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LETTER TO THE EDITOR

Electronic states in GaAs/AlAs lateral-surface superlattices

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Abstract. The electronic energy subband structures and energy minigaps in quasi-two-dimensional electronic systems with periodic modulation potentials along the lateral directions due to the periodic modulation of the widths of the systems, such as those produced by deposition of AlAs and GaAs fractional layers on (001) vicinal GaAs substrates, were predicted by numerical calculations. A coordinate transformation was introduced which transforms the systems with periodically structured interfaces to quantum wells with planar interfaces, so that the boundary conditions of the electron wavefunctions are considerably simplified. The dependence of the electronic subband structures and energy minigaps on the structural parameters of the systems, such as the periods and shapes of their periodically structured interfaces, are investigated in detail.

Much interest is currently being devoted to the two-dimensional electronic systems with periodic modulation potentials along the lateral directions, that is the so called lateral-surface superlattices (LSSLs). A variety of interesting electronic and optical phenomena associated with the energy band structures of the LSSLs have been discovered experimentally [1–9]. Of the various structures of the LSSLs proposed, the one produced by deposition of AlAs and GaAs fractional layers on (001) vicinal GaAs substrates seems to offer the greatest potential for wide applications in microelectronics and electrooptics [4, 5, 8, 10], due to the possibility of producing large periodic structures on LSSL interfaces with periods comparable with the electron wavelengths and the large band offsets between GaAs and AlAs materials, which enhance the effect of interface structures on the motions of the electrons in the LSSLs. In a previous paper [11], one of the present authors proposed a simple method to calculate the electronic energy subband structures in this kind of LSSL where the periodic modulation potentials arise from the periodic modulation of the widths of the LSSLs. A coordinate transformation was found to transform the LSSL structures to quantum wells with planar interfaces and periodic potential perturbations along the lateral directions. In the previous paper [11], a simple two-wave approximation was used to calculate the electronic subband structures of the LSSLs with the potential barriers between the well GaAs and barrier AlAs assumed to be infinitely high. In this letter, we present the results of a more rigorous numerical calculation with the potential barriers between GaAs and AlAs assumed to be finite and the electron wave functions along the lateral direction expanded with the planar waves.

We consider the same LSSL system as that described in the previous paper [11], which is produced by deposition of AlAs and GaAs fractional layers on the (001) vicinal GaAs

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substrate with interfaces separating the well GaAs and barrier AlAs at $z = \pm L_z/2 + f_\pm(x)$, where L_z is the average width and $f_\pm(x)$ describes the periodically structured interfaces of the LSSL structure. In the effective mass approximation, the Hamiltonian of the system is:

$$H = -(\hbar^2/2m_c)\nabla_r^2 + V(r) \tag{1}$$

where m_c is the electron band mass in GaAs and $V(r)$ is the quasi-two-dimensional electron potential given by:

$$V(r) = \begin{cases} 0 & \text{for } -L_z/2 + f_-(x) < z < L_z/2 + f_+(x) \\ \Delta V_c & \text{otherwise} \end{cases} \tag{2}$$

with ΔV_c the band offset between bulk GaAs and AlAs.

For a model calculation, the periodic interface structures are assumed to be:

$$f_-(x) = 0 \qquad f_+(x) = \Delta L_z \tan^{-1}[\lambda \sin(2\pi x/L_x)]/\tan^{-1}(\lambda) \tag{3}$$

where L_x and ΔL_z are the period and amplitude of the periodic interface structure.

The shape of the interface changes from a sine-shaped structure to a periodic square-welled structure if one adjusts the parameter λ in equation (3) from $\lambda = 0$ to $\lambda \longrightarrow \infty$.

The boundary conditions of the electronic wavefunction are determined by requiring the electron probability density and its probability current density to be continuous, which requires the electronic wavefunction and its derivative normal to the interfaces to be continuous at the interfaces. The complicated boundary condition can be simplified by introducing the same coordinate transformation as that in the previous paper [11], which transforms the LSSL structure in space r to a quantum well with planar interfaces at $z' = \pm L_z$ in space r'. The simplified boundary conditions in the transformed space are given by (hereinafter we denote r' by r again to simplify the notation)

$$\psi(r)|_{z=(\pm L_z/2)^-} = \psi(r)|_{z=(\pm L_z/2)^+} \tag{4}$$

and

$$\partial\psi(r)/\partial z|_{z=(\pm L_z/2)^-} = \partial\psi(r)/\partial z|_{z=(\pm L_z/2)^+} \tag{5}$$

where we have neglected the mass difference between GaAs and AlAs, which is the same approximation as used in the previous calculations of energy subband structures in GaAs/AlAs LSSLs [8, 10]. The effective Hamiltonian of the system in the transformed space can be written as

$$H_{\text{eff}} = H_0 + H_1 \tag{6}$$

with H_0 the Hamiltonian of a quantum well with two planar interfaces and a well width equal to the average width L_z of the LSSL, and H_1 a periodic modulation perturbation along the x direction due to the periodic interface structures. The orthonormalization relation of the electronic wavefunctions becomes

$$\int_{-\infty}^{\infty} \mathrm{d}r\, \psi_i^*(r)\, J(r)\, \psi_j(r) = \delta_{ij} \tag{7}$$

where $J(r)$ is the Jacobian determinant introduced in the coordinate transformation. The detailed derivations of the above formulae are given in [11].

The trial electronic wavefunctions of the system are expanded with the eigen-wavefunctions of H_0:

$$\psi_k(r) = \sum_{n=-\infty}^{\infty} A_n\, \varphi_0(z)\, \exp[\mathrm{i}(k - Q_n)\cdot x]/\sqrt{L_0} = \sum_{n=-\infty}^{\infty} A_n\, \psi_{nk}(r) \tag{8}$$

where k is the electron wave vector in the lateral direction, $L_0 = NL_x$ ($N \to \infty$) is the length of the LSSL structure in the lateral direction, $Q_n = 2n\pi/L_x$ with $n = 0, \pm 1, \pm 2, \ldots$ is the reciprocal lattice wave vector, and $\varphi_0(z)$ is the electron ground-state wavefunction of the quantum well H_0. For LSSL structures, the magnitudes of the interface modulations must be much less than the average widths of the LSSLs ($\Delta L_z/L_z \ll 1$), so that the modulation potentials induced by the interface structures are not strong enough to prevent the electrons from travelling along the lateral directions of the LSSLs. This is why in the trial wavefunction $\psi_k(r)$, we have neglected the overlaps of the ground- and high-level states in the z direction caused by the perturbation H_1 in H_{eff}.

It is easy to show that $\psi_k(r)$ satisfies the boundary conditions (4) and (5) (because $\varphi_0(z)$ satisfies the boundary conditions) and orthogonal relation (7) for different k when k is restricted within the first Brillouin zone $|k| < Q/2$ with $Q = Q_1$. By minimizing the expectation value of H_{eff} with respect to A_n with the trial wave function $\psi_k(r)$ satisfying the normalization relation (7), we obtaining the following equation which determines the energy subband structure $E_n(k)$ of the LSSL as a function of the electron wave vector k:

$$\det \| H_{\text{eff}}^{(ij)}(k) - E_n(k) J^{(ij)}(k) \| = 0 \tag{9}$$

with the matrix elements

$$H_{\text{eff}}^{(ij)}(k) = \langle \psi_{ik}(r) | H_{\text{eff}}(r) | \psi_{jk}(r) \rangle \tag{10}$$

and

$$J^{(ij)}(k) = \langle \psi_{ik}(r) | J(r) | \psi_{jk}(r) \rangle. \tag{11}$$

The numerical calculation is carried out for GaAs/AlAs LSSL structures where $m_c = 0.0665 m_0$ and $\Delta V_c = 1.06$ eV [12]. In figure 1, we give the three lowest-energy subband dispersions $E_n(k)$ of the GaAs/AlAs LSSL as functions of the electron wave vector k. The structural parameters of the LSSL are $L_z = 100$ Å, $\Delta L_z = 10$ Å and $L_x = 200$ Å for a sine-shaped interface (full curves in figure 1 with $\lambda = 0$ in equation (3)) and a square-welled interface (chain curves in figure 1 with $\lambda = 10$ in equation (3)). Twenty-one planar waves were used in $\psi_k(r)$ in equation (8) ($n = 0, \pm 1, \ldots \pm 10$) for the calculation. Also given in figure 1 are the energy dispersions $E_n^{(0)}(k)$ (broken curves) for a quantum well without interface structures. In table 1, the minigaps ΔE_m of several lowest-energy subbands at the edge of the Brillouin zone are listed for the same LSSL structures as described above. It is easy to see that the minigaps of the subbands decrease quickly for high subbands. Also the energy dispersions of the LSSL systems we considered depend strongly on the exact shapes of the interface structures ($\lambda = 0$ and 10). This becomes more obvious in figure 2 where the energy minigaps ΔE_1 between the first and second subbands as functions of the parameter λ are given, with other structural parameters of the LSSLs being the same as those described above.

To study the electronic and optical properties of the GaAs/AlAs LSSLs, Sham [8] also put forward a variational approach. Working in the original coordinate space r, Sham writes the Hamiltonian (1) of the LSSL as $H = H_0 + H_1$, where H_0 is the Hamiltonian of an imaginary quantum well with planar interfaces and a width L_z equal to the average width of the LSSL. The trial wavefunction of H is composed of the eigen wavefunctions of H_0, which takes exactly the same form as our wavefunction $\psi_k(r)$ in equation (8). The differences between Sham's method and ours are that the former works in the original coordinate space, where the boundary conditions are given on the structured interfaces of the systems which are not satisfied by the trial wavefunction. In addition, the effective periodic potential H_1 induced

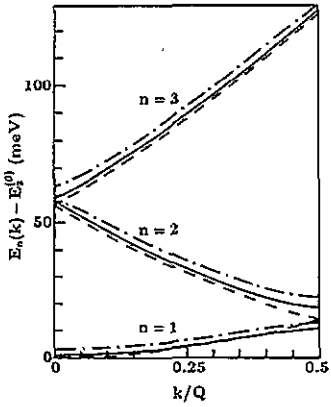

Figure 1. The three lowest-energy subband dispersions $E_n(k)$ of a GaAs/AlAs LSSL as functions of the electron wave vector k along the lateral direction, where the electron band mass $m_c = 0.0665m_0$, the potential barrier between GaAs and AlAs $\Delta V_c = 1.06$ eV [12] and the structural parameters of the LSSL are $L_z = 100$ Å, $\Delta L_z = 10$ Å and $L_x = 200$ Å for a sine-shaped interface (full curves with $\lambda = 0$ in equation (3)) and a square-welled interface (chain curves with $\lambda = 10$ in equation (3)). Twenty-one planar waves were used in $\psi_k(r)$ for the calculation. Also given are the energy dispersions $E_n^{(0)}(k)$ (broken curves) for a quantum well without interface structures. The results are given with the ground-state energy $E_z^{(0)}$ of the electron z direction motion in a quantum well without interface structures subtracted.

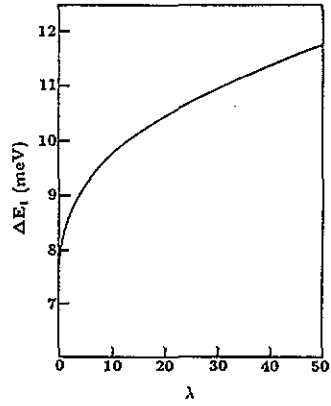

Figure 2. The energy minigaps ΔE_1 between the first and second subbands of the LSSLs at the edge of the Brillouin zone $k = Q/2$ as functions of the parameter λ, which changes the shape of the interface structures, with other structural parameters of the LSSLs being the same as those described in figure 1.

Table 1. The three lowest-electron-energy minigaps ΔE_m in meV of the LSSL's subbands at the edge of the Brillouin zone $k = Q/2$ with the structural parameters $L_z = 100$ Å, $\Delta L_z = 10$ Å and $L_x = 200$ Å for a sine-shaped interface ($\lambda = 0$ in (3)) and a square-welled interface ($\lambda = 10$ in (3)). Twenty-one planar waves were used in the trial wavefunction $\psi_k(r)$ for the calculation with the potential barriers between GaAs and AlAs and the electron band mass assumed to be $\Delta V_c = 1.06$ eV and $m_c = 0.0665m_0$ [12], respectively.

	$m = 1$	$m = 2$	$m = 3$
$\lambda = 0$	7.6	0.4	0.0
$\lambda = 10$	9.8	5.0	3.3

by the interface structures are different in the original space (Sham's method) and in the transformed space (our method). In figure 3, we give the energy dispersions $E'_n(k) - E_n^{(0)}(k)$ as functions of k calculated for the same GaAs/AlAs structure with Sham's method (broken curves in figure 3) and our method (full curves in figure 3), where $E_n^{(0)}(k)$ is the subband dispersion of a quantum well H_0 with planar interfaces, which is the same for both Sham's method and ours (see the broken curves in figure 1). The prime on $E'_n(k)$ indicates that the calculations for figure 3 were carried out with a two-wave approximation (only two planar waves ($n = 0, 1$) are used in $\psi_k(r)$ in equation (8)) as used by Sham [8]. The structural parameters of the LSSL are $L_z = 100$ Å, $\Delta L_z = 10$ Å, and $L_x = 200$ Å for a sine-shaped interface. From figure 3, the energy minigap between the first and second subbands at the edge of the Brillouin zone is 7.67 meV from our method and 10.9 meV from Sham's method. The difference of the results represents the effect of the boundary conditions of

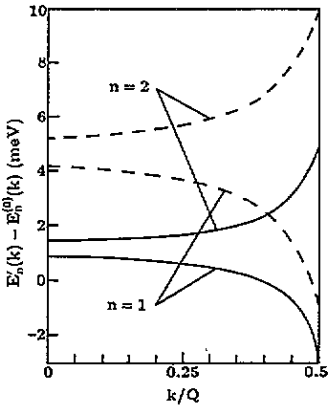

Figure 3. The energy dispersions $E'_n(k) - E_n^{(0)}(k)$ as functions of k calculated with Sham's method (broken curves) and our method (full curves) for the same GaAs/AlAs LSSL structure with the electron band mass $m_c = 0.0665m_0$, the potential barrier between GaAs and AlAs $\Delta V_c = 1.06$ eV [12] and the structural parameters $L_z = 100$ Å, $\Delta L_z = 10$ Å, and $L_x = 200$ Å for a sine-shaped interface. $E_n^{(0)}(k)$ is the subband dispersion of a quantum well H_0 with planar interfaces, which is the same for both Sham's method and ours (see the broken curves in figure 1). Only two planar waves ($n = 0, 1$) are used in $\psi_k(r)$ for the calculation.

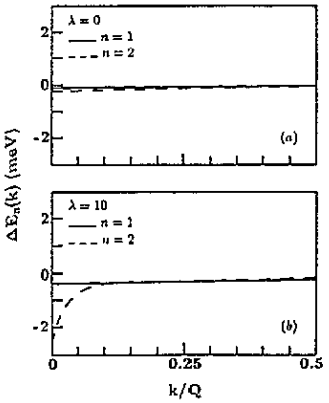

Figure 4. The differences of the first two subband dispersions, $\Delta E_n(k) = E_n(k) - E'_n(k)$, as functions of k calculated with the planar wave expansion $E_n(k)$ and two-wave approximation $E'_n(k)$ for the same LSSL structures as described in figure 1 for a sine-shaped interface (figure 4(a) with $\lambda = 0$ in equation 3)) and a square-welled interface (figure 4(b) with $\lambda = 10$ in equation (3)).

the electron wavefunctions which are not satisfied in Sham's method.

In figure 4 we give the differences of the first two subband dispersions, $\Delta E_n(k) = E_n(k) - E'_n(k)$, as functions of k calculated with the planar wave expansion $E_n(k)$ and two-wave approximation $E'_n(k)$ for the same LSSL structures as described in figure 1 for a sine-shaped interface (figure 4 (a) with $\lambda = 0$ in equation (3)] and a square-welled interface [figure 4 (b) with $\lambda = 10$ in equation (3)). It is obvious that for the two lowest subbands, the two-wave approximation gives very accurate results.

The LSSL structures with periodic modulation of the widths of the LSSLs can be also fabricated, for instance, by directly etching GaAs/$Al_xGa_{1-x}As$ heterojunction quantum wells grown by molecular-beam epitaxy [7, 13, 14]. In figure 5, we give the lowest-subband minigap ΔE_1 as a function of the barrier ΔV_c between GaAs and $Al_xGa_{1-x}As$ (the full curve in figure 5). The structural parameters of the LSSL are $L_z = 100$ Å, $\Delta L_z = 10$ Å, and $L_x = 200$ Å for a sine-shaped interface. Also indicated in figure 5 (the broken line) is the same minigap $\Delta E_1^{(0)}$ for the same LSSL structure with infinitely high potential barriers between GaAs and $Al_xGa_{1-x}As$. The subband minigaps depend strongly on the barriers between GaAs and $Al_xGa_{1-x}As$. The minigaps of the LSSLs are overestimated by about 50% if infinitely high potential barriers between GaAs wells and $Al_xGa_{1-x}As$ barriers are assumed.

In conclusion, the electronic energy subband structures and energy minigaps in quasi-two-dimensional electronic systems with periodic modulation potentials along the lateral directions due to the periodic modulation of the widths of the systems were predicted by numerical calculations. A coordinate transformation was introduced which transforms the systems with periodically structured interfaces to quantum wells with planar interfaces so that the boundary conditions of the electron wavefunctions are considerably simplified. The first minigap of typical LSSLs, such as those produced by deposition of AlAs and GaAs

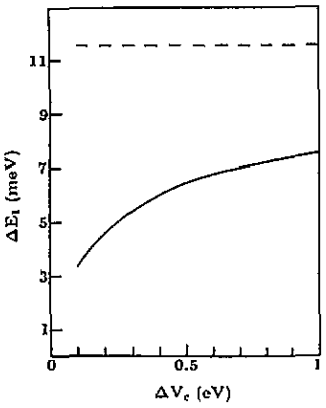

Figure 5. The lowest subband minigap ΔE_1 (full curve) as a function of the band offset ΔV_c between GaAs and $Al_xGa_{1-x}As$ materials for an LSSL with the structural parameters $L_z = 100$ Å, $\Delta L_z = 10$ Å, and $L_x = 200$ Å for a sine-shaped interface. Also indicated in figure 5 (broken line) is the same minigap $\Delta E_1^{(0)}$ for the same LSSL structure calculated with infinitely high potential barriers between GaAs and $Al_xGa_{1-x}As$ materials.

fractional layers on (001) vicinal GaAs substrates, is about 5–10 meV, which is large enough to be tested experimentally, for instance, by far-infrared spectrum measurements. The minigaps depend sensitively on the exact structures and the potential barrier heights between the wells and barriers of the LSSLs. The infinitely high potential barrier approximation is not good enough in calculating the energy subbands, while a two-wave approximation gives very accurate results for the first and second subbands in the LSSLs.

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