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Optical absorption spectra associated with an impurity in lateral-surface superlattice quantum well wires

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Abstract. We calculate the optical absorption spectra associated with an impurity in quasi-one-dimensional GaAs/AlAs quantum well wires with periodic lateral surface structures. The results indicate that there is an energy-forbidden region for optical transitions from acceptors to conduction minibands, and no forbidden region for optical transitions from valence minibands to donors. The dependence of optical absorption spectra on the interface amplitude is discussed.

1. Introduction

In the past few years, the quantum well with periodic lateral structures on its interfaces, referred to as a lateral-surface superlattice (LSSL), has attracted considerable attention. Because of the existence of the lateral-surface structures which act as periodic potentials on electrons, many interesting electronic and optical phenomena have been discovered in this system experimentally [1–5]. Technically now we are also able to fabricate quantum well wires with periodic structures on 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 [6, 7], for instance. It is expected that the peculiar electronic and optical properties observed in LSSLs may be greatly enhanced in LSSLWs.

Using a coordinate transformation which transforms the structured interfaces of the wires into planar interfaces so that the boundary conditions of electronic wavefunctions can be satisfied exactly on the interfaces, we have studied the electronic and impurity states in LSSLWs in our previous papers [8–11]. It is found that energy minigaps (EMGs) appear in the electronic energy dispersions in LSSLWs at the boundaries of the Brillouin zone, and the impurity binding energies extend on the maximum and minimum sides compared with those in the quantum well wires with planar interface structures. In this paper, we study the optical absorption spectra associated with an impurity in LSSLWs further. The dependence of optical absorption spectra on the interface amplitude will be discussed.

Because the binding energies for impurities in wires with comparable shapes are most closely correlated to the cross sectional area and the shape effects on binding energies are of little importance [12], we consider only the LSSLW with a circular cross section as in our recent paper [11]. In section 2, we outline the theoretical framework. The results and discussion are presented in section 3.

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2. Theory

The Hamiltonians describing the motion of an electron in the GaAs/AlAs LSSLW with circular cross section excluding and including an impurity can be written

$$H^{(0)}(r) = \frac{|P|^2}{2m} + V(r) \tag{1}$$

and

$$H(r) = \frac{|P|^2}{2m} - \frac{e^2}{\kappa|r - r_i|} + V(r) \tag{2}$$

where m is the electron-band effective mass in GaAs, $\kappa = 13.1$ is the dielectric constant of GaAs and r_i is the position of impurity in the LSSLW. The electron-confining potential well $V(r)$ is given by

$$V(r) = \begin{cases} 0 & \rho < R_0 + f(r) \\ \infty & \text{elsewhere} \end{cases} \tag{3}$$

where R_0 is the average radius of the LSSLW and

$$f(r) = \Delta \sin\left(\frac{2\pi}{L_d} z\right) \tag{4}$$

describes the periodic structures on its interfaces with Δ and L_d the amplitude and the period, respectively, of the interface structures.

The following coordinate transformation transforms the structured interfaces of the LSSLW into flat interfaces [11].

$$\begin{aligned} \rho' &= \rho \frac{R_0}{R_0 + f(r)} \\ \theta' &= \theta \\ z' &= z \end{aligned} \tag{5}$$

In the new coordinate system, the Hamiltonians without and with an impurity become the effective Hamiltonians which are the periodic functions in the z direction [11], and the wavefunction satisfies the boundary condition (hereafter we denote r' by r to simplify the notation):

$$\psi(r)|_{\rho=R_0} = 0. \tag{6}$$

For optical transitions from valence minibands to a donor level, we have for the initial state

$$|i\rangle = [A\varphi_{k_z}^{(1)}(r) + B\varphi_{k_z}^{(2)}(r)]u_i(r) \tag{7}$$

with

$$\varphi_{k_z}^{(1)}(r) = (\pi R_0^2 L_0)^{-1/2}[J_1(\beta_{01})]^{-1} J_0(\beta_{01}\rho/R_0)\exp(ik_z z) \tag{8}$$

and

$$\varphi_{k_z}^{(2)}(r) = (\pi R_0^2 L_0)^{-1/2}[J_1(\beta_{01})]^{-1} J_0(\beta_{01}\rho/R_0)\exp[i(k_z - k_d)z] \tag{9}$$

where β_{01} is the first zero of the Bessel function, $L_0 = NL_d$ ($N \to \infty$) is the length of the LSSLW, $k_d = 2\pi/L_d$ is the first reciprocal-lattice vector, and A and B are the variational parameters which have been determined in our previous paper [11]. For the final state, the wavefunction is

$$|f) = NJ_0(\beta_{01}\rho/R_0)\exp(-|r - r_i|/\lambda)u_f(r) \tag{10}$$

where N is the normalization constant and λ is the variational parameter [11]. In equations (7) and (10), $u_i(r)$ and $u_f(r)$ are the periodic parts of the Bloch state for the initial and final states, respectively.

Taking the energy origin at the bottom of the first conduction miniband as depicted later in figure 1, we have for the energy of the initial state

$$E_i = -\epsilon_g - E^v(k_z) \tag{11}$$

where $E^v(k_z)$ is the energy dispersion of valence minibands [11] and

$$\epsilon_g = E_g + \frac{\hbar^2}{2m_c}\frac{\beta_{01}^2}{R_0^2} + \frac{\hbar^2}{2m_v}\frac{\beta_{01}^2}{R_0^2} \tag{12}$$

with E_g being the bulk GaAs band gap and $m_c(m_v)$ the effective mass of the conduction (valence) and in GaAs. The energy of the final state is

$$E_f = -E_b(r_i) \tag{13}$$

where $E_b(r_i)$ is the binding energy of the donor impurity [11].

The transition probability per unit time for transitions from the valence minibands to the donor impurity associated with the impurity located at the position r_i is proportional to the square of the matrix element of the electron–photon interaction H_{int} between the wavefunctions of the initial state (valence) and final (impurity) state [13–16]

$$W(\omega, r_i) = \frac{2\pi}{\hbar}\sum_i |(f|H_{int}|i)|^2\delta(E_f - E_i - \hbar\omega) \tag{14}$$

with $H_{int} = Ce\cdot p$, where e is the polarization vector in the direction of the electric field of the radiation, p is the momentum operator and C is a pre-factor that describes the effects of the photon vector potential [17]. Following the effective-mass approximation, the above matrix element may be written [13–16]

$$\langle f|H_{int}|i\rangle \simeq Ce\cdot P_{fi}S_h \tag{15}$$

with

$$P_{fi} = \frac{1}{\Omega}\int_\Omega u_f^*(r)pu_i(r)\,dr \tag{16}$$

and

$$S_{fi} = \int F_f^*(r) F_i(r)\, dr \tag{17}$$

where Ω is the volume of the unit cell and $F_f(r)$ ($F_i(r)$) is the envelope function for the final (initial) state. Then equation (14) can be simplified further:

$$W(\omega, r_i) = \frac{2\pi}{\hbar}|C|^2|e \cdot P_{fi}|^2 |S_{fi}(r_i, k_z(\Delta))|^2 g(\Delta) \tag{18}$$

where $g(\Delta)$ is the density of states of valence minibands [11] and

$$\Delta = \hbar\omega + E_b(r_i) - \epsilon_g. \tag{19}$$

Assuming that the circular cross section of the LSSLW is not too small, we could treat the impurity position as a continuous random variable. Provided that the impurities exist only inside the LSSLW and there is not intentional doping, the total transition probability per unit time can be obtained:

$$W(\omega) = \frac{2\pi}{\hbar}|C|^2|e \cdot P_{fi}|^2 \frac{1}{V_0} \int_{v_0} |S_{fi}(r_i, k_z(\Delta))|^2 g(\Delta)\, dr_i. \tag{20}$$

where V_0 is the volume of LSSLW in half the lateral period due to the geometric symmetry of the LSSLW [11]. Also, the transition probability for transitions from acceptors to conduction minibands can be obtained in the same way as described above [16].

3. Results and discussion

In our practical calculation, the conduction band effective mass m_c in GaAs is taken to be $0.067m_0$ with m_0 the free-electron mass and the valence band effective mass m_v in GaAs is $0.30m_0$ with the mixing of the light- and heavy-hole bands neglected [13]. Figure 1 shows the possible valence minibands$\longrightarrow$donor band transitions, where $\Delta E_g^c(1)$ and $\Delta E_g^v(1)$ are the first EMGs of conduction minibands and valence minibands [11] respectively, which result from the periodic potentials along the quantum wire caused by the interface structures of LSSLW. In figure 1, $\hbar\omega_1$ represents the transition energy from the top edge of the first valence miniband to the bottom edge of the donor band, $\hbar\omega_2$ represents the transition energy from the bottom edge of the first valence miniband to the top edge of the donor band and $\hbar\omega_3$ represents the transition energy from the top edge of the second valence miniband to the bottom edge of the donor band. For the acceptor band$\longrightarrow$conduction minibands transitions, $\hbar\omega_1$ is the transition energy from the top edge of the acceptor band to the bottom edge of the first conduction miniband, $\hbar\omega_2$ is the transition energy from the bottom edge of the acceptor band to the top edge of the first conduction miniband and $\hbar\omega_3$ is the transition energy from the top edge of the acceptor band to the bottom edge of the second conduction miniband [11,16]. The optical transition spectra associated with donors and acceptors in LSSLWs with different amplitudes of interface structures are shown in figures 2 and 3, where $E_j = \hbar\omega_j - E_g$ ($j = 1$–3).

Figure 2 shows the optical absorption spectra of impurity$\overrightarrow{\longleftarrow}$minibands transitions in the LSSLW, where the average radius of the LSSLW is $R_0 = 50$ Å, and the amplitude and period of the interface structures of the LSSLW are $\Delta = 5$ Å and $L_d = 100$ Å, respectively. From

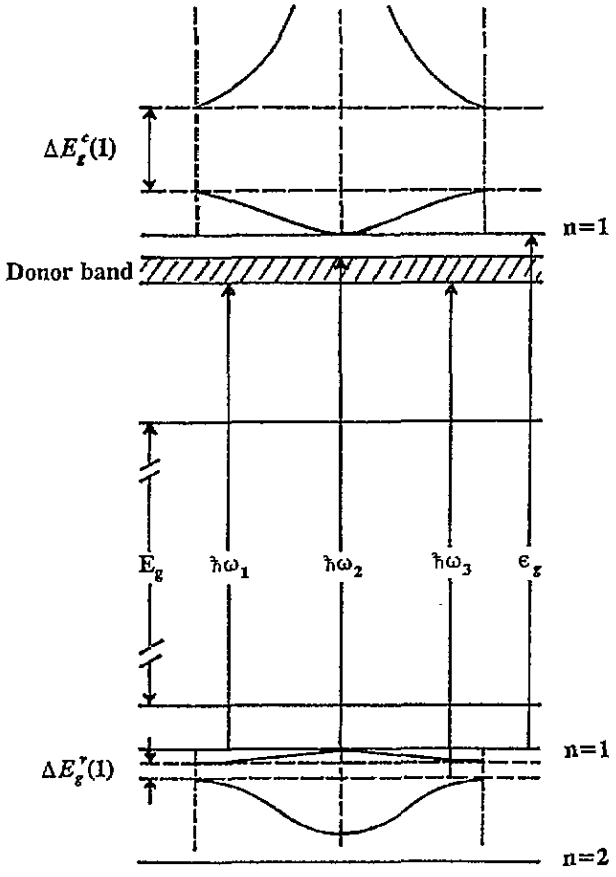

Figure 1. Schematic representation of some possible optical transitions from the valence minibands to the donor band in the LSSLW, where the parabolae represent the energy dispersions of the first two conduction and valence minibands in the first Brillouin zone of z direction.

figure 2(*a*), we can see that the spectrum structures for the valence minibands⟶donor band transitions are complicated and no energy-forbidden region exists. The situation for the acceptor band⟶conduction mimband transitions is different and an energy-forbidden region between the transition energies E_3 and E_2 appears, as shown in figure 2(*b*).

Figure 3 also shows the optical absorption spectra associated with an impurity in the LSSLW, where the average radius of the LSSLW is $R_0 = 50$ Å, and the amplitude and period of the interface structures of the LSSLW are $\Delta = 10$ Å and $L_d = 100$ Å, respectively. Compared with the results in figure 2, we found that the energy-forbidden region for the acceptor band⟶conduction minibands transitions with the amplitude $\Delta = 10$ Å is much larger than that with the amplitudes $\Delta = 5$ Å, as shown in figure 3(*b*). However, the absorption spectra for valence minibands⟶donor band transitions with the amplitude $\Delta = 10$ Å have no apparent change except some movement of absorption peaks, and also no energy-forbidden region appear, as shown in figure 3(*a*).

The above results are interesting and their physical interpretation is as follows. The electron motion in quantum wires consists of plane waves in the direction along the wires. The periodic structures on the interfaces of the LSSLW act as periodic potentials which cause

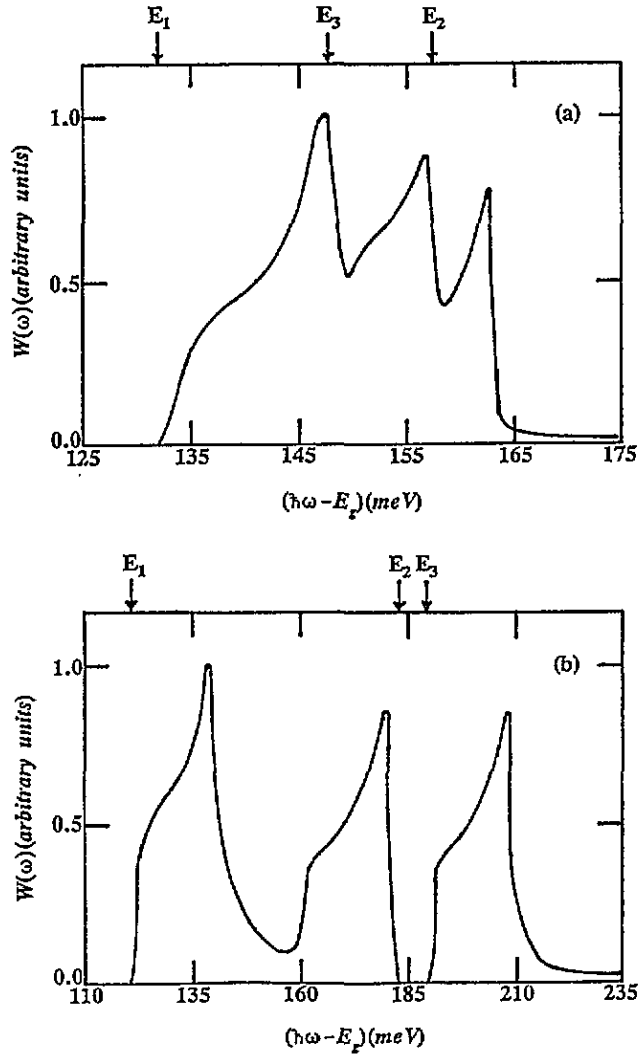

Figure 2. Optical absorption probability per unit time for the transitions (*a*) from the valence minibands to the donor band and (*b*) from the acceptor band to the conduction minibands as a function of $\hbar\omega - E_g$, where the average radius of the LSSLW is $R_0 = 50$ Å, and the amplitude and period of the interface structures of the LSSLW are $\Delta = 5$ Å and $L_d = 100$ Å, respectively.

reflections of the electron plane waves. EMGs appear in the electronic energy dispersions of the LSSLW at the boundary of the Brillouin zone [8, 11]. The effects of the periodic potentials on impurity states in the LSSLW are not as drastic on free-electron states, and only some broadenings and shifts in the peaks of the impurity density of states are caused [11]. If the EMG is larger than the width of impurity band, i.e. the transition energy $\hbar\omega_3 > \hbar\omega_2$ and $E_3 > E_2$, an energy-forbidden region could appear for the impurity$\overleftarrow{\longrightarrow}$miniband optical transitions owing to the energy conservation law [11]. This happens for the acceptor band$\longrightarrow$conduction minibands transitions where an energy-forbidden region exists, because the first conduction EMG $\Delta E_g^c(1) = 26.3$ meV is larger than the width of the acceptor band,

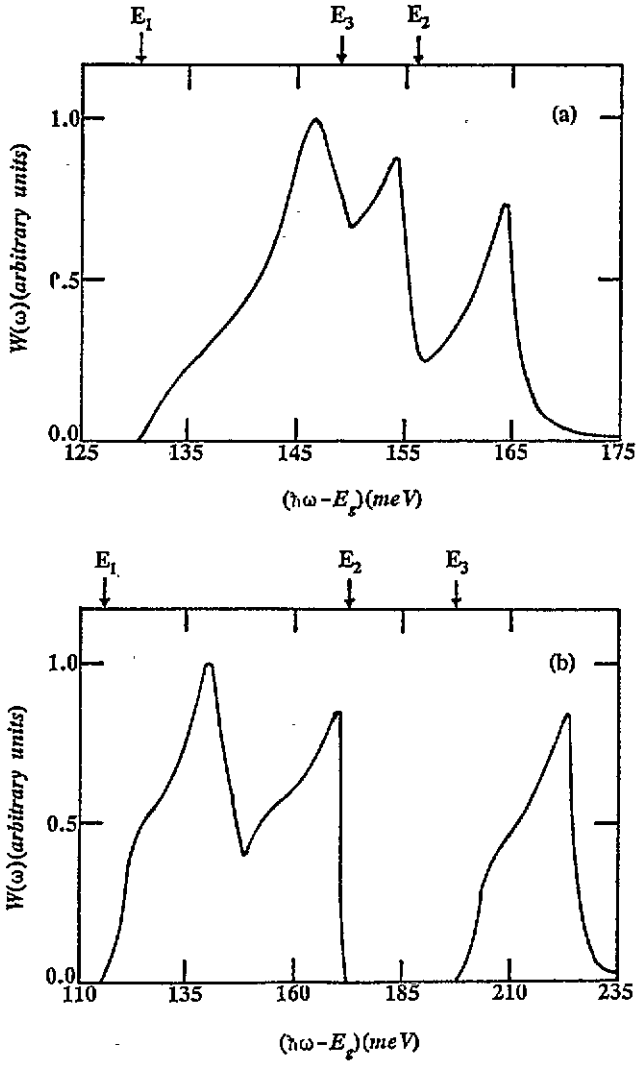

Figure 3. Optical absorption probability per unit time for the transitions (*a*) from the valence minibands to the donor band and (*b*) from the acceptor band to the conduction minibands as a function of $\hbar\omega - E_g$ where the average radius of the LSSLW is $R_0 = 50$ Å, and the amplitude and period of the interface structures of the LSSLW are $\Delta = 10$ Å and $L_d = 100$ Å, respectively.

$\Delta E_A = 20.2$ meV, when the amplitude $\Delta = 5$ Å, as shown in figure 2(*b*) ($E_3 > E_2$), and the first conduction EMG $\Delta E_g^c(1) = 52.6$ meV is larger than the width of the acceptor band, $\Delta E_A = 26.0$ meV, when the amplitude $\Delta = 10$ Å, as shown in figure 3(*b*) ($E_3 > E_2$). The same situation does not happen for the valence minibands⟶donor band transitions where no energy-forbidden region exists, because the first valence EMG $\Delta E_g^v(1) = 5.9$ meV is smaller than the width of the donor band, $\Delta E_D = 13.1$ meV, when the amplitude $\Delta = 5$ Å, as shown in figure 2(*a*) ($E_3 < E_2$), and the first valence EMG $\Delta E_g^v(1) = 11.7$ meV is smaller than the width of the donor band, $\Delta E_D = 15.7$ meV, when the amplitude $\Delta = 10$ Å, as shown in figure 3(*a*) ($E_3 < E_2$). In fact, the width of the energy-forbidden region is

equal to $\Delta E_F = E_3 - E_2$. When ΔE_F is positive, the energy-forbidden region appears and, when ΔE_F is negative, the energy-forbidden region does not exist. For the acceptor band⟶conduction minibands transitions, $\Delta E_F = 26.2$ meV with the amplitude $\Delta = 10$ Å is much larger than $\Delta E_F = 6.1$ meV with the amplitude $\Delta = 5$ Å, and the energy-forbidden region shown in figure 3(*b*) is much wider than that shown in figure 2(*b*). In addition, the optical absorption peaks appearing in figures 2 and 3 are related to the peaks of the density of states at the edges of the impurity band and at the edges of the conduction or valence minibands.

Summing up, we have studied the optical absorption spectra associated with an impurity in the LSSLW. The results show that there is an energy-forbidden region for acceptor band⟶conduction miniband transitions and no forbidden region for valence minibands⟶donor band transitions, and the width of the energy-forbidden region for acceptor band⟶conduction miniband transitions is large when the amplitude of the interface structures of the LSSLW becomes large. We hope that our theoretical results stimulate further experimental investigations.

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