Energy subband structures in lateral-surface superlattices

1992 J. Phys.: Condens. Matter 4 L213

(http://iopscience.iop.org/0953-8984/4/12/004)

J. Phys.: Condens. Matter 4 (1992) L213–L219. Printed in the UK

LETTER TO THE EDITOR

Energy subband structures in lateral-surface superlattices

Hong Sun†
Centre of Theoretical Physics, CCAST (World Laboratory), Beijing 100080, People's Republic of China and International Centre for Material Physics, Academie Sinica, Shenyang 110015, People's Republic of China

Received 14 January 1992

Abstract. The electronic energy subbands and minigaps in lateral-surface superlattices (LSSLs) produced by deposition of AlAs and GaAs fractional layers on (001) vicinal GaAs substrates were calculated variationally. The results were compared with those calculated with other theories. It was found that energy minigaps induced by periodic structures on LSSL interfaces are much smaller than those induced by periodic structures inserted in the middle of LSSLs, and the approximation of infinitely high potential barriers between GaAs and AlAs interfaces is not as good in calculating the energy subbands in LSSLs as it is in the case of quantum wells.

Ever since the idea of lateral-surface superlattices (LSSLs) was put forward some fifteen years ago [1], a great deal of work has been done both theoretically and experimentally in order to understand the electronic and optical properties of this novel system [2–12]. The main experimentally observed and theoretically predicted notable results associated with the LSSL structure, where periodic structures are introduced artificially into or on the interfaces of electronic two-dimensional systems, are the following:

(i) Magnetoresistance oscillations with magnetic fields in high-mobility AlGaAs/GaAs LSSLs were observed which shows that the behaviour deviates from the well-known Shubnikov–de Haas oscillations [4, 5].

(ii) Strong anisotropies in the ratios of the electron–light-hole–exciton peak intensities to the electron–heavy-hole–exciton peak intensities were reported in AlAs/GaAs LSSLs [6, 7].

(iii) Exciton–polariton localizations in AlGaAs/GaAs LSSLs with lateral interface structure widths of below 150 nm were demonstrated [8].

(iv) New infrared optical absorption peaks associated with the electronic energy minigaps of the LSSL structures were predicted [10].

Of the various structures of 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 application in microelectronics and electrooptics [6, 7, 10, 13]. This

† Address to which all correspondence should be sent: Department of Physics and Institute of Condensed Matter Physics, Shanghai Jiao Tong University, Shanghai 200030, People's Republic of China.

0953-8984/92/120213 + 07 $04.50

is due to its potential to produce large periodic structures on interfaces of electronic two-dimensional systems, such as quantum wells, with periods comparable with electron wave lengths and the large conduction band offsets between GaAs and AlAs materials, which enhance the effect of interface structures on the motion of electrons in LSSLs. In this letter, we present a theory to allow the study of electronic energy dispersions in this kind of LSSL system.

We consider an LSSL system produced by deposition of AlAs and GaAs fractional layers on a (001) vicinal GaAs 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 of the LSSL and $f_\pm(x)$ represents the periodic structures on the interfaces. For LSSL structures, we must have $|f_\pm(x)| \ll L_z$, so that the effective potential induced by the interface structure is not strong enough to prevent the electron in the LSSL from travelling along the superlattice direction.

In the effective mass approximation, the Hamiltonian of the system reads:

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

where m_c is the electron band mass. Because the bulk AlAs and GaAs materials have very large conduction band offsets ($\Delta V_c = 1.06$ eV) [14], it is reasonable to simplify the calculation by assuming that the barrier between GaAs and AlAs is infinitely high, that is we take

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

To be consistent with the above approximation, the boundary condition of the electron wave function ψ is given by

$$\psi|_{z=\pm L_z/2+f_\pm(x)} = 0. \tag{3}$$

The electronic energies of the LSSL system can be obtained with variational calculations, taking the minimum of the following quantity:

$$F = \int_{-\infty}^{\infty} dx\, dy \int_{-L_z/2+f_-(x)}^{L_z/2+f_+(x)} dz\, \psi_i^*(r) H(r) \psi_i(r) \tag{4}$$

with the trial wave function $\psi_i(r)$ satisfying the boundary condition (3), being orthogonal to other eigen functions $\psi_j(r)$ which have lower energy levels than that of $\psi_i(r)$, and normalized in space r. That is, $\psi_i(r)$ must satisfy the orthonormalization relation

$$\int_{-\infty}^{\infty} dx\, dy \int_{-L_z/2+f_-(x)}^{L_z/2+f_+(x)} dz\, \psi_j^*(r)\psi_i(r) = \delta_{ij}. \tag{5}$$

The difficulty in obtaining the energy dispersions of the Hamiltonian $H(i)$ is that it is not easy to find a reasonable trial wave function which satisfies the boundary condition (3). We avoid this difficulty by introducing a coordinate transformation that transforms the coordinate space r to space $\tilde{r}$, where the interfaces at $z = \pm L_z/2 + f_\pm(x)$ in space r become planar interfaces at $\tilde{z} = \pm L_z/2$. The coordinate transformation we need is given by

$$\begin{aligned} \tilde{x} &= x \\ \tilde{y} &= y \\ \tilde{z} &= [z - \tfrac{1}{2}(f_+(x) + f_-(x))]\, L_z/[L_z + f_+(x) - f_-(x)]. \end{aligned} \tag{6}$$

It is easy to show from (6) that when $z = \pm L_z/2 + f_\pm(x)$, we have $\tilde{z} = \pm L_z/2$. The interfaces of the LSSL in space $\tilde{r}$ become planar ones. In the transformed space, $\tilde{r}$, the quantity F becomes

$$F = \int_{-\infty}^{\infty} d\tilde{x}\, d\tilde{y} \int_{-L_z/2}^{L_z/2} d\tilde{z}\ \tilde{\psi}_i^*(\tilde{r}) H_{\text{eff}}(\tilde{r}) \tilde{\psi}_i(\tilde{r}) \tag{7}$$

where $\tilde{\psi}_i(\tilde{r})$ is the transformed wave function of $\psi_i(r)$ in space $\tilde{r}$, and

$$H_{\text{eff}}(\tilde{r}) = J(\tilde{x}, \tilde{y}, \tilde{z}) \tilde{H}(\tilde{x}, \tilde{y}, \tilde{z}), \tag{8}$$

with $\tilde{H}(\tilde{r})$ the transformed Hamiltonian of H (i) and $J(\tilde{r})$ the Jacobian determinant introduced into the integration (7) in the coordinate transformation (6). In space $\tilde{r}$, the boundary condition (3) becomes

$$\tilde{\psi}|_{\tilde{z}=\pm L_z/2} = 0 \tag{9}$$

and the orthonormalization relation (5) becomes

$$\int_{-\infty}^{\infty} d\tilde{x}\, d\tilde{y} \int_{-L_z/2}^{L_z/2} d\tilde{z}\ \tilde{\psi}_j^*(\tilde{r}) J(\tilde{r}) \tilde{\psi}_i(\tilde{r}) = \delta_{ij}. \tag{10}$$

The electronic energy dispersions of the LSSL system are obtained by minimizing F (7) with the wave function $\tilde{\psi}_i(\tilde{r})$ satisfying (9) and (10) in space $\tilde{r}$.

To make further calculations, we must specify the periodic interface structure. For a model calculation, we assume

$$f_-(x) = 0 \qquad \text{and} \quad f_+(x) = \Delta L_z \arctan[K \sin(2\pi x/L_x)]/\arctan(K). \tag{11}$$

By adjusting the parameter K in (11), we can change the interface structure from a sine-shaped structure ($K = 0$) to a periodic square-well structure ($K = \infty$), which enables us to investigate how sensitive the electronic energy dependences are to the exact shape of the interface structure. In figure 1, we give $f_+(x)/\Delta L_z$ as a function of x for $K = 0$ and 20.

In what follows, we remove the tilde on $\tilde{\psi}$ and $\tilde{r}$ to simplify the notation but one must keep in mind that we are working in transformed space. Substituting $f_\pm(x)$ into H_{eff}, we obtain

$$H_{\text{eff}} = H_0 + H_1 \tag{12}$$

where H_0 is the Hamiltonian of a quantum well with two planar interfaces and a width equal to the average width L_z of the LSSL, and H_1 is a small perturbation which is periodic in the superlattice direction with a period L_x and vanishes as $\Delta L_z/L_z$ goes to zero. The interface structure now is transformed into an effective potential H_1 acting upon the electron in a quantum well H_0. New energy subbands appear with energy minigaps at the edge of the Brillouin zone.

In this letter, we use a very simple two-wave approximation to calculate the electronic energy dispersions of the first and second subbands in the LSSL. That is, the trial wave function is composed of two eigen wave functions of H_0

$$\psi_k(r) = A\varphi_k^{(1)}(r) + B\varphi_k^{(2)}(r) \tag{13}$$

with

$$\varphi_k^{(1)}(r) = (e^{ikx}/\sqrt{L_0})\sqrt{2/L_z}\cos(\pi z/L_z) \tag{14a}$$

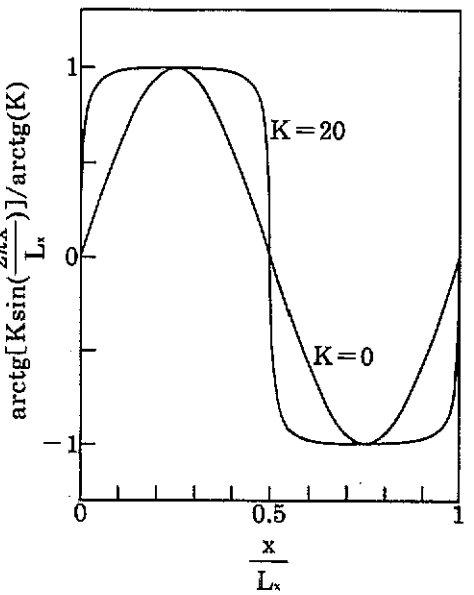

Figure 1. The periodic interface structure on one of the interfaces of the GaAs/AlAs LSSLs considered in the text with the parameter K determining the interface structure being 0 and 20.

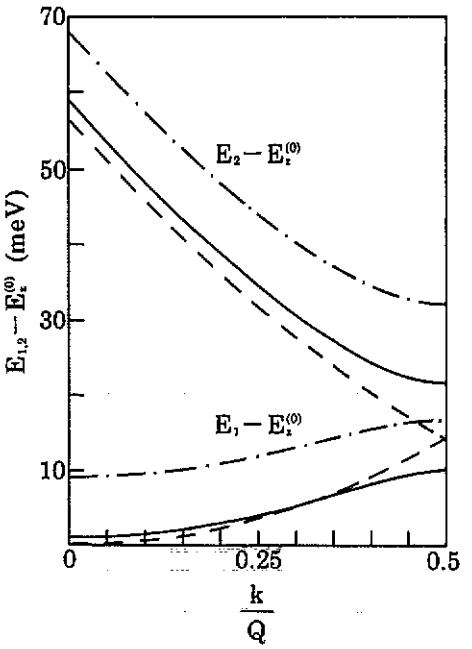

Figure 2. The first and second subbands of electron energy dispersions $E_{1,2} - E_1^{(0)}$ of a GaAs/AlAs LSSL as functions of the electron wave vector k in the superlattice direction, where the average width L_z of the LSSL is 100 Å; the periodic structure on one of its interfaces is given in figure 1 with a period $L_x = 200$ Å and an amplitude $\Delta L_z = 10$ Å. $E_2^{(0)}$ is the first subband energy in a quantum well with two planar interfaces and a width L_z. Q is the first reciprocal lattice vector. The full curves are the results for the interface with the parameter $K = 0$, the dash-dotted curves are those for $K = 20$ and the dashed curves are the results with no interface structures ($\Delta L_z = 0$).

and

$$\varphi_k^{(2)}(\boldsymbol{r}) = (e^{i(k-Q)x}/\sqrt{L_0})\sqrt{2/L_z}\cos(\pi z/L_z) \tag{14b}$$

where k is the electron wave vector in the superlattice direction, $L_0 = NL_x$ ($N \to \infty$) is the length of the LSSL structure and $Q = 2\pi/L_x$ is the first reciprocal lattice vector. It is easy to show that $\psi_k(\boldsymbol{r})$ (13) satisfies the boundary condition (9) and orthogonal relation (10) when k is restricted to within the first Brillouin zone. (To prove (10), one must notice that the Jacobian determinant $J(\boldsymbol{r})$ is also periodic in the x direction with a period L_x.) The first and second electronic energy dispersions $E_{1,2}(k)$ are obtained by minimizing F (7) with $\psi_k(\boldsymbol{r})$ satisfying the normalization relation (10), which gives the following equation

$$\det\|H_{\text{eff}}^{(ij)}(k) - E_{1,2}(k)\,J^{(ij)}(k)\| = 0 \qquad (i,j = 1,2) \tag{15}$$

with the matrix elements

$$H_{\text{eff}}^{(ij)}(k) = \langle\varphi_k^{(i)}(\boldsymbol{r})|H_{\text{eff}}(\boldsymbol{r})|\varphi_k^{(j)}(\boldsymbol{r})\rangle \tag{16}$$

and

$$J^{(ij)}(k) = \langle \varphi_k^{(i)}(r)|J(r)|\varphi_k^{(j)}(r)\rangle. \tag{17}$$

The numerical calculation of (15) is carried out for a GaAs/AlAs LSSL with $L_z = 100$ Å, $\Delta L_z = 10$ Å and $L_x = 200$ Å. The calculated electronic energy dispersions $E_{1,2}(k) - E_z^{(0)}$, with $E_z^{(0)} = (\hbar^2/2m_e)(\pi/L_z)^2$ the first subband energy in a quantum well H_0 where $m_e = 0.0665\, m_0$ [14], is shown in figure 2 where the full curves are the first and second subbands of the electronic energy dispersions in the LSSL with a sine-shaped interface structure ($K = 0$), the dash-dotted curves are those with a periodic square-well structure ($K = 20$) and the dashed curves are the results without interface structures ($\Delta L_z = 0$).

The energy minigap ΔE between the first and second subbands at the edge of the Brillouin zone ($k = Q/2$) is given in figure 3 as a function of the period L_x of the interface structure for the same LSSL system described above. ΔE becomes almost independent of L_x when L_x is larger than 300 Å. However, when L_x is comparable with the average width L_z of the LSSL, ΔE becomes strongly dependent on L_x and on the exact shape of the interface structures.

Using the finite-element calculation method, Sugawara *et al* [13] have calculated the subband structures in an LSSL where AlAs grids were inserted periodically in the middle of a GaAs/AlAs quantum well with the width of the quantum well $L_z = 116$ Å and the separation between the grids and the width of the grids both equal to 81 Å. They found that the energy minigap ΔE between the first and second subbands is 22.7 meV when the thickness of the grids is 2.83 Å, and 63.4 meV when the thickness is 14.2 Å. If we move the AlAs grids in the middle of the quantum well to one of its interfaces, the LSSL becomes the one we studied in this letter. With the theory we developed above, we found that for the same structural parameters, ΔE is 0.73 meV when the grid thickness is 2.83 Å and 4.2 meV when the thickness is 14.2 Å. The energy minigap is much smaller than that in the LSSL structure described by Sugawara *et al* [13]. Physically, this is obvious. Because of the AlAs barriers outside LSSLs, electrons distribute mainly in the middle of the structures. Electrons feel much stronger periodic potentials when periodic structures are in the middle of LSSLs than when periodic structures are on the interfaces of LSSLs. However, structures in the middle of LSSLs also cause strong electron scattering. For applications where one requires high electron mobility, LSSLs with periodic structures on interfaces are favoured.

With the theory developed above, we also calculated electron energy minigaps in LSSLs where the structures on both interfaces were the same (i.e. $f_+(x) = f_-(x)$), that is, we considered LSSLs where their widths do not change while their central lines curve periodically in the superlattice direction. The results show that apart from causing a small and parallel shift of the undisturbed energy dispersions, given as dashed curves in figure (2), the interface structures induce no minigaps in the energy dispersions. The minigaps in GaAs/AlAs LSSLs produced by deposition of GaAs and AlAs fractional layers on (001) vicinal GaAs substrates are mainly caused by periodic changes of the widths of the LSSLs.

To study the electronic and optical properties of the GaAs/AlAs LSSLs, Sham also put forward a variational approach [10]. 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 a quantum well with planar interfaces and a width L_z equal to the average width of the LSSL. Within the two-wave approximation, the trial wave function of H is composed of two eigen wave functions of H_0, which takes exactly the same form of trial wave function

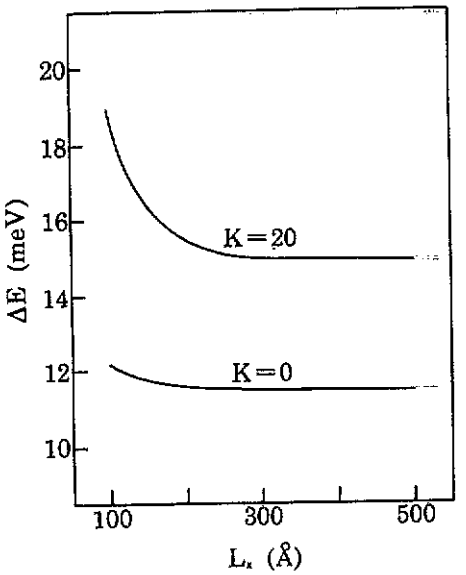

Figure 3. The energy minigaps ΔE between the first and second subbands as functions of the period L_x of the interface structure for LSSLs with other structural parameters being the same as those described for figure 2, where the parameter K determining the interface structure takes the values 0 and 20.

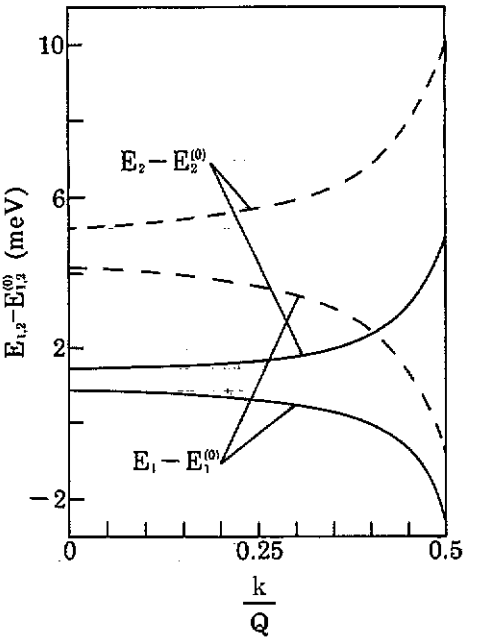

Figure 4. The energy dispersions $E_{1,2} - E_{1,2}^{(0)}$, calculated with Sham's method (dashed curves) and ours (full curves), for the same LSSL structure as described in figure 2 except that the potential barrier between GaAs and AlAs is finite ($\Delta V_c = 1.06$ eV) [14], where $E_{1,2}^{(0)}$ are the first and second subbands of an LSSL with no interface structures, thus being the same for both Sham's method and ours. The parameter K determining the interface structure is 0 in the calculation.

(13) as ours. The differences between Sham's method and ours is that the former works in the original coordinate space where the boundary condition is given by (3), which is not satisfied by the trial wave function, and the latter works in transformed coordinate space where the boundary condition is (9), which is satisfied by the trial wave function. In addition, the effective potential H_1 induced by the interface structures are different in the original space (Sham's method) and in the transformed space (our method). Because both methods are variational calculations, the better of the two is determined to be the one which gives lower electron energies. In figure (4) we give the energy dispersions $E_{1,2}(k) - E_{1,2}^{(0)}(k)$ calculated with both methods as functions of k for the same LSSL structure as that in figure (2) with a finite conduction band offset $\Delta V_c = 1.06$ eV, where $E_{1,2}^{(0)}(k)$ are the first and second energy subbands in an LSSL with no interface structures (similar to the dashed curves in figure (2)). Our results (full curves in figure (4)) give lower energy subbands than those (dashed curves) calculated with Sham's method. From figure (4), the energy minigap at the edge of the Brillouin zone is 7.67 meV from our method and 10.9 meV from Sham's method.

It is also noteworthy from figures (2) and (4) that for the same LSSL structure, the minigap ΔE is 11.6 meV if one assumes an infinitely high potential barrier between GaAs and AlAs, and ΔE is 7.67 meV for the finite potential barrier ($\Delta V_c = 1.06$ eV). The infinitely high potential barrier approximation seems not to work as well in cal-

culating the energy subbands in LSSLs as it does in the case of quantum wells. The detailed calculations, where finite potential barriers between GaAs and AlAs are used, will be given elsewhere.

This work is supported by the National Natural Science Foundation of China under Grant No 19004006.

References

[1] Sakaki H, Wagatsuma K, Hamasaki J and Saito S 1976 *Thin Solid Films* **36** 497
[2] Warren A C, Antoniadis D A, Smith H I and Melngailis J 1985 *IEEE Electron. Device Lett.* **EDL-6** 294
[3] Stormer H L, Pfeiffer L N, Baldwin K W, West K W and Spector J 1991 *Appl. Phys. Lett.* **58** 726
[4] Gerhardts R R, Weiss D and Klitzing K V 1989 *Phys. Rev. Lett.* **62** 1173
[5] Winkler R W, Kotthaus J P and Ploog K 1989 *Phys. Rev. Lett.* **62** 1177
[6] Tanaka M and Sakaki H 1988 *Japan. J. Appl. Phys.* **27** L2025
[7] Tsuchiya M, Gaines J M, Yan R H, Simes R J, Holtz P O, Coldren L A and Petroff P M 1989 *Phys. Rev. Lett.* **62** 466
[8] Kohl M, Heitmann D, Grambow P and Ploog K 1990 *Phys. Rev.* B **42** 2941
[9] Shchukin V A and Efetov K B 1991 *Phys. Rev.* B **43** 14 164
[10] Sham L J 1990 Electronic and optical properties in semiconductor heterostructures *Int. Seminar Phys. of Semiconductor Interfaces and Heterostructures (Beijing, 1990)*
[11] Brinkop F, Hansen W, Kotthaus J P and Ploog K 1988 *Phys. Rev.* B **37** 6547
[12] Demel T, Heitmann D, Grambov P and Ploog K 1988 *Phys. Rev.* B **38** 12 732
[13] Sugawara H, Schulman J N and Sakaki H 1991 *J. Appl. Phys.* **69** 2722
[14] Kumagai M and Takagahara T 1989 *Phys. Rev.* **40** 12 359