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Energy levels in rectangular quantum well wires based on a modified profile of the heterojunction

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Abstract. The effect of a spatially dependent effective mass on the energy levels in a rectangular quantum wire with finite barrier potential is considered. The heterojunction is modelled by an error function rather than a step function to more accurately model the material transition region at the interface between the two materials. The carrier ground state is calculated using the envelope function approximation for $Ga_{0.47}In_{0.53}As/InP$ and $GaAs/Ga_{0.63}Al_{0.37}As$ systems. The results are lower than those reported before, and are in better agreement with the experimental points.

Keywords. Envelope function; heterojunction; quantum confinement.

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Nowadays, the fabrication technology of semiconductor quantum well structures of nanometer size is being developed. These structures will form the basis of the electronic devices of the future. It has been proved that transistors and lasers made of quantum wires (QWR) demonstrate excellent characteristics [1]. Among all these structures, quantum well wires have attracted attention because of a combination of the confinement across a quantum well wire and the free motion of a charge carrier along the quantum wire axis.

The first rectangular quantum wires were made of $Ga_{0.47}In_{0.53}As$ [2,3] or GaAs [4] for the well and InP or $Ga_{0.63}Al_{0.37}As$ for the barrier, respectively. The height of the potential barrier for an electron in both cases was about 250 meV. A detailed investigation of optical properties of rectangular GaAs/AlAs quantum wires has been carried out in [5] where the anisotropy of PL and PLE spectra has been studied.

In order to find the energy levels for a well with finite barrier height, the Schrödinger equation must be solved with appropriate boundary conditions. This cannot be done analytically except for the case with the spherical structural symmetry. A few numerical methods have been suggested to solve the Schrödinger equation for quantum wires with a rectangular cross-section and with a finite height of the barrier potential. In [6] the eigenenergies in the rectangular $GaAs/Ga_{0.63}Al_{0.37}As$ quantum wire have been calculated for an electron and a

hole using the finite-element method. In [7,8] calculations have been carried out for the $Ga_{0.47}In_{0.53}As/InP$ quantum wire expressing electron and hole wave functions in terms of a two-dimensional Fourier series. A quantum wire subjected to no external field is usually modelled by a step profile which is discontinuous at the heterojunctions [9]. In this case the electronic states of the system are determined by the method of the effective mass approximation:

$$\left[\mathbf{P}\,\frac{1}{2m_i^*}\,\mathbf{P}+V_i\right]F_i = EF_i, \tag{1}$$

where F_i, m_i^*, V_i, E and $\mathbf{P}$ are the wave function (envelope function), the effective mass, the potential, the energy eigenvalue and the generalized momentum, respectively. The required boundary conditions at the heterojunctions are: (1) the continuity of the envelope function and its first derivative, or (2) the continuity of the envelope function and its first derivative divided by the effective mass [10].

For the rectangular quantum wire, the numerical method should be applied and a search for an approximate envelope function must be carried out. In this situation the gradient of the effective mass (which is not considered by Gershoni *et al* [7] and by Gangopadhyay and Nag [8] in the study of different heterojunctions) should be included. In the previous work, the gradient of the effective mass was considered as a suitable Dirac delta function [11]. But in the real world, the effective mass cannot change abruptly across the heterojunction, because, the discontinuity of the square quantum well model implies an infinite internal electric field at the heterojunctions, and this is not physically possible. In reality, the effective mass changes over a few monolayers for a perfect microscopic interface [12]. In this paper the method of envelope function is used and a suitable error function for the variation of the effective mass at the boundary is considered.

First, we consider a two-dimensional quantum wire with a rectangular cross-section. In this case the electrons and the holes are confined in the xy plane and move freely along the wire axis (z direction). The Schrödinger equation in the envelope function approximation is written as

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

The potential $V(x,y)$ is equal to zero in the well region and equal to V_0 in the barrier region. The wave function can be expanded in terms of a complete orthonormal set of functions:

$$\begin{aligned}F(x,y)=\sum_{lm}a_{lm}\varphi_{lm}&=\sum_{lm}a_{lm}\frac{2}{\sqrt{(L_xL_y)}}\sin l\pi\\&\times\left(\frac{1}{2}-\frac{x}{L_x}\right)\sin m\pi\left(\frac{1}{2}-\frac{y}{L_y}\right),\end{aligned} \tag{3}$$

where $l,m=1,2,....$

Expression (3) is substituted into eq. (2); the terms are then multiplied by $\varphi_{l'm'}$ and integrated over the cross-section $L_x\times L_y$. The functions being orthogonal, the following secular equation is obtained:

$$|H_{lml'm'} - E\delta_{ll'}\delta_{mm'}| = 0. \tag{4}$$

The elements of the Hamiltonian matrix can be written as

$$\begin{aligned} H_{lml'm'} = \frac{\hbar^2}{2m_0}\Bigg[\frac{I_1}{m_b} - \left(\frac{1}{m_b} - \frac{1}{m_w}\right) \\ \Bigg[\int_{-L_1/2}^{\frac{L_1}{2}}\int_{-L_2/2}^{L_2/2}\left(\frac{\mathrm{d}\varphi_{lm}(x,y)}{\mathrm{d}x}\frac{\mathrm{d}\varphi_{l'm'}(x,y)}{\mathrm{d}x}\right. \\ \left. + \frac{\mathrm{d}\varphi_{lm}(x,y)}{\mathrm{d}y}\frac{\mathrm{d}\varphi_{l'm'}(x,y)}{\mathrm{d}y}\right)\mathrm{d}x\,\mathrm{d}y\Bigg]\Bigg] + V_0 I_2 \\ -V_0\int_{\frac{-L_1}{2}}^{\frac{L_1}{2}}\int_{\frac{-L_2}{2}}^{\frac{L_2}{2}}\varphi_{lm}(x,y)\varphi_{l'm'}(x,y)\,\mathrm{d}x\mathrm{d}y + \langle T\rangle_{lml'm'}, \end{aligned} \tag{5}$$

where I_1, I_2 and $\langle T\rangle_{lml'm'}$ were introduced in [8] and [11], respectively. For the study of the effects of the spatially dependent effective mass on the energy levels, the carrier's effective mass can be expressed in terms of error functions as

$$\begin{aligned} m^*_\mu(\nu) = m_w + \frac{1}{2}(m_b - m_w)\Bigg\{2 + \mathrm{erf}\left[\frac{1}{\sqrt{(2)}\sigma_\mu}\left(\nu - \frac{L_\nu}{4}\right)\right] \\ + \mathrm{erf}\left[\frac{1}{\sqrt{(2)}\sigma_\mu}\left(-\nu - \frac{L_\nu}{4}\right)\right]\Bigg\}, \end{aligned} \tag{6}$$

where $\mu = e$, (lh, hh), $\nu = x, y$ and σ is a dispersive factor which designate the change rates of the carrier effective mass at the heterojunctions. Substituting eq. (6) in $\langle T\rangle_{lml'm'}$, we obtain

$$\begin{aligned} \langle T\rangle_{lml'm'} = -\frac{\hbar^2\sqrt{(\pi)}(m_b - m_w)}{m_0\sqrt{(2)}\sigma_\mu} \\ \times\left\{\left(\frac{l}{L_x^2}\delta_{mm'}\right)B[l', l] + \left(\frac{m}{L_y^2}\delta_{ll'}\right)B[m', m]\right\} \end{aligned} \tag{7}$$

with

$$\begin{aligned} B[\lambda', \lambda] = \int_{-L_\nu/2}^{L_\nu/2}\frac{1}{m^{*2}(\nu)}\sin\lambda'\pi\left(\frac{1}{2} - \frac{\nu}{L_\nu}\right) \\ \times\left[\mathrm{e}^{-((\nu - \frac{L_\nu}{4})^2/2\sigma_\mu^2)} - \mathrm{e}^{-((\nu + \frac{L_\nu}{4})^2/2\sigma_\mu^2)}\right]\cos\lambda\pi\left(\frac{1}{2} - \frac{\nu}{L_\nu}\right)\mathrm{d}\nu, \end{aligned} \tag{8}$$

where $\lambda = l, m$ and $\nu = x, y$, respectively. Sufficiently large numbers of component functions (ϕ_{lm}) must be taken to ensure that the eigenvalues are equal to their asymptotic values. For the rectangular quantum wire the condition is achieved with uncertainty less than 0.1% when fifteen component functions are considered.

Table 1. Energy eigenvalues with (E) and without (E_G) boundary effect in rectangular QWRs (meV).

Material	Cross-section (Å^2)	Electron		Heavy hole		Light hole	
		E	E_G	E	E_G	E	E_G
$GaAs/Ga_{0.63}Al_{0.37}As$	50×50	145.60	155.2	46.19	46.57	104.62	110.63
	50×100	102.24	111.2	30.67	31.0	75.07	79.77
	100×100	57.40	63.47	15.00	15.03	44.48	46.02
$Ga_{0.47}In_{0.53}As/InP$	50×50	129.79	162.4	40.17	43.4	110.20	
	50×100	93.72	121.5	26.39	28.3	81.11	
	100×100	55.94	76.0	12.54	13.1	50.10	

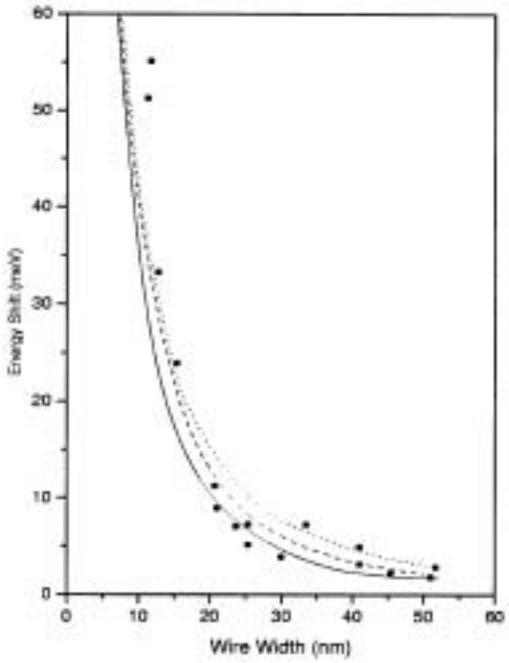

Figure 1. Energy shift of electron for 5 nm thick $Ga_{0.47}In_{0.53}As/InP$ QWRs vs. wire width. Closed circles are the experimental work of Notomi [2], the dotted and the dashed curves are the works done by Gangopadhyay and Nag [8] and Barati and Sadeghi [11], respectively. The solid curve is the result of the present calculation including the boundary effect.

Energy eigenvalues are calculated for two-dimensional $GaAs/Ga_{0.63}Al_{0.37}As$ and $Ga_{0.47}In_{0.53}As/InP$ quantum wires by using the parameter values given in [8]. The dispersive factor of effective masses of the electron (e), heavy holes (hh) and the light holes (lh) are assumed to be equal for simplicity. Namely, $\sigma_e = \sigma_{lh} = \sigma_{hh} = \sigma = 2.83$ Å (one monolayer of the GaAs lattice).

The ground state energies obtained here including the boundary effects (E) are presented in table 1. Values calculated by Gangopadhyay and Nag [8] for rectan-

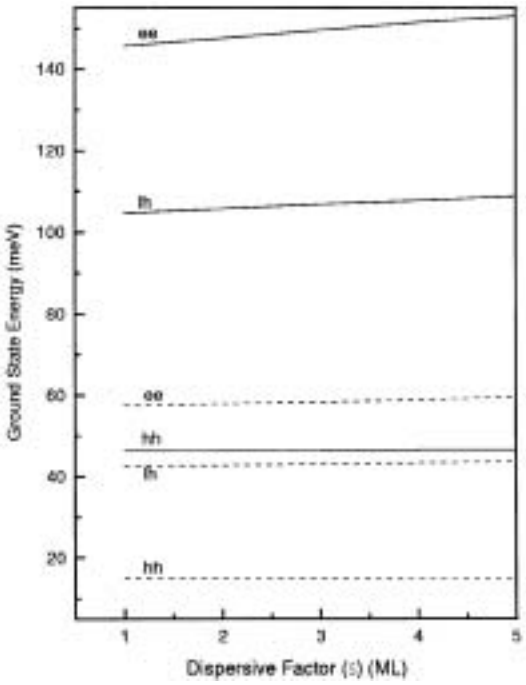

Figure 2. Ground state energies of carriers vs. dispersive factor for GaAs/$Ga_{0.63}Al_{0.37}As$ QWRs with 5×5 nm^2 (solid curves) and 10×10 nm^2 (dotted curves) cross-section.

gular quantum wire excluding the effects of effective mass variation (E_G) are also quoted. It is interesting to note that the ground state energy eigenvalues are reduced when the effect of boundary is included in the envelope function. The reduction of the ground state energy in $Ga_{0.47}In_{0.53}As$/InP quantum wire is about 32.6 and 3.2 meV for 5×5 nm^2 cross-section and about 20 and 0.6 meV for 10×10 nm^2 for the electrons and heavy holes, respectively. This reduction in GaAs/$Ga_{0.63}Al_{0.37}As$ is about 10, 0.4 and 6 meV for 5×5 nm^2 and reduces to 6, 0.03 and 1.5 meV for 10×10 nm^2. It is also interesting to note that the two sets of the energy eigenvalues for the electron in $Ga_{0.47}In_{0.53}As$/InP indicate large differences in comparison with the other types of investigated carriers, which is most likely due to the large variation of the effective mass of the electron carriers at the boundary. The energy shift of electron in $Ga_{0.47}In_{0.53}As$/InP QWR with 5 nm thickness vs. the wire width is shown in figure 1. For comparison, the numerical analysis by Gangopadhyay and Nag [8] and the experimental results of Notomi *et al* [2] in a photoluminescence investigation are also presented in figure 1. For a wire width smaller than 20 nm, our results are lower than the experimental reported values. For higher width the experimental error is relatively large. However, our theoretical results pass through the scattered experimental points. The energy shift calculated with delta function approximation is also plotted in this figure [11]. As seen, the difference between the two results for wire with a smaller width is significantly larger than those with

a larger width. The effect of band non-parabolicity has not been included in these calculations. However, the band non-parabolicity increases the energy eigenvalues significantly and the increase is larger for electrons than for heavy holes. Inclusion of the effect of non-parabolicity 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.

The ground state energies of the electron, heavy and the light-hole as a function of the dispersive factor for the $GaAs/Ga_{0.63}Al_{0.37}As$ quantum wires including the gradient of the effective mass at the boundary are shown in figure 2. As seen the energy eigenvalues of the electron and the light hole for 5×5 nm^2 quantum wire increase monotonically as the dispersive factor increases, while this increase is slower for 10×10 nm^2 QWR. This is because the position-dependent effective mass modifies the real potential energy in the fashion that the lower half of the quantum well (in each direction) is narrowed and the upper half is widened. As the dispersive factor increases, the lower half of the quantum well wire becomes narrower, and therefore the energy eigenvalues are pushed to higher values. This effect is more apparant in smaller cross-sections. The energy eigenvalues of the heavy hole remain almost unchanged for any two cross-sections.

References

[1] M Asada, Y Miyamoto and Y Suematsu, *Jpn. J. Appl. Phys.* **24**, L95 (1985)
[2] M Notomi, M Naganuma, T Nishida, T Tamamura, H Iwamura, S Nojima and M Okamoto, *Appl. Phys. Lett.* **58**, 720 (1991)
[3] P Ils, M Michel, A Forchel, I Gyuro, M Klenk and E Zielinski, *Appl. Phys. Lett.* **64**, 498 (1994)
[4] J Cibert, P M Petroff, G J Dolan, S J Pearson, A C Gossard and J H English, *Appl. Phys. Lett.* **49**, 1275 (1986)
[5] T Sogawa, H Ando, S Ando and H Kanbe, *Phys. Rev.* **B56**, 1958 (1997)
[6] J Shertzer and L R Ram-Mohan, *Phys. Rev.* **B41**, 9994 (1990)
[7] D Gershoni, H Temkin, G J Dolan, J Dunsmuir, S N G Chu and M B Panish, *Appl. Phys. Lett.* **53**, 995 (1988)
[8] S Gangopadhyay and B R Nag, *Phys. Status Solidi* **B195**, 123 (1996)
[9] B Gerlach, J Wusthoff, M O Dzero and M A Smondyrev, *Phys. Rev.* **B58**, 10568 (1998)
[10] G T Einevoll, P C Hemmer and J Thomsen, *Phys. Rev.* **B42**, 3485 (1990)
[11] M Barati and E Sadeghi, *Iranian J. Sci. Tech.* **A24**, 385 (2000)
E Sadeghi, *Iranian J. Phys. Res.* **3**, 289 (2003)
[12] L Li Tsung and J Kuhn Kelin, *Phys. Rev.* **B47**, 12760 (1993)