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## Binding energies of hydrogenic impurities in lateral surface superlattice quantum well wires

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**Abstract.** A variational calculation of hydrogenic impurity binding energies in quasi-one-dimensional GaAs/AlAs quantum well wires with periodic lateral surface structures was carried out. By a coordinate transformation, the structured interfaces of the wires are transformed into planar interfaces so that the boundary conditions of the electronic wavefunctions can be satisfied exactly at the interfaces. The dependences of the binding energies on the positions of the impurities and on the lateral surface structures are studied.

### 1. Introduction

In the past few years, the interesting physical properties of quantum well wires with dimensions comparable with the electronic de Broglie wavelength have attracted considerable attention. The studies have concerned electronic structures, transport properties and excitonic levels, as well as the impurity binding energies in quantum wires. Because of the quantum confinement in two directions, the binding energies of excitons and impurity states are greatly enhanced in wires compared with those in quasi-two-dimensional quantum well structures [1-11].

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 a lateral surface superlattice (LSSL), has shown interesting behaviours of its electronic and optical properties [12-16]. Technically now we are also able to fabricate quantum well wires with periodic structures at their interfaces, referred to as lateral surface superlattice wires (LSSLWs), by ion beam implantation on LSSLs produced by deposition of AlAs and GaAs fractional layers on (001) vicinal GaAs substrates [15-19], 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 the electron to light-hole to exciton peak intensities and the ratios of the electron to heavy-hole to exciton peak intensities, etc [12-15], may be greatly enhanced in LSSLWs. The difficulty in calculating the electronic and optical properties

of LSSLWS is that the boundary conditions of the electronic wavefunctions are not easily satisfied on the periodically structured interfaces.

In this paper, we use the coordinate transformation suggested in our previous paper [20] which avoids this difficulty and the binding energies of hydrogenic impurities in one single wire in which the lateral walls have a periodic undulation are studied. In our consideration, 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 practical experiments, there are many irregularities in the periodic structured interfaces in LSSLs, but their main structures are periodic [12–15], and we examine only exact periodic LSSLWS here. In addition, in this paper we consider mainly the ground electronic states whose energies (less than 150 meV) are much smaller than the conduction band offset between AlAs and GaAs (equal to 1.07 eV [15]); so the potential barrier between AlAs and GaAs is assumed to be infinitely high.

The paper is organized as follows. In section 2 we explain the theory, i.e. the coordinate transformation and the definition of impurity binding energy. The numerical results and discussion are presented in section 3.

## 2. Theory

Let us consider a quantum wire of GaAs surrounded by AlAs, which is assumed to have a rectangular cross section and an 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

$$H^{(0)}(\mathbf{r}) = |\mathbf{P}|^2/2m + V(\mathbf{r}) \quad (1)$$

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

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

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

When a hydrogenic impurity is placed in the quantum wire, the Hamiltonian becomes

$$H(\mathbf{r}) = |\mathbf{P}|^2/2m - e^2/\kappa|\mathbf{r} - \mathbf{r}_i| + V(\mathbf{r}) \quad (3)$$

where  $\kappa = 13.1$  is the dielectric constant of GaAs and  $\mathbf{r}_i$  is the position of the hydrogenic impurity in the quantum wire.

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

$$\begin{aligned} x' &= \left\{ x - \frac{1}{2}[f_1(\mathbf{r}) + f_2(\mathbf{r})] \right\} 2d_x / [2d_x + f_1(\mathbf{r}) - f_2(\mathbf{r})] \\ y' &= \left\{ y - \frac{1}{2}[f_3(\mathbf{r}) + f_4(\mathbf{r})] \right\} 2d_y / [2d_y + f_3(\mathbf{r}) - f_4(\mathbf{r})] \\ z' &= z. \end{aligned} \quad (4)$$

In the transformation, we note that

$$\begin{aligned} \int_V \psi^*(\mathbf{r}) H^{(0)}(\mathbf{r}) \psi(\mathbf{r}) d\tau &= \int_{V'} \tilde{\psi}^*(\mathbf{r}') J(\mathbf{r}') \tilde{H}^{(0)}(\mathbf{r}') \tilde{\psi}(\mathbf{r}') d\tau' \\ &= \int_{V'} \tilde{\psi}^*(\mathbf{r}') H_{\text{eff}}^{(0)}(\mathbf{r}') \tilde{\psi}(\mathbf{r}') d\tau' \end{aligned} \quad (5)$$

where  $J(\mathbf{r}')$  is the Jacobian determinant, and the effective Hamiltonians without and with an impurity are defined, respectively, as

$$H_{\text{eff}}^{(0)}(\mathbf{r}') = J(\mathbf{r}') \tilde{H}^{(0)}(\mathbf{r}') \quad (6)$$

and

$$H_{\text{eff}}(\mathbf{r}') = J(\mathbf{r}') \tilde{H}(\mathbf{r}'). \quad (7)$$

The normalization condition becomes

$$\int_{V'} \tilde{\psi}^*(\mathbf{r}') \tilde{\psi}(\mathbf{r}') J(\mathbf{r}') d\tau' = 1. \quad (8)$$

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

$$\tilde{V}(\mathbf{r}') = \begin{cases} 0 & |x'| < d_x \quad |y'| < d_y \\ \infty & \text{elsewhere.} \end{cases} \quad (9)$$

In the new coordinate system the wavefunction satisfies the boundary conditions

$$\tilde{\psi}(\mathbf{r}')|_{x'=\pm d_x} = 0 \quad \tilde{\psi}(\mathbf{r}')|_{y'=\pm d_y} = 0. \quad (10)$$

In this paper, we consider two typical cases as follows: case (i) is

$$\begin{aligned} f_1(\mathbf{r}) &= -f_2(\mathbf{r}) = \Delta \sin[(2\pi/L_d)z] \\ f_3(\mathbf{r}) &= -f_4(\mathbf{r}) = \Delta \sin[(2\pi/L_d)z] \end{aligned} \quad (11)$$

and case (ii) is

$$\begin{aligned} f_1(\mathbf{r}) &= f_2(\mathbf{r}) = \Delta \sin[(2\pi/L_d)z] \\ f_3(\mathbf{r}) &= f_4(\mathbf{r}) = \Delta \sin[(2\pi/L_d)z] \end{aligned} \quad (12)$$

where  $\Delta$  and  $L_d$  are the amplitude and period, respectively, of the interface structures of the LSSLWs. Case (i) represents an LSSLW where the central line is straight but its widths fluctuate periodically, as shown in figure 1(b), while case (ii) represents an LSSLW where the widths do not change but its central line curves periodically, as shown in figure 1(c).

In the new coordinate spaces, the trial electronic wavefunction of  $H_{\text{eff}}^{(0)}(\mathbf{r}')$  in the quantum well wire without any impurity can be written as

$$\tilde{\phi}_{nmk_z}(\mathbf{r}') = N_0 \sin[(n\pi/2d_x)(d_x + x')] \sin[(m\pi/2d_y)(d_y + y')] \exp(ik_z z') \quad (13)$$

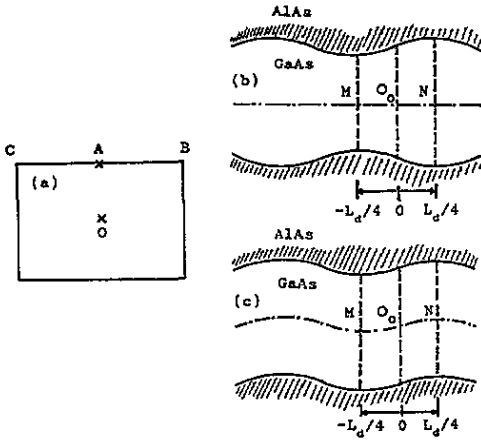


Figure 1. The diagrams of the two types of LSSLW that we considered. (a) The rectangular cross section of a quantum wire. O, A, B and C are the centre, the centre of one side and the corners of the quantum wire, respectively. (b) The surface periodic structures of an LSSLW in case (i). M, O<sub>0</sub> and N lie at  $z' = -L_d/4, 0$  and  $L_d/4$ , respectively, on the central line of the quantum wire. (c) The surface periodic structures of the LSSLW in case (ii). The positions of M, O<sub>0</sub> and N are the same as those in (b).

where  $N_0$  is the normalization constant, and  $n$  and  $m$  are positive integers. Here, the periodic potential due to the LSSLs is much smaller than the electronic kinetic energy, and the electronic wavefunction moving along the quantum wire could be viewed as a plane wave. The electronic wavefunction in the ground state is

$$\tilde{\phi}_{11}(\mathbf{r}') = N_0 \cos[(\pi/2d_x)x'] \cos[(\pi/2d_y)y'] \tag{14}$$

The trial wavefunction of  $H_{\text{eff}}(\mathbf{r}')$  we take as analogous to that used in [4, 7] and it is written for the ground impurity state as

$$\tilde{\psi}(\mathbf{r}') = N \cos[(\pi/2d_x)x'] \cos[(\pi/2d_y)y'] \exp[-|\mathbf{r}' - \mathbf{r}'_i|/\lambda] \tag{15}$$

where  $N$  is the normalization constant and  $\lambda$  is the variational parameter. This wavefunction reproduces the 3D results when  $d_x, d_y \rightarrow \infty$  and 1D results when  $d_x, d_y \rightarrow 0$ . The trial wavefunction (15) satisfies the boundary conditions (10).

As usual, we define the impurity binding energy as the energy difference between the bottom of the electronic conduction band without the impurity and the ground level of impurity state in the LSSLW, i.e.

$$E_i = \langle \tilde{\phi}_{11}(\mathbf{r}') | H_{\text{eff}}^{(0)}(\mathbf{r}') | \tilde{\phi}_{11}(\mathbf{r}') \rangle - \min_{\lambda} \langle \tilde{\psi}(\mathbf{r}') | H_{\text{eff}}(\mathbf{r}') | \tilde{\psi}(\mathbf{r}') \rangle \tag{16}$$

The above integrals were calculated numerically.

### 3. Results and discussion

According to the geometric symmetry shown in figure 1, we consider only the impurity binding energies in half the lateral period,  $L_d/2$ , in the  $z'$  direction. The following typical points and lines in LSSLWs are selected. In figure 1, O, A and B are the centre, the centre of one side and the corner of the cross section, respectively; M, O<sub>0</sub> and N lie at  $z' = -L_d/4, 0$  and  $L_d/4$ , respectively, on the central line of the quantum wires. Because of the peculiar situation of the LSSLW in case (ii), another corner C of the cross section is also considered.

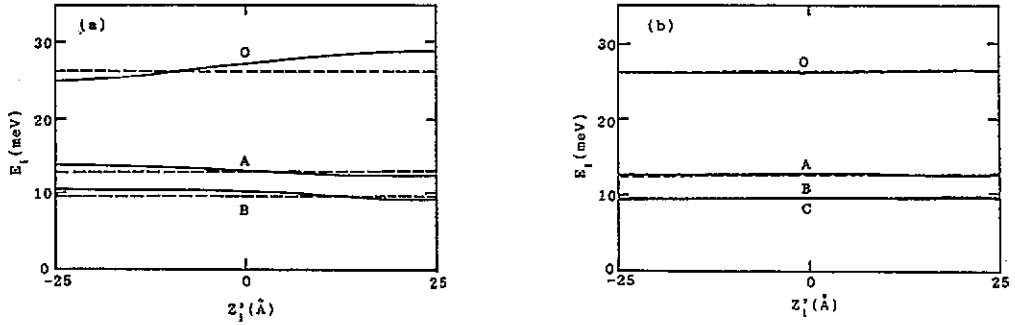
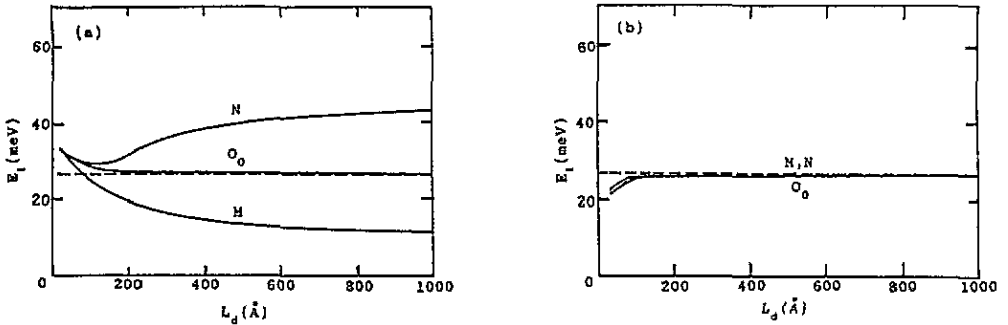


Figure 2. Numerical results for impurity binding energies on different lines along a quantum wire for two types of LSSLW, where  $d_x = d_y = 50 \text{ \AA}$ ,  $\Delta/d_x = \Delta/d_y = 0.10$  and  $L_d = 100 \text{ \AA}$ : ---, corresponding impurity binding energies without lateral surface structures. (a) The variations in impurity binding energy with the positions on different lines (O, A and B) along the quantum wire in case (i). (b) The variations in impurity binding energy with the positions on different lines (O, A, B and C) along the quantum wire in case (ii).

Figure 2 shows the variations in the impurity binding energy with its position on different lines along the quantum wire for two types of LSSLW, where we consider the cross section sizes  $d_x = d_y = 50 \text{ \AA}$ , the relative fluctuation  $\Delta/d_x = \Delta/d_y = 0.10$  and the lateral period  $L_d = 100 \text{ \AA}$ . In figure 2, the broken lines represent the corresponding numerical results when the quantum wire has no lateral surface structures.

From figure 2(a), it is apparent that the impurity binding energy in case (i) changes with its position along the  $z'$  direction. The difference between the maximum binding energy and the minimum binding energy on the central line (O) (3.85 meV) is larger than that on the centre line of one side (A) (1.40 meV) or on the line of the corner (B) (1.28 meV). From figure 2(b), we can also see that the variations in the impurity binding energy along the  $z'$  direction in case (ii), where the widths of the LSSLW do not change, are smaller than those in case (i), where the widths of the LSSLW fluctuate periodically. In case (ii), the difference between the maximum binding energy and the minimum binding energy on the central line is 0.12 meV, that on the central line of one side is 0.35 meV and those on the lines of the corners B and C are 0.12 meV and nearly zero, respectively.

Figure 3 shows the variations in the impurity binding energy with lateral period  $L_d$  at different points on the central line for two types of LSSLW, where we set the cross section sizes  $d_x = d_y = 50 \text{ \AA}$  and the relative fluctuation  $\Delta/d_x = \Delta/d_y = 0.10$ . The broken lines in figure 3 represent the corresponding impurity binding energy on the central line without lateral surface structures. The variations in case (i) as shown in figure 3(a) are very different from those in case (ii) as shown in figure 3(b). In case (i), the binding energy at position N decreases for small  $L_d$  with increasing lateral period, reaches a minimum in the vicinity of the effective Bohr radius of GaAs ( $a^* \simeq 100 \text{ \AA}$ ) and then increases again; when  $L_d$  is infinite, it reaches a limiting value. The binding energies at positions  $O_0$  and M decrease monotonically with increasing  $L_d$ ; when  $L_d$  becomes infinite, the binding energy at  $O_0$  is the same as that without lateral surface structures and the binding energy at M reaches a minimum limit. However, in case (ii), the binding energies at positions M,  $O_0$  and



**Figure 3.** The variations in impurity binding energy with lateral period  $L_d$  at different positions on the central line for two types of LSSLW, where  $d_x = d_y = 50 \text{ \AA}$  and  $\Delta/d_x = \Delta/d_y = 0.10$ : ---, corresponding impurity binding energies on the central line of a quantum wire without lateral surface structures. (a) The variations in impurity binding energy with lateral period  $L_d$  at positions M,  $O_0$  and N on the central line of the quantum wire in case (i). (b) The variations in impurity binding energy with lateral period  $L_d$  at positions M,  $O_0$  and N on the central line of the quantum wire in case (ii).

$N$  increase monotonically with increase in the lateral period  $L_d$ , where the binding energies at M and N are the same because of the geometric symmetry. The variations in the binding energy at the three points on the central line in case (ii) are much smaller than those in case (i). In addition, in case (ii) the binding energies at M and N are slightly larger than those at  $O_0$  and, when  $L_d$  becomes infinite, their binding energies reach the values obtained without lateral surface structures.

The results obtained above are interesting, and their physical interpretation and discussion are as follows. By the coordinate transformation that we suggested, the structured interfaces of the LSSLWs are transformed into planar interfaces and the Hamiltonian of the electron is transformed into the effective Hamiltonian in the new coordinate system, which is a periodic potential along a quantum wire, i.e. the lateral surface periodic structures in the LSSLW could be viewed as a periodic potential along a quantum wire which acts on the electron moving in the  $z'$  direction. When a hydrogenic impurity is placed in the LSSLW, the electron moving in the quantum wire is affected by the impurity potential and the periodic potential in the  $z'$  direction, and the sums of the potentials around an impurity are different for different impurity positions on the central line or on the boundary lines along the quantum wire. Hence, in figure 2 the impurity binding energy changes along the quantum wire. Because the effective periodic potential due to the lateral surface structures in case (i), where the widths of the LSSLW fluctuate periodically, is larger than that in case (ii), where the widths of the LSSLW do not change [20], therefore the variations in impurity binding energy on the central line or on the boundary lines in case (i) are greater than the corresponding values in case (ii).

The results in figure 3(a) may cause some misunderstanding. When the lateral period  $L_d$  is infinite, the binding energy at position N, where the widths of the LSSLW are  $d_x + \Delta$ ,  $d_y + \Delta > d_x$ ,  $d_y$ , reaches a maximum limit which is larger than the corresponding binding energy without lateral surface structures. On the other hand, when the lateral period  $L_d$  becomes infinite, the binding energy at position M, where the widths of the LSSLW are  $d_x - \Delta$ ,  $d_y - \Delta < d_x$ ,  $d_y$ , reaches a minimum limit which is smaller than the corresponding binding energy without lateral surface

structures. These contradict the usual results [1–11] in which the impurity binding energy increases when the cross section dimensions of the quantum wire decrease. In order to understand this peculiar phenomenon, we must examine the definition (16) of the impurity binding energy in LSSLWs firstly. From equation (16) it is easily seen that the ground-state electronic kinetic energy without any impurity in the LSSLW is the expectation value of the effective Hamiltonian  $H_{\text{eff}}^{(0)}(r')$  and is not dependent on the electron and impurity positions in the LSSLW. When the lateral period  $L_d$  is infinite, the ground-state electronic kinetic energies at the positions M,  $O_0$  and N, where they have different cross section sizes, are the same. These are different from the usual ground-state electronic kinetic energy in a quantum well wire without lateral surface structures, where the different cross section sizes result in different ground-state electronic kinetic energies. Hence, when the lateral period becomes infinite, the impurity binding energies at the positions M,  $O_0$  and N reach different limiting values and these results are different from the usual conclusion. However, the situation in case (ii) is different, as shown in figure 3(b). When the lateral period  $L_d$  is infinite, its structure is the same as that without lateral surface structures, and the binding energies at the positions M,  $O_0$  and N are the same as the corresponding value without lateral surface structures.

From figure 2 we can also see that, different from the impurity binding energy dispersion in quantum well wires without lateral surface structures, the maximum and minimum of the impurity binding energies in an LSSLW change when impurities move along the  $z'$  direction. These would change the distribution of the density of impurity states, would change the centre of gravity of the impurity band and could affect the features in the transition spectra of a doped quantum wire.

In conclusion, by a coordinate transformation, the structured interfaces of the wires are transformed into planar interfaces so that the boundary conditions of the electronic wavefunctions can be satisfied exactly at the interfaces. In this paper, the hydrogenic impurity binding energies are calculated with a variational approach for two types of GaAs/AlAs LSSLW: one in which its central line is straight but the widths fluctuate periodically, and the other where the widths do not change but the central line curves periodically. The results have shown that the binding energies change along the  $z'$  direction and change with different lateral periods  $L_d$  for the two types of LSSLW. The variations in binding energy with the impurity position and with the lateral period in case (i) are larger than those in case (ii). When the lateral period  $L_d$  becomes infinite, the binding energies at the positions M,  $O_0$  and N on the central line in case (ii) are the same as those without lateral surface structures, but the corresponding values in case (i) reach different limits and are different from the usual results. In addition, because of the extension of the impurity binding energy in maximum and minimum sides the density of impurity states would be changed. These could affect the features in the transition spectra of a doped quantum wire.

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