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# Energy subband structures in lateral surface superlattices under normally applied electric fields

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**Abstract.** The electronic energy subband structures in quasi-two-dimensional electronic systems under normally applied electric fields with periodic modulation potentials along the lateral directions due to 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, are established by numerical calculations. A coordinate transformation is introduced which transforms systems with periodically structured interfaces into quantum wells with planar interfaces, so that the boundary conditions of the electron wavefunctions are considerably simplified. The changes of the electronic density of states and energy minigaps as functions of the normally applied electric fields and the structural parameters of the systems are investigated in detail.

## 1. Introduction

Much interest is currently being devoted to two-dimensional electronic systems with periodic modulation potentials along the lateral directions. These systems are called lateral surface superlattices (LSSLs) if the periodic modulation potentials along the lateral directions are not strong enough to prevent the electrons from travelling in these directions. A variety of interesting electronic and optical phenomena associated with the energy band structures of LSSLs have been discovered experimentally [1–9]. Of the various structures proposed for the LSSLs, the one produced by deposition of AlAs and GaAs fractional layers on (001) vicinal GaAs substrates seems to offer the greatest potential for wide application in microelectronics and electrooptics [4, 5, 8, 10]. This is because of 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. Indeed, electronic wave interference devices using the GaAs/AlAs LSSL have been designed [11].

In a previous paper [12], 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 calculations [12], it was found that the electronic subband gaps caused by the periodic structures on the interfaces of GaAs/AlAs LSSLs are much less than the subband gaps caused by the periodic structures buried in the middle of the LSSLs because the electrons

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are distributed mainly in the middle of the GaAs wells. The situation changes if electric fields are applied normally to the LSSLs; this shifts the electron distributions towards the GaAs/AlAs interfaces and so increases lateral periodic potentials on the electrons caused by the periodic structures on the interfaces of the LSSLs. The minigaps of the subband structures of the GaAs/AlAs LSSLs can be adjusted continuously by normally applied electric fields.

In this paper, we present the results of numerical calculations on the electronic subband structures of GaAs/AlAs LSSLs under normally applied electric fields using the method we developed previously [12].

## 2. Theory

We consider the same LSSL system as that described in [12], which is produced by deposition of AlAs and GaAs fractional layers on the (001) vicinal GaAs substrate with interfaces separating the well GaAs and barrier AlAs at $z = \pm\frac{1}{2}L_z + f_\pm(x)$, where $L_z$ is the average width and $f_\pm(x)$ describes the periodically structured interfaces of the LSSL structure. The potential barrier between the GaAs/AlAs interfaces is assumed to be infinite for simplicity. In the effective mass approximation, the Hamiltonian of the system reads

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

where $m_c$ is the electron band mass in GaAs, $F$ is the external electric field strength applied normally to the LSSL and $V(r)$ is the quasi-two-dimensional electron potential which is given, if we assume an infinitely high potential barrier between GaAs/AlAs interfaces, by

$$V(r) = \begin{cases} 0 & \text{for } -\frac{1}{2}L_z + f_-(x) < z < \frac{1}{2}L_z + f_+(x) \\ \infty & \text{otherwise.} \end{cases} \tag{2}$$

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

$$f_-(x) = 0 \quad \text{and} \quad f_+(x) = \Delta L_z \sin(2\pi x/L_x) \tag{3}$$

where $L_x$ and $\Delta L_z$ are the period and amplitude of the periodic interface structure, respectively. The interface structure given by equation (3) produces a periodic fluctuation of the width of the GaAs well along the lateral $x$ direction, which is mainly responsible for the periodic potential along the lateral $x$ direction of the LSSLs [12].

The boundary condition of the electronic wavefunction is that the wavefunction vanishes to zero on the GaAs/AlAs interfaces required by the infinitely high potential barriers between GaAs/AlAs interfaces. The complicated boundary condition can be simplified by introducing the same coordinate transformation as in [12]

$$\begin{aligned} x' &= x \\ y' &= y \\ z' &= \{z - \tfrac{1}{2}[f_+(x) + f_-(x)]\}L_z/[L_z + f_+(x) - f_-(x)] \end{aligned} \tag{4}$$

which transforms the LSSL structure in space $r$ to a quantum well with planar interfaces at $z' = \pm\frac{1}{2}L_z$ in space $r'$. The simplified boundary condition in the transformed space is given by (hereafter we denote $r'$ by $r$ to simplify the notation):

$$\psi(r)|_{z=(\pm L_z/2)^-} = 0. \tag{5}$$

The effective Hamiltonian of the system in the transformed space can be written as

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

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

$$\int_{-\infty}^{\infty} \mathrm{d}\boldsymbol{r}\, \psi_k^*(\boldsymbol{r}) J(\boldsymbol{r}) \psi_{k'}(\boldsymbol{r}) = \delta_{k,k'} \tag{7}$$

where $J(\boldsymbol{r})$ is the Jacobian determinant introduced in the coordinate transformation. Detailed derivations of the above formulae are given in [12].

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

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

where $k$ and $L_0 = NL_x$ ($N \to \infty$) are the electron wave vector and the length of the LSSL structure in the lateral $x$ direction, respectively, $Q_n = 2n\pi/L_x$ with $n = 0, \pm 1, \pm 2, \ldots$ is the reciprocal lattice wave vector, and $\varphi_0(z, \beta)$ is the electron ground-state wavefunction of the quantum well $H_0$. Under a normally applied electric field, we take the trial wavefunction $\varphi_0(z, \beta)$ as that suggested by Bastard [13],

$$\varphi_0(z, \beta) = N(\beta) \cos(\pi z/L_z) \exp[-\beta(z/L_z + \tfrac{1}{2})] \tag{9}$$

where $\beta$ is a variational parameter and $N(\beta)$ is the normalization constant. For LSSL structures, the magnitudes of the interface structures must be much less than the average widths of the LSSLs ($\Delta L_z/L_z \ll 1$), so that the periodic 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 $\psi_k(\boldsymbol{r}, \beta)$ we have neglected the overlaps of the ground and high-level states in the $z$ direction caused by the perturbation $H_1$ in $H_{\text{eff}}$.

It is easy to show that $\psi_k(\boldsymbol{r}, \beta)$ satisfies the boundary condition (5) (because $\varphi_0(z, \beta)$ satisfies the boundary condition (5)) and orthogonal relation (7) for different $k$ when $k$ is restricted within the first Brillouin zone $|k| < \frac{1}{2}Q$ with $Q = Q_1$. By first minimizing the expectation value of $H_{\text{eff}}$ with respect to $A_n$ with the trial wavefunction $\psi_k(\boldsymbol{r}, \beta)$ satisfying the normalization relation (7) and then minimizing the lowest subband energy $E_1(k, \beta)$ with respect to $\beta$ to determine $\beta$, we obtain the following equations which determine the energy subband structures $E_n(k)$ of the LSSL as a function of the electron wave vector $k$ in the lateral $x$ direction:

$$\det \| H_{\text{eff}}^{(ij)}(k, \beta) - E_n(k, \beta) J^{(ij)}(k, \beta) \| = 0 \tag{10}$$

and

$$\mathrm{d}E_1(k, \beta)/\mathrm{d}\beta = 0 \tag{11}$$

with the matrix elements

$$H_{\text{eff}}^{(ij)}(k, \beta) = \langle \psi_{ik}(\boldsymbol{r}, \beta) | H_{\text{eff}}(\boldsymbol{r}, ) | \psi_{jk}(\boldsymbol{r}, \beta) \rangle \tag{12}$$

and

$$J^{(ij)}(k, \beta) = \langle \psi_{ik}(\boldsymbol{r}, \beta) | J(\boldsymbol{r}) | \psi_{jk}(\boldsymbol{r}, \beta) \rangle. \tag{13}$$

## 3. Numerical results and discussion

The numerical calculation is carried out for GaAs/AlAs LSSL structures where $m_c = 0.0665m_0$ [14]. In figure 1, we give two lowest-energy subband dispersions $E_{1,2}(k)$ 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. The electric field strength is $FL_z = -170$ (broken curve), 0 (full curve) and 170 mV (chain curve), which corresponds to $eFL_z/E_z^{(0)} = -3$, 0 and 3 with $E_z^{(0)} = \hbar^2\pi^2/2m_cL_z^2$ the electron ground-state energy in a quantum well of width $L_z$ without the external electric fields. Eleven planar waves were used in $\psi_k(r, \beta)$ in equation (8) ($n = 0, \pm1, \ldots, \pm5$) for the calculation. To further increase the number of the planar waves in $\psi_k(r, \beta)$ changes the numerical results of the first two lowest subbands by less than 1%.

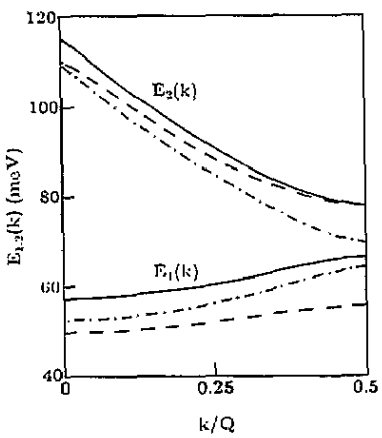


**Figure 1.** The two lowest-energy subband dispersions $E_{1,2}(k)$ of a GaAs/AlAs LSSL as functions of the electron wave vector $k$ along the lateral $x$ direction within the first Brillouin zone $k < \frac{1}{2}Q$, where the electron band mass $m_c = 0.0665m_0$ [14], the potential barrier between the GaAs/AlAs interfaces is assumed to be infinitely high and the structural parameters of the LSSL are $L_z = 100$ Å, $\Delta L_z = 10$ Å and $L_x = 200$ Å. The electric field strength is $eFL_z/E_z^{(0)} = -3$ (broken curve), 0 (full curve) and 3 (chain curve) with $E_z^{(0)}$ the electron ground-state energy in a quantum well of width $L_z$ with planar interfaces and without external electric fields.

It is obvious that when the electric field ($eFL_z/E_z^{(0)} = -3$) shifts the electron distribution towards the interface with the interface structures, $z = \frac{1}{2}L_z + \Delta L_z \sin(2\pi x/L_x)$, the miniband gap at the edge of the first Brillouin zone $k = \frac{1}{2}Q$ is much larger than that when the electric field ($eFL_z/E_z^{(0)} = 3$) shifts the electron towards the planar interface, $z = -\frac{1}{2}L_z$. In figure 2, the first minigap between the second and first subbands, $\Delta E = E_2(\frac{1}{2}Q) - E_1(\frac{1}{2}Q)$, is given as a function of the applied electric field $F$ for the same LSSL structures described above, except with $L_z = 80$ Å and $\Delta L_z/L_z = 0.1$ (broken curve), $L_z = 100$ Å and $\Delta L_z/L_z = 0.1$ (full curve) and $L_z = 150$ Å and $\Delta L_z/L_z = 0.1$ (chain curve). The first minigaps of the typical GaAs/AlAs LSSLs produced by deposition of AlAs and GaAs fractional layers on (001) vicinal GaAs substrates, with $L_z = 100$ Å and $\Delta L_z = 10$ Å, change continuously from about 6 to 20 meV when the electric fields normally applied to the LSSL change from $eFL_z/E_z^{(0)} = 3$ to $-3$. The results in figure 2 also show that, the thinner the LSSL structure, the stronger its subband gap depends on the normally

applied electric field. This sensitive dependence of the electronic subband energy gaps on the normally applied electric fields might be used to design optical detectors covering a large far-infrared region.

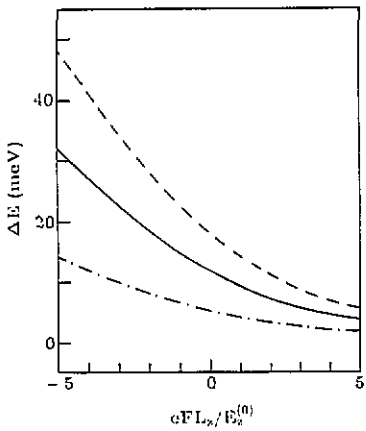


**Figure 2.** The energy minigaps $\Delta E$ between the second and first subbands of the GaAs/AlAs LSSL at the edge of the Brillouin zone $k = \frac{1}{2}Q$ as functions of the normally applied electric field $F$. The structural parameters of the LSSL are the same as those described in figure 1, except that $L_z = 80$ Å and $\Delta L_z/L_z = 0.1$ (broken curve), $L_z = 100$ Å and $\Delta L_z/L_z = 0.1$ (full curve) and $L_z = 150$ Å and $\Delta L_z/L_z = 0.1$ (chain curve).

The electron energy dispersions in quantum wells with planar interfaces under normally applied electric fields are given by $E^{(0)}(q) = E_z(F) + \hbar^2 q^2/2m_c$ with $q$ the in-plane electron wave vector of the electron and $E_z(F)$ the electron ground-state energy in a quantum well with planar interfaces under a normally applied electric field $F$. The electron density of states associated with the energy dispersions $E^{(0)}(q)$ are given by $g_0(E) = g_0\theta[E - E_z(F)]$, where $\theta(E)$ is the step function and $g_0 = m_c S/2\pi\hbar^2$ is a constant, with $S$ the area of the interface of the quantum well. Apart from causing a shift of the edge $E = E_z(F)$ of the electron density of states, the electric field does not change the profiles of the electron density of states in the quantum wells with planar interfaces. The electron energy dispersions in LSSLs are given by $E_n(q) = E_n(q_x) + \hbar^2 q_y^2/2m_c$, with $E_n(q_x)$ determined by equations (10)–(13). From the results in figure 1, it is obvious that the applied electric field will change not only the edge $E = E_1(0)$ of the electron density of states, but also the dependence of the electron energy dispersions on the wave vector $q_x$, and so changes the profiles of the electron density of states in the LSSLs for different $F$. In figure 3, we give the calculated electron density of states $g(E)$ for the GaAs/AlAs LSSL structures described in figure 1 with electric field strength $eFL_z/E_z^{(0)} = -3$ (broken curve), 0 (full curve) and 3 (chain curve). The electron density of states differ significantly from those of quantum wells with planar interfaces mainly in the energy range of the energy minigaps of the LSSL which change greatly for different electric field strength $F$ (see figure 2). It is expected that optical transitions associated with the electron subbands of the LSSLs will have a strong dependence on the normally applied electric field.

In figure 4, we give the calculated optical absorption coefficient $\alpha(\hbar\omega)$ associated with the electron transitions between the first and second conduction subbands for the same GaAs/AlAs LSSL described in figure 1. The normally applied electric field is $eFL_z/E_z^{(0)} = 3$

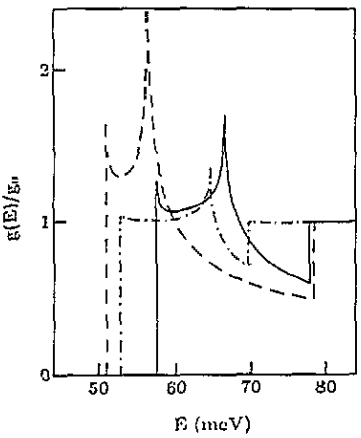


**Figure 3.** The calculated electron density of states $g(E)$ for the GaAs/AlAs LSSL described in figure 1 with electric field strength $eFL_z/E_z^{(0)} = -3$ (broken curve), 0 (full curve) and 3 (chain curve), where $g_0 = m_e S/2\pi\hbar^2$ with $S$ the area of the interface of the LSSL.

(full curve) and 0 (broken curve). The electric field not only shifts the positions of the absorption peaks, it also changes the half-height widths of the absorption spectra. Detailed results and discussions of the subband optical absorptions in GaAs/AlAs LSSLs under normally applied electric fields will be given elsewhere.

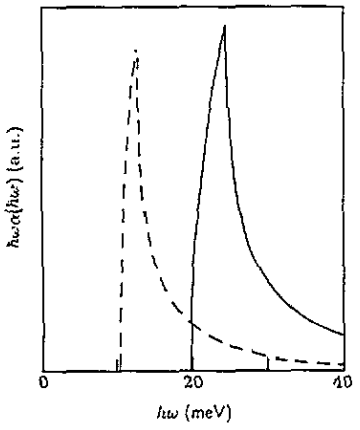


**Figure 4.** The calculated $\hbar\omega\alpha(\hbar\omega)$, which is proportional to the optical transition rate between the first and second conduction subbands of the GaAs/AlAs LSSL, is given as functions of the photon energy $\hbar\omega$ for different electric field strength $eFL_z/E_z^{(0)} = -3$ (full curve) and 0 (broken curve) with the structural parameters of the GaAs/AlAs LSSL being the same as those described in figure 1.

In our calculation, we have assumed that the potential barrier between the well GaAs and barrier GaAs is infinitely high. The justification for this infinitely high potential barrier approximation (IHPBA) is discussed below. For a quantum well with a finite potential barrier $V_0$ between the well and barrier, the electronic wavefunction inside the barrier area for the

zero electric field case ($F = 0$) is

$$\varphi(z) \propto \exp(-(\alpha_1/L_z)|z \mp L_z|)$$

where $\alpha_1 = [(V_0 - E_z)2mL_z^2/\hbar^2]^{1/2}$ with $E_z$ the ground-state energy for the quantum well with finite potential barrier $V_0$. The decay length of the electronic wavefunction inside the barrier is $L_z/\alpha_1$. If $\alpha_1 \gg 1$, the electronic wavefunction is confined mainly inside the well, which indicates that the IHPBA is appropriate. When a electric field is applied normally to the quantum well, the maximum potential change caused by the electric field inside the well is $\frac{1}{2}eL_zF$. So if $\alpha_2 = eL_zF/2V_0 \ll 1$, the discussion for the zero electric field case is still valid.

Another factor that describes the effect of the electric field on the electronic wavefunction is $\alpha_3 = eFL_z/\alpha_1 V_0$, where $eFL_z/\alpha_1$ gives the electric potential change from the interfaces to the place where the electronic wavefunction decays to $e^{-1}$ inside the barrier of the quantum well. So the criterion for the validity of the IHPBA is $\alpha_1 \gg 1$ and $\alpha_2,\ \alpha_3 \ll 1$. For a GaAs/AlAs quantum well, we have $V_0 = 1.06$ eV. When $eFL_z/E_z^{(0)} = 3$ and $L_z = 100$ Å, we have $\alpha_1 \approx 13$, $\alpha_2 \approx 0.08$ and $\alpha_3 \approx 0.01$. When $eFL_z/E_z^{(0)} = 3$ and $L_z = 50$ Å, we have $\alpha_1 \approx 6$, $\alpha_2 \approx 0.3$ and $\alpha_3 \approx 0.1$. So for the GaAs/AlAs quantum well, even when $L_z = 50$ Å and $|eFL_z/E_z^{(0)}| \leqslant 3$, the IHPBA is a fairly good approximation, due to the large potential barrier $V_0 = 1.06$ eV between the well and barrier materials. For a GaAl/AlAs quantum well with $L_z = 100$ Å, IHPBA is valid even when $|eFL_z/E_z^{(0)}| \leqslant 5$.

LSSL structures can also be fabricated with quantum wells of planar interfaces where the periodical potentials along the lateral directions arise from outside fields, for instance, by a gate voltage applied to the periodic metallic wires laid lithographically on top of the LSSLs. The electronic potentials in this kind of LSSL can be written as $V(z) + \Delta V(x)$, where $V(z)$ are the quantum well potentials confining the electrons in the quantum wells and $\Delta V(x)$ are the periodic potentials along the lateral $x$ direction [15]. The difference between this LSSL structure and the one we have discussed is that the lateral periodical potential $V(x)$ of the former is independent of the $z$ coordinate of the electron. The Hamiltonian of the system can be separated into $H(x, z) = H_\parallel(x) + H_\perp(z)$, with $H_\parallel(x)$ independent of the normally applied electric field. If we perform the same numerical calculation as we did in this paper by averaging the Hamiltonian $H(x, z)$ over the electron ground-state wavefunction $\varphi_0(z, \beta)$ in the $z$ direction, the effective Hamiltonian which determines the subband structures of the LSSLs is given by

$$H_{\text{eff}}(x) = H_\parallel(x) + \langle \varphi_0(z, \beta) \mid H_\perp(z) \mid \varphi_0(z, \beta) \rangle = H_\parallel(x) + E_z(F).$$

Apart from causing a parallel shift $E_z(F)$ of the electronic subband structures, a normally applied electric field does not change the lateral periodic potential of the LSSLs, and so does not change the minigaps, the energy dispersion relations and the electronic density of states of the LSSLs. The subband optical absorptions of the LSSLs, which depends only on the subband energy difference, are independent of the normally applied electric fields.

In conclusion, the electronic energy subband structures in quasi-two-dimensional electronic systems under normally applied electric fields with periodic modulation potentials along the lateral directions due to the periodic modulation of the widths of the systems have been established 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 minigaps of the typical LSSLs, such as those produced by

deposition of AlAs and GaAs fractional layers on (001) vicinal GaAs substrates, change continuously from about 6 to 20 meV when the electric fields normally applied to the LSSLs change from $eFL_z/E_z^{(0)} = 3$ to $-3$, which are large enough to be tested experimentally, for instance, by far-infrared spectrum measurements. The electron density of states differ significantly from those of quantum wells with planar interfaces in the energy range of the energy minigaps of the LSSLs which change greatly for different electric field strength $F$. It is expected that any optical transitions associated with the electron subbands of the LSSLs, such as valence to conduction band, acceptor to conduction band, exciton and conduction subband to subband optical absorptions, will have a strong dependence on the normally applied electric field. The detailed results of the optical properties of more realistic LSSL models with finite potential barriers between GaAs/AlAs interfaces in external electric fields will be given elsewhere.

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