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Energy Eigenvalues in Square and Rectangular Quantum Wires with Finite Barrier Potential

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Energy eigenvalues have been calculated for square and rectangular quantum wires with finite barrier potential of GaAs/$Ga_{0.63}Al_{0.37}As$ and $Ga_{0.47}In_{0.53}As$/InP systems, by expressing the wave function in terms of a two-dimensional Fourier series. Calculated values are compared with those obtained earlier by using the finite element method and by using equivalent circular or elliptic wires. Experimental values of the energy shift of $Ga_{0.47}In_{0.53}As$/InP wires are also compared with the calculations.

1. Introduction

Quantum wires in which the electron motion is confined in two directions have been receiving much attention. It has been predicted that transistors and lasers made with quantum wires will have better performance characteristics [1 to 3]. Attempts have been made therefore to realize experimentally quantum wire structures. Some success has been achieved by using the technique of electron beam lithography [4] and etching, and also by using the technique of selective growth on SiO_2 patterned substrates [5]. Quantum wires with rectangular geometry have been obtained by the former technique [6] while wires of triangular cross-sections have been obtained by the latter technique [7]. The observed blue shift in the energy levels has been considered as evidence of two-dimensional confinement. Agreement of the calculated value of energy with experiment has been reported in both cases. However, no details of the method of calculation and material constants have been given.

The experimental quantum wires have been made by using either $Ga_{0.47}In_{0.53}As$ or GaAs as the well material. The wire has been covered by InP in the case of $Ga_{0.47}In_{0.53}As$ wire and by $Ga_{0.63}Al_{0.37}As$ in the case of GaAs wire. The barrier potential in both cases is of the order of 250 meV. Energy eigenvalues are significantly altered for finite barrier potential, but the Schrödinger equation cannot be solved analytically for wires of square or rectangular cross-sections when the barrier potential is finite. An analytic solution may, however, be obtained for circular or elliptic cross-section by using Bessel or Mathieu functions. The present authors reported such solutions for $Ga_{0.47}In_{0.53}As$/InP wires in [8]. The solutions were used to estimate the energy eigenvalues for wires of square or rectangular cross-sections by assuming that the values are identical to those for the circular and elliptic cross-sections having areas equal to $(0.96)^2$ times the cross-

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sectional areas of square or rectangular cross-sections. The factor of $(0.96)^2$ was obtained by considering the solutions for wires of infinite barrier height. The calculated values of energy shift, however, differed considerably from the experimental values.

The Schrödinger equation for quantum wires of rectangular cross-sections and finite barrier potential may, however, be solved numerically. Shertzer and Ram-Mohan [9] calculated the energy eigenvalues for electrons and holes in $GaAs/Ga_{0.63}Al_{0.37}As$ quantum wires by using the finite element method. Notomi et al. [4] expressed the wave function as a linear combination of the functions for a two-dimensional well in one dimension and obtained a differential equation for the expansion coefficient in the other direction. Eigenvalues were obtained by solving the differential equation. Gershoni et al. [10], on the other hand, obtained the energy eigenvalues for electrons by using a two-dimensional Fourier series for the wave function and compared these values with those obtained from photoluminescence excitation spectroscopy in $Ga_{0.47}In_{0.53}As$ wires.

We have used the method suggested by Gershoni et al. [10] to calculate the energy shift of the photoluminescence peak in rectangular $Ga_{0.47}In_{0.53}As$ quantum wires for comparison with the experimental results of Notomi et al. [4]. We have calculated also the values of energy levels in rectangular $Ga_{0.63}Al_{0.37}As/GaAs$ quantum wires by this method for comparison with the results reported by Shertzer and Ram-Mohan [9].

Calculations have also been done to find out if the eigenvalues for rectangular or square wires may be estimated from the results for elliptic and circular wires with an equivalent cross-sectional area [8]. It should be mentioned that the incorporation of the energy dependence of the effective mass is not easy for the numerical methods but such incorporation may be easily done in analytical methods [8]. The effect of energy band nonparabolicity in square or rectangular quantum wires with finite barrier may be estimated for the square or rectangular wires from the analytic solutions for equivalent circular or elliptic wires.

The method of solution is briefly outlined in Section 2 and results are presented in Section 3. Implications of the results are discussed in the concluding section.

2. Theory

Energy eigenvalues for the rectangular quantum wire of dimensions L_1 and L_2 are required to be obtained from the Schrödinger equation in the envelope function approximation [11] as

$$-(\hbar^2/2m_0)\,[\nabla(1/m^*(x, y))\,\nabla]\,F(x, y) + V(x, y)\,F(x, y) = EF(x, y)\,, \tag{1}$$

where $m^*(x, y)$ represents the effective mass of the carrier for different values of x and y. It is equal to m_W, the effective mass of the well material in the well region and equal to the effective mass for the barrier material m_B in the barrier region. $V(x, y)$ is the potential as a function of x, y. It is equal to zero in the well region and equal to V_B, the barrier potential, in the barrier region. E is the energy eigenvalue. The wave function $F(x, y)$ may be expanded in a two-dimensional Fourier series with periods of L_x and L_y in the x and y directions, respectively. The values of L_x and L_y are chosen arbitrarily but should be significantly large so that the actual wave functions become insignificantly small for these values of x and y. In practice their values are chosen to be such that the eigenvalues do not change significantly when their values are increased.

Accordingly, the wave function is written as

$$F(x, y) = \sum_{l,m} a_{lm}\varphi_{lm} = \sum_{l,m} a_{lm} \sin l\pi\left(\frac{1}{2} - \frac{x}{L_x}\right) \sin m\pi\left(\frac{1}{2} - \frac{y}{L_y}\right), \tag{2}$$

$l, m = 1, 2, 3 \ldots$.

For the evaluation of the energy eigenvalues, the wave function, as assumed above, is substituted in the Schrödinger equation. The equation is then converted to a matrix equation by using the orthonormality property of the constituent functions. The matrix equation is,

$$(A_{lml'm'} - E\delta_{ll'}\delta_{mm'})\,\varphi_{lm} = 0\,, \tag{3}$$

where the matrix element $A_{lml'm'}$ is given by

$$A_{lml'm'} = \frac{\hbar^2}{2m_0}\left[\frac{I_1}{m_\mathrm{B}} - \left(\frac{1}{m_\mathrm{B}} - \frac{1}{m_\mathrm{W}}\right)\left[\int_{\frac{-L_1}{2}}^{\frac{L_1}{2}}\int_{\frac{-L_2}{2}}^{\frac{L_2}{2}} \frac{\mathrm{d}\varphi_{lm}(x, y)}{\mathrm{d}x}\,\frac{\mathrm{d}\varphi'_{l'm'}(x, y)}{\mathrm{d}x}\,\mathrm{d}x\,\mathrm{d}y + \int_{\frac{-L_1}{2}}^{\frac{L_1}{2}}\int_{\frac{-L_2}{2}}^{\frac{L_2}{2}} \frac{\mathrm{d}\varphi_{lm}(x, y)}{\mathrm{d}y}\,\frac{\mathrm{d}\varphi'_{l'm'}(x, y)}{\mathrm{d}y}\,\mathrm{d}x\,\mathrm{d}y\right]\right] + VI_2 - V\int_{\frac{-L_1}{2}}^{\frac{L_1}{2}}\int_{\frac{-L_2}{2}}^{\frac{L_2}{2}} \varphi_{lm}(x, y)\,\varphi'_{l'm'}(x, y)\,\mathrm{d}x\,\mathrm{d}y\,, \tag{4}$$

where

$$I_1 = \int_{\frac{-L_x}{2}}^{\frac{L_x}{2}}\int_{\frac{-L_y}{2}}^{\frac{L_y}{2}} \frac{\mathrm{d}\varphi_{lm}(x, y)}{\mathrm{d}x}\,\frac{\mathrm{d}\varphi'_{l'm'}(x, y)}{\mathrm{d}x}\,\mathrm{d}x\,\mathrm{d}y + \int_{\frac{-L_x}{2}}^{\frac{L_x}{2}}\int_{\frac{-L_y}{2}}^{\frac{L_y}{2}} \frac{\mathrm{d}\varphi_{lm}(x, y)}{\mathrm{d}y}\,\frac{\mathrm{d}\varphi'_{l'm'}(x, y)}{\mathrm{d}y}\,\mathrm{d}x\,\mathrm{d}y\,, \tag{5}$$

$$I_2 = \int_{\frac{-L_x}{2}}^{\frac{L_x}{2}}\int_{\frac{-L_y}{2}}^{\frac{L_y}{2}} \varphi_{lm}(x, y)\,\varphi'_{l'm'}(x, y)\,\mathrm{d}x\,\mathrm{d}y\,, \tag{6}$$

$I_1 \neq 0$, $I_2 \neq 0$ only for $l = l'$, $m = m'$, for other combinations of l, l', m, m' $I_1 = 0$, $I_2 = 0$.

$\varphi'_{l'm'}$ can be obtained by putting l', m' in place of l, m respectively in the expression of φ_{lm}.

Eigenvalues for the matrix are then obtained by using the IMSL software.

Table 1
Energy eigenvalues in square and rectangular quantum wires

material	dimension (nm^2)	energy levels (meV)					
		conduction electron		heavy hole		light hole	
		a	b	a	b	a	b
$GaAs/Ga_{0.63}Al_{0.37}As$	5 × 5	155.2	155.3	46.57	46.5	110.63	110.7
	10 × 10	63.47	63.5	15.03	15.1	46.02	46.0
	10 × 10	111.2	111.1	31.0	30.9	79.77	79.8

a: present calculation, b: Shertzer and Ram-Mohan [9].

3. Results

To judge the accuracy of the method, calculations were first done for GaAs rectangular quantum wires for which calculated values obtained by the finite element method were reported earlier [9]. In Table 1 are presented the energy eigenvalues for rectangular GaAs wires calculated by using the following parameter values:
Conduction electron: $m_W = 0.0665m_0$, $m_B = 0.0858m_0$, $V_B = 276$ meV; light hole: $m_W = 0.0905m_0$, $m_B = 0.1107m_0$, $V_B = 184$ meV; heavy hole: $m_W = 0.3774m_0$, $m_B = 0.3865m_0$, $V_B = 184$ meV.

It is seen that our calculated values are almost the same as those obtained by Shertzer and Ram-Mohan [9] by using the finite element method.

In Table 2 are presented the energy eigenvalues of $Ga_{0.47}In_{0.53}As/InP$ for square or rectangular quantum wires. Calculations were done with the following values of physical constants:
Conduction electron: $m_W = 0.042m_0$, $m_B = 0.079m_0$, $V_B = 240$ meV; heavy hole: $m_W = 0.47m_0$, $m_B = 0.61m_0$, $V_B = 370.6$ meV.

Values calculated by Gershoni et al. [10] for rectangular wires are also quoted. Also, energy eigenvalues for cylindrical and elliptic quantum wires with a cross-sectional area equal to $(0.96)^2$ times the area of the corresponding square or rectangular wire are given.

Table 2
Energy eigenvalues in square and rectangular quantum wires

material	dimension (nm^2)	energy levels (meV)				
		conduction electron			heavy hole	
		a	b	c	a	c
$Ga_{0.47}In_{0.53}As/InP$	5 × 5	162.4		163.8	43.4	44.3
	10 × 10	76.0		77.5	13.1	13.2
	20 × 20	28.1		28.4	3.6	3.63
	10 × 5	121.5	160.0	103.0	28.3	22.7
	25 × 5	96.0	105.0		22.9	

a: present calculation, b: Gershoni et al. [10], c: equivalent cylindrical or elliptic quantum wire

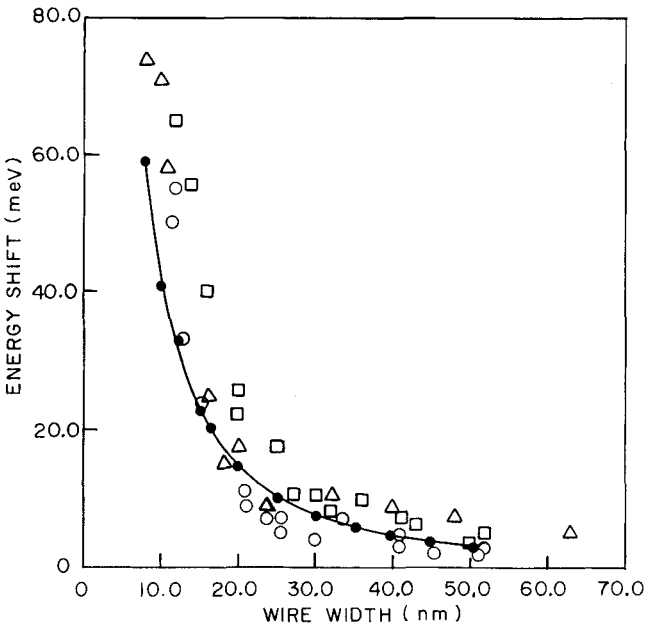

Fig. 1. Energy shift for rectangular $Ga_{0.47}In_{0.53}As/InP$ quantum wires with a smaller dimension 5 nm and different larger dimensions. ○ experimental points obtained by Notomi et al. [4], △ and □; experimental points obtained by Ils et al. [5]; the solid line gives the calculated values

We find that the values for the circular wires agree to within 2% with the values obtained for the corresponding square wires. We may hence conclude that the energy eigenvalues for square wires may be estimated quite accurately from the values for circular wires with the equivalent cross-sections as was done in [8].

The value for the elliptic wire is, however, found to be significantly lower than the corresponding rectangular wire. This difference may be due to the fact that the eigenvalues of the elliptic wires were calculated with a limited number of Mathieu functions. It may also indicate that the numerical factor for the equivalence does not apply to rectangular wires with finite barrier potential. Values calculated by Gershoni et al. [10] are also found to be about 20% higher than those obtained by us. As the values of physical constants (particularly the band offset) used by Gershoni et al. [10] are not given, we cannot comment on this difference.

The energy shift in a rectangular $Ga_{0.47}In_{0.53}As/InP$ wire calculated with physical constants given earlier are presented in Fig. 1. For comparison with the experiments of Notomi et al. [4] and of Ils et al. [5], the dimension of one side was taken 5 nm and the dimension of the other side was varied from 8 to 50 nm. In Fig. 1 are also presented the experimental points of [4, 5]. We find that our results are close to the experimental values [4, 5]. It should, however, be noted that there is a large amount of scatter in the experimental results [4, 5]. For some wire widths the experimental values of energy shifts differ by a factor of two or more. Our calculated values for a wire width larger than 20 nm agree with the average values. However, for widths less than 20 nm the calculated values are significantly lower. The effect of band nonparabolicity has not been included in our calculations. However, the band nonparabolicity increases significantly the energy

eigenvalues and the increase is larger for electrons than for heavy holes. Inclusion of the effect of nonparabolicity will therefore increase the value of energy shift particularly for dimensions of the order of 3 to 10 nm, and bring the calculated values closer to the experimental points.

4. Conclusion

We may conclude from the present study that the method of calculating the energy eigenvalues for square or rectangular wires by expressing the wave function as a two-dimensional Fourier series gives results identical to those obtained by the finite element method [9]. It is also found that energy eigenvalues for a square wire may be estimated from those for an equivalent circular wire [8]. However, for a rectangular wire the values are significantly different from those obtained for an equivalent elliptic wire by using only two Mathieu functions [8]. The energy shifts in rectangular $Ga_{0.47}In_{0.53}As/InP$ wires are found to be close to the experimental results.

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