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Electronic states in lateral-surface-superlattice quantum well wires

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Abstract. Energy minigaps caused by lateral-surface structures in quasi-one-dimensional quantum well wires are calculated using the variational and degenerate-perturbational approaches for GaAs/AlAs wires. By a coordinate transformation, the structured interfaces of the wires are transformed into planar ones so that the boundary conditions of the electronic wave functions can be satisfied exactly on the interfaces. The dependences of the energy minigaps on the lateral-surface structures are discussed.

Owing to the great efforts of a large number of researchers, the electronic properties in quasi-one-dimensional quantum well wires are now well understood. Because of the quantum confinement in two directions, the binding energies of excitons and impurity states in the wires are greatly enhanced as compared with those in quasi-two-dimensional quantum well structures [1, 2]. Recently with the rapid development of crystal growth techniques, it has become possible to fabricate quantum wells with periodic structures on their interfaces which act as periodic potentials on electrons. This novel system, referred to as that of lateral-surface superlattices (LSSLs), has shown interesting behaviours in its electronic and optical properties [3–7]. Technically, we are now also able to fabricate quantum well wires with periodic structures on their interfaces—referred to as lateral-surface-superlattice wires (LSSLWs) hereinafter—by ion beam implantation on LSSLs produced by deposition of AlAs and GaAs fractional layers on (001) vicinal GaAs substrates [6, 7], for instance. The peculiar electronic and optical properties observed in LSSLs, such as magnetoresistance oscillations with magnetic fields and strong anisotropies in the ratios of electron–light-hole-exciton and electron–heavy-hole-exciton peak intensities [3–6], may be greatly enhanced in LSSLWs. The difficulty in calculating electronic and optical properties in LSSLWs is that the boundary conditions of the electronic wave functions are not easily satisfied on the periodically structured interfaces. In this paper, we present a theory that avoids this difficulty, and the electronic states in one single wire in which the lateral walls

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have a periodic undulation are studied. In our considerations, we ignore the tunnelling between the two adjacent quantum well wires, which means that the distance between them is assumed to be very large. In the practical experiments, there are many irregularities in the periodically structured interfaces in LSSLs, but their main structures are periodic [3–6], and we only examine the exact periodic LSSLWs here. In addition, in this paper we considered mainly the ground electronic states whose energies (< 150 meV) are much smaller than the conduction band offset between AlAs and GaAs ($= 1.07$ eV); hence the potential barrier between AlAs and GaAs is assumed to be infinitely high. Further investigations on other properties of LSSLWs will be published subsequently.

Let us consider a quantum wire of GaAs surrounded by AlAs, which is assumed to have rectangular cross section and infinitely high potential barrier between GaAs and AlAs. In the effective-mass approximation, the Hamiltonian describing the motion of an electron in the quantum wire can be written as

$$H = \frac{|p|^2}{2m} + V(r) \tag{1}$$

where p and r are the electron momentum and coordinate respectively, and m is the electron-band effective mass which is $m = 0.067m_0$ in the GaAs with m_0 the free-electron mass. The electron-confining potential well $V(r)$ is given by

$$V(r) = \begin{cases} 0 & \text{for } \begin{cases} -d_x + f_2(r) < x < d_x + f_1(r) \\ -d_y + f_4(r) < y < d_y + f_3(r) \end{cases} \\ \infty & \text{elsewhere} \end{cases} \tag{2}$$

where $2d_x$ and $2d_y$ are the average widths of the rectangular quantum wire and $f_i(r)$ ($i = 1, 2, 3, 4$) describes the periodic structures on the quantum wire interfaces.

The following coordinate transformation transforms the quantum wire interfaces into flat ones:

$$\begin{aligned} x' &= \{x - \tfrac{1}{2}[f_1(r) + f_2(r)\} \frac{2d_x}{2d_x + f_1(r) - f_2(r)} \\ y' &= \{y - \tfrac{1}{2}[f_3(r) + f_4(r)\} \frac{2d_y}{2d_y + f_3(r) - f_4(r)} \\ z' &= z. \end{aligned} \tag{3}$$

In the transformation, we note that

$$\begin{aligned} \int_V \psi^*(r) H(r) \psi(r)\, \mathrm{d}\tau &= \int_{V'} \tilde{\psi}^*(r') J(r') \tilde{H}(r') \tilde{\psi}(r')\, \mathrm{d}\tau' \\ &= \int_{V'} \tilde{\psi}^*(r') H_{\text{eff}}(r') \tilde{\psi}(r')\, \mathrm{d}\tau' \end{aligned} \tag{4}$$

where $J(r')$ is the Jacobian determinant, and the effective Hamiltonian is defined as

$$H_{\text{eff}}(r') = J(r') \tilde{H}(r'). \tag{5}$$

The normalization condition becomes

$$\int_{V'} \tilde{\psi}^*(r')\tilde{\psi}(r')J(r')\,\mathrm{d}\tau' = 1. \tag{6}$$

After the coordinate transformation, the electron-confining potential well $\tilde{V}(r')$ is

$$\tilde{V}(r') = \begin{cases} 0 & |x'| < d_{x'}|y'| < d_y \\ \infty & \text{elsewhere.} \end{cases} \tag{7}$$

Also, in the new coordinate system the wave function satisfies the boundary conditions

$$\tilde{\psi}(r')|_{x'=\pm d_x} = 0 \qquad \tilde{\psi}(r')|_{y'=\pm d_y} = 0. \tag{8}$$

In this paper, we consider two typical cases as follows:

$$\left.\begin{aligned} f_1(r) = -f_2(r) = \Delta\sin(2\pi/L_d)z \\ f_3(r) = -f_4(r) = \Delta\sin(2\pi/L_d)z \end{aligned}\right\} \quad \text{case (i)} \tag{9}$$

$$\left.\begin{aligned} f_1(r) = f_2(r) = \Delta\sin(2\pi/L_d)z \\ f_3(r) = f_4(r) = \Delta\sin(2\pi/L_d)z \end{aligned}\right\} \quad \text{case (ii)} \tag{10}$$

where Δ and L_d are the amplitude and period of the interface structures of the LSSLW, respectively. Case (i) represents a LSSLW where the central line keeps straight, but its widths fluctuate periodically, while case (ii) represents a LSSLW where the widths do not change but its central line curves periodically.

We first calculate the energy minigaps (EMGs) of the LSSLW at the boundaries of the Brillouin zone using the variational approach:

$$\begin{aligned} E &= \int_V \psi^*(r)H(r)\psi(r)\,\mathrm{d}\tau \Big/ \int_V \psi^*(r)\psi(r)\,\mathrm{d}\tau \\ &= \int_{V'} \tilde{\psi}^*(r')H_{\mathrm{eff}}(r')\tilde{\psi}(r')\,\mathrm{d}\tau' \Big/ \int_{V'} \tilde{\psi}^*(r')\tilde{\psi}(r')J(r')\,\mathrm{d}\tau' \end{aligned} \tag{11}$$

where $\tilde{\psi}(r')$ represents the variational wave function in the new coordinate spaces.

To satisfy the boundary conditions (8), the following trial wave function is adopted:

$$\tilde{\psi}(r') = \sin[k_x(x' + d_x)]\sin[k_y(y' + d_y)](A\mathrm{e}^{\mathrm{i}k_z z'} + B\mathrm{e}^{\mathrm{i}k'_z z'}) \tag{12}$$

where A and B are variational parameters, $k_x = n_x\pi/2d_x$ ($k_y = n_y\pi/2d_y$) with $n_x(n_y)$ positive integers, and $k_z = n\pi/L_d$ ($k'_z = -n\pi/L_d$), with n the integers at the boundaries of the Brillouin zone. Inserting the trial wave function (12) and effective Hamiltonian (5) into equation (11), the variational calculation gives the following results. For case (i) the first EMG can be obtained as

$$\Delta E_g(1) = 2\delta_x(\hbar^2/2m)k_x^2 + 2\delta_y(\hbar^2/2m)k_y^2 \tag{13}$$

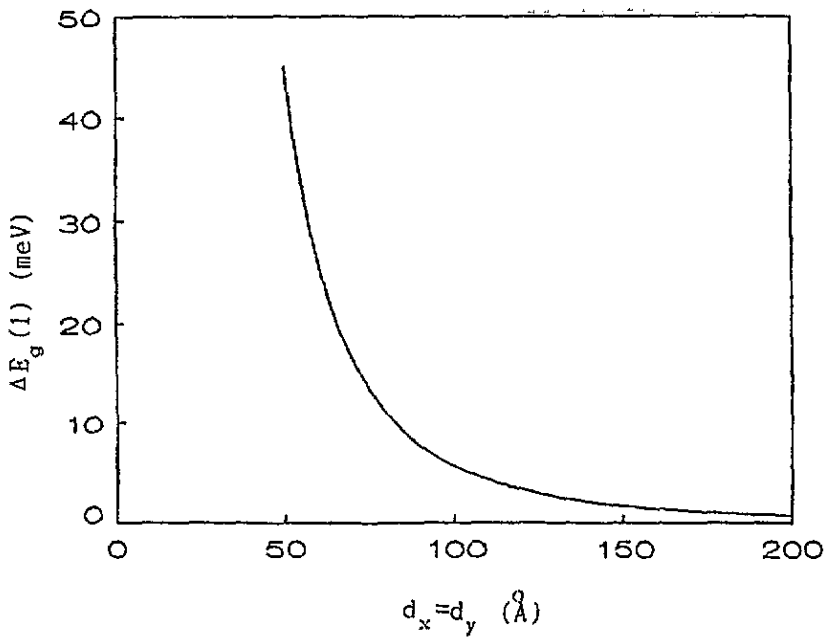

Figure 1. Numerical results for the first EMG, $\Delta E_g(1)$, as a function of the cross section sizes $d_x = d_y$ for the ground state ($n_x = n_y = 1$) in case (i), where the amplitude of the fluctuation of the interface structures is $\Delta = 10$ Å.

where $\delta_x = \Delta/d_x$, $\delta_y = \Delta/d_y$ are the relative fluctuations of the LSSLW in the x, y directions, referred to as radial roughness. For case (ii) the first EMG is zero and the second EMG becomes

$$\Delta E_g(2) = 2\pi^2(\Delta/L_d)^2(h^2/2m)(k_x^2 + k_y^2) \tag{14}$$

where Δ/L_d is the relative curvature of the LSSLW in the z direction, referred to as longitudinal roughness.

At the same time, the degenerate–perturbational approach is used to calculate the EMGs. It is found that the results obtained are the same for both approaches. Then we further calculated the second, third, ... EMGs in case (i) using the degenerate–perturbational approach and found that the larger the number n the smaller the EMG.

From the analytical results (13) and (14), it is easy to see that in case (i) the first EMG, $\Delta E_g(1)$, is not dependent on the LSSLW period L_d. By fixing the amplitude of fluctuation as $\Delta = 10$ Å, we obtained the numerical results given in figure 1, for the case of a square cross section $d_x = d_y$ and the ground state $n_x = n_y = 1$. Figure 1 shows the dependence of the first EMG, $\Delta E_g(1)$, on the cross section dimensions $d_x = d_y$. In addition, in case (i) a circular-cross-section LSSLW is also considered; the results obtained with the method developed in this paper are very similar to those for the square cross section, and the first EMG of the square-cross-section case is slightly larger than that of the circular-cross-section case when they have equal areas.

In case (ii) the first EMG, $\Delta E_g(1)$, is zero and the second EMG, $\Delta E_g(2)$, shows a strong dependence on the LSSLW period L_d as shown in figure 2 where we consider

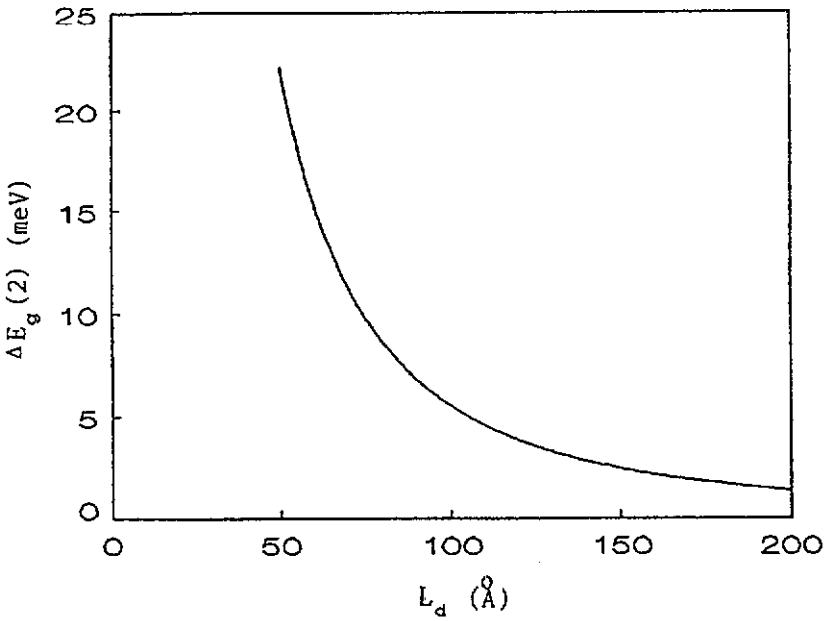

Figure 2. Numerical results for the second EMG, $\Delta E_g(2)$, as a function of the lateral period L_d for the ground state ($n_x = n_y = 1$) in case (ii), where the amplitude of the fluctuation of the interface structures is $\Delta = 10$ Å and the cross section sizes are $d_x = d_y = 100$ Å.

$\Delta = 10$ Å, $d_x = d_y = 100$ Å and the ground state $n_x = n_y = 1$. The results indicate that $\Delta E_g(2)$ increases with the decrease of the LSSLW period L_d.

From the above results, it is interesting to note that the EMGs in case (i), where the widths of the LSSLW fluctuate periodically, are proportional to the first order of the radial roughness Δ/d_x (Δ/d_y) and independent of the lateral period L_d. However, the EMGs in case (ii), where the central line of the LSSLW curves periodically, are proportional to the second order of the longitudinal roughness Δ/L_d and so depend strongly on the lateral period L_d. By reducing the lateral period L_d, the EMGs in case (ii) can be made comparable to those in case (i). This indicates a very useful LSSLW structure where the EMGs can be adjusted by changing the lateral period L_d, which is achieved by turning the vicinal angles of the GaAs substrates in GaAs/AlAs LSSLWs produced by the method described at the beginning of the paper. The EMGs of LSSLWs can be detected by infrared absorptions; we hope that our theoretical predications can soon be tested experimentally.

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