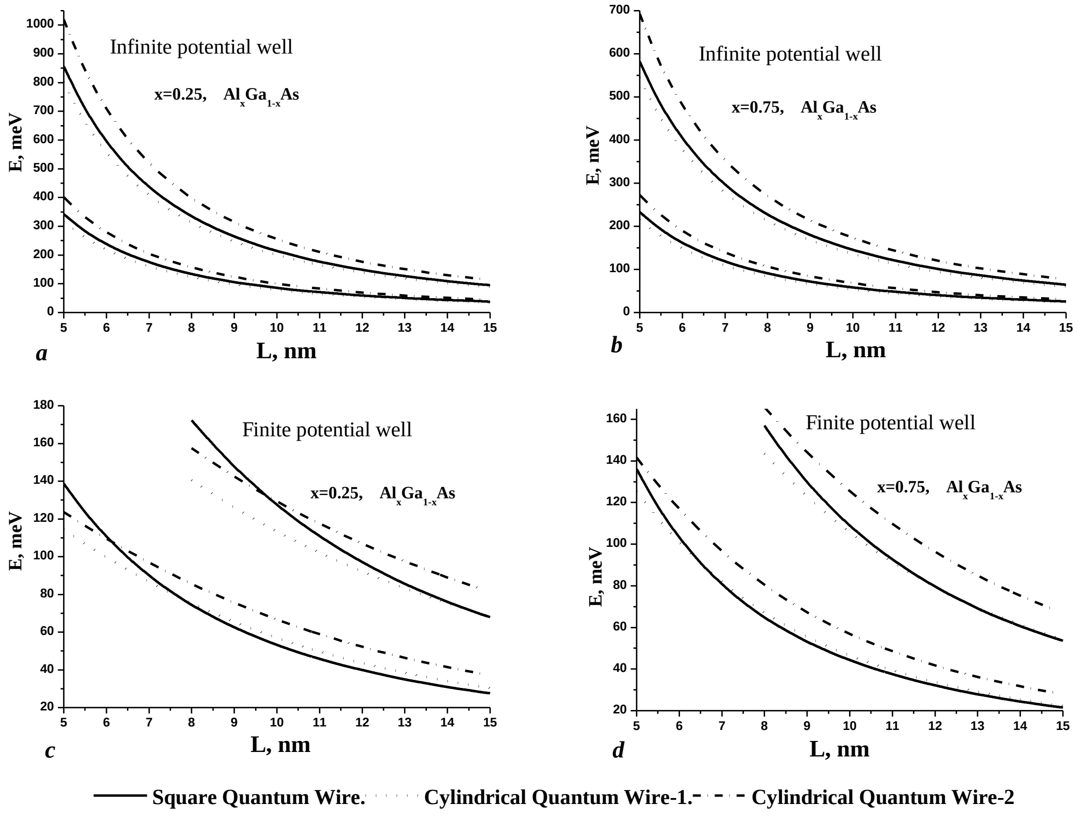

Fig. 2 – Dependences of the electron energy of the $Al_xGa_{1-x}As$ quantum wire on its shape and size: a) a quantum wire with infinitely high walls ($x = 0.25$-$Al_xGa_{1-x}As$), b) a quantum wire with an infinite potential ($x = 0.75$-$Al_xGa_{1-x}As$), c) a quantum wire with a finite potential ($x = 0.25$-$Al_xGa_{1-x}As$), d) a quantum wire with a finite potential ($x = 0.75$-$Al_xGa_{1-x}As$)

the rectangular wire. This replacement greatly simplifies the calculation of the electron concentration, density of energy states, heat capacity, electrical conductivity, and entropy of the electron gas in cylindrical quantum wires.

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Енергія електронів у прямокутних та циліндричних квантових дротах

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Вивчено вплив форми поперечного перерізу квантового дроту на енергетичний спектр електронів. Проводиться розрахунок рівнів енергії електронів у квантовому дроті. Для квантового дроту $Al_xGa_{1-x}As$ з нескінченною та кінцевою глибиною були отримані спектри енергетичних рівнів. Розраховано дисперсійну залежність з параболічним законом у квантовому дроті з кінцевою та нескінченною висотою потенційного бар'еру на основі $Al_{0.25}Ga_{0.75}As$ та $Al_{0.75}Ga_{0.25}As$ та отримано графіки дисперсійних залежностей. Результати отримано для лінійних розмірів квантового дроту в межах від 5 нм до 15 нм. Знайдено поперечні розміри циліндричних та прямокутних квантових дротів з близькими рівнями енергії. Проведено аналіз енергетичних рівнів в циліндричних та прямокутних квантових дротах та виявлено їх схожість. Показано, що рівні енергії близькі один до одного, коли площі поперечного перерізу прямокутних і циліндричних квантових дротів стають рівними. Представлено розв'язки рівняння Шредінгера, коли розв'язок для циліндричного дроту можна замінити розв'язком для прямокутного дроту.

Ключові слова: Квантовий дріт, Потенційна яма, Енергетичні рівні.