Quantum wells with corrugated interfaces: Theory of electron states

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We present realistic effective-mass calculations of electron and exciton states in [311] GaAs/AlAs corrugated quantum wells (QW's) taking into consideration a finite barrier potential and flux-conserving boundary conditions. One-dimensional minibands are formed in the periodic lateral corrugation potential. Light- and heavy-hole exciton binding energies are calculated as a function of QW effective width and discussed in connection with existing experimental data.

The unique properties of low-dimensional electron systems are of fundamental interest and important for device applications. With progress in crystal growth techniques it has become possible to fabricate heterojunctions and quantum-well (QW) structures with atomic scale perfection.[1] However, the precise formation of structures with a dimensionality lower than two is still a challenging problem. The widely spread method of patterning quasi-two-dimensional (2D) heterostructures with lithographic techniques[2] has led to objects with lateral dimensions that are an order of magnitude larger than the vertical dimension. These objects show optical signatures of the additional lateral confinement, although—as a result of the small energy separation—the individual subbands are masked by the level broadening.

Several direct approaches including growth of fractional layers on vicinal substrates[3] and the cleaved edge overgrowth method[4,5] have been developed. An alternative method makes use of the spontaneous formation of periodic 1D channels on the [311] GaAs surface.[6] This ordered surface structure was transferred to the interface during conventional molecular-beam epitaxy and AlAs/GaAs/AlAs QW's with corrugated interfaces were fabricated.[7–9] Potentially, structures with comparable lateral and vertical confinement can be achieved by use of these direct growth techniques.

The comparison of the experimental data with theoretical calculations provides a test for structure parameters and theoretical concepts. However, from the mathematical point of view an exact solution of the multidimensional Schrödinger equation with arbitrary potential is essentially a numerical problem. In some limiting cases, e.g., when one size drastically dominates another one, an effective separation of variables can be achieved which leads to an analytical solution.[10,11] Frequently, the quantum mechanics of quasi-1D systems is treated in simplifying approximations (like the so-called infinite-barrier model[12–15]), which fails to give quantitative results comparable with experimental data for structures with sizes on the nanometer scale. A few schemes of realistic calculations have been recently performed. Based on the Fourier series expansion the method of Ref. 16 becomes inconvenient for complex structure geometries. Others[17,18] make use of the crystal simulation on the microscopic level.

In this paper we report on realistic effective-mass calculations of the electron states in the corrugated GaAs/AlAs QW's grown along the [311] direction taking into account finite potential barrier at interfaces as well as flux-conserving boundary conditions. We present also the excitonic calculations for QW's with corrugated interfaces. The results are compared with experimental data.

We employ the free-relaxation method[19] in order to find the electron states in an arbitrary potential: in the time-dependent Schrödinger equation $i\hbar\partial\phi/\partial t = H\phi$ we formally change the variable t to $-i\tau$ and consider the τ-dependent evolution of the arbitrary wave function ψ. We can expand the initial state $\psi(0)$ over the eigenstates ϕ_i (with energies E_i) of the time-independent Schrödinger equation $H\phi = E\phi$

$$\psi(0) = \sum_i C_i \phi_i$$

and express the evolution of ψ in the form

$$\psi(\tau) = \sum_i C_i \phi_i e^{-E_i \tau/\hbar} .$$

With increasing τ the terms with larger E_i disappear faster, so $\psi(\tau) \rightarrow C_1 \phi_1 \exp(-E_1 \tau/\hbar)$. An accurate truncation of the electron ground state ϕ_1 in the initial function ψ_0 permits one to find the second level and so on. In model calculations we have mapped the original problems on the rectangular mesh thus replacing the Schrödinger equation with the flux-conserving boundary conditions by the difference equations. Standard relaxation routines[19] were used to solve them numerically.

In the following, we consider a QW of effective width a with triangular corrugation of period d along $[01\bar{1}]$ and height h (see Fig. 1). The structure is supposed to be uniform in the third direction ($[\bar{2}33]$).

Figure 2 presents the shape of the electron density $|\phi_1|^2$ at the bottom of the lowest subband for (a) the limiting

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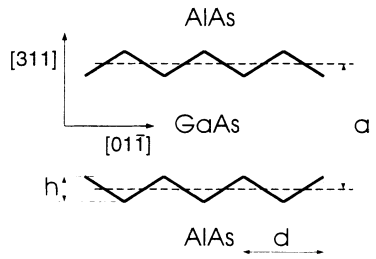

FIG. 1. [311] QW of effective width a with 1D triangular corrugation of period d and height h.

case of the regular chain of rhombic clusters ($a=h$) and (b) three times thicker corrugated QW. The parameters used in the calculations are as follows: electron effective masses $m(\text{GaAs})=0.067m_0$ and $m(\text{AlAs})=0.15m_0$,[20] free electron mass m_0, GaAs/AlAs conduction-band offset $V_0=1.1094$ eV, $d=32$ Å, and $h=10.2$ Å.[7] One can see the clear breaking of the wave function derivative at the interfaces due to the correct boundary conditions. Even in the limiting case $a=h=10.2$ Å the barriers between neighboring GaAs facets do not prevent delocalization of the lowest state [Fig. 2(a)]. The effect of faceted interfaces is small for thicker wells [Fig. 2(b)].

The dependence of E_1 on the QW effective width a is shown in Fig. 3 by a solid line. For comparison we

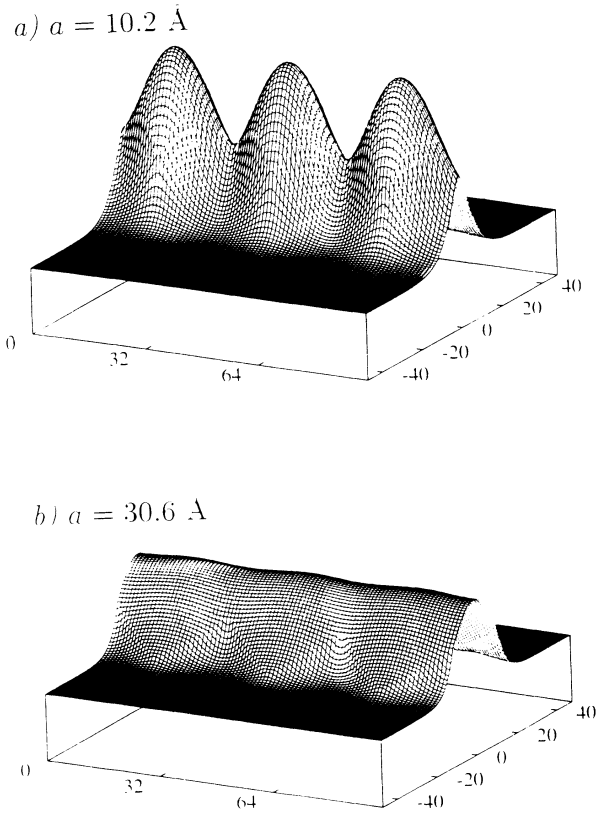

FIG. 2. The electron density $|\phi_1|^2$ in the corrugated QW is shown for (a) the regular chain of clusters (the limiting case $a=h$) and (b) thicker QW ($a=3h$). Lengths in Å.

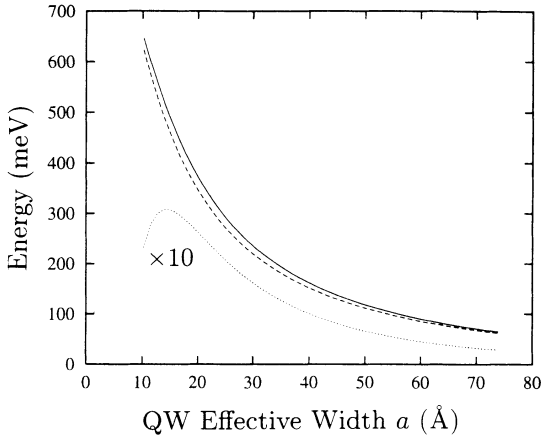

FIG. 3. Dependence of the lowest electron state in corrugated (solid curve) and simple (dashed curve) QW's on the effective width a. Their difference is shown as a dotted line.

presented on this graph the similar dependence for the QW with flat interfaces (dashed curve). The first subband energy for faceted QW exceeds E_1^0 for the simple QW of the same width. This can be demonstrated analytically in the case of thick QW's considering the corrugation of interfaces as a perturbation. In the simple case of equal effective masses in the well and barrier the perturbation potential V_p is a chain of alternating triangular regions with positive and negative potential value $\pm V_0$ (see Fig. 1). The integral $\int V_p|\phi_1^0|^2 d\mathbf{r}$, where ϕ_1^0 is the wave function of the lowest state in the uncorrugated QW, is the first-order correction to the energy E_1^0. Since the electron density $|\phi_1^0|^2$ is larger in the well region than in the barrier, this correction is positive. The second-order correction for the lowest state is unconditionally negative, so one can predict a change in the relative behavior of E_1 and E_1^0 when the corrugation is not small. The dotted line in Fig. 3 displays the difference $E_1-E_1^0$ as a function of the corrugated QW effective width a. The dependence is nonmonotonic in agreement with the qualitative consideration.

The formation of minibands due to the lateral periodic potential is demonstrated by calculating the dispersion of the lowest quasi-2D miniband for wave vectors parallel and perpendicular to facets [solid line in Fig. 4(a)]. The isotropic dispersion of electrons in the simple QW, $E_1^0(\mathbf{k})$, is shown for comparison (dashed line). The difference between the two dispersion curves at $\mathbf{k}=\mathbf{0}$ is identical to the quantity shown in Fig. 3 (dotted line) for $a=20.4$ Å. The miniband formation leads to the anisotropy of the electron effective mass at the bottom of the band. The miniband effective mass as a function of the QW effective width is shown in Fig. 4(b) for propagation parallel and perpendicular to the 1D facets (solid lines). With decreasing a the longitudinal mass $m_\parallel$ increases as a result of the electron penetration into the barrier material, as well as for the uncorrugated QW (dotted line). In contrast, $m_\perp$ increases much stronger due to renormalization by the potential of corrugation.

In order to construct the exciton states in corrugated

QW's we used the simplest approximation for hole states: Light and heavy holes were decoupled and considered as simple particles with anisotropic masses defined by the diagonal terms in Luttinger's Hamiltonian. Additional effects of the [311] crystallographic direction compared with [100] have been omitted. Inclusion of the nonparabolicity in the bulk conduction band and of the full Luttinger Hamiltonian for the holes would improve our calculations. This would allow one to estimate quantitatively the effects of the high-index crystallographic direction and of the additional lateral confinement on the optical anisotropy of the direct electron transitions. A blueshift of light- (LH*) and heavy-hole (HH*) exciton continua reflects the influence of corrugation on single-particle states in heterostructure (Table I), which corresponds to data from luminescence excitation experiments.[7-9] The light-hole states in corrugated QW's are essentially distorted by the interface faceting due to the large value of the in-plane mass, similar to the finding of Ref. 17 for a different geometry and method. E_1 for light holes occurs even lower than E_1^0 in ultrathin QW's.

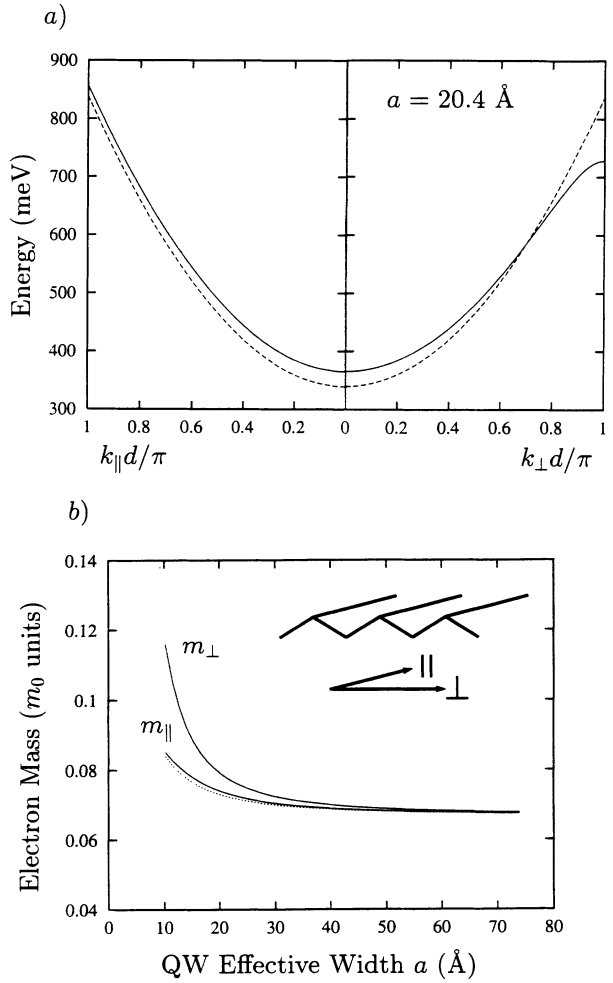

FIG. 4. (a) The dispersion of the lowest 2D miniband in a corrugated QW along (||) and perpendicular to (⊥) facets (solid curves). The same dependence for a simple QW is presented for comparison by dashed line. (b) The electron effective masses parallel ($m_\parallel$) and perpendicular to ($m_\perp$) facets at the bottom of the lowest miniband as functions of the QW effective width a. For comparison, the in-plane electron effective mass in a simple QW is shown by the dotted line.

TABLE I. Blueshift of electron-hole continuum, and heavy- and light-hole exciton binding energies in corrugated and simple QWs.

QW effective width a (Å)	10.2	20.4	30.6	45.9
Blueshift of HH* (meV)	59.5	42.1	22.7	10.4
E_B(HH) in corrugated QW (meV)	15.0	12.1	11.1	10.2
E_B(HH) in simple QW (meV)	13.5	11.8	11.0	10.1
Blueshift of LH* (meV)	18.6	31.4	20.6	10.6
E_B(LH) in corrugated QW (meV)	17.2	14.1	12.9	11.8
E_B(LH) in simple QW (meV)	15.5	13.8	12.7	11.7

A conventional variational procedure with two parameters of the exciton lateral extension along and perpendicular to facets has been used to estimate the effect of corrugation on the exciton binding energy (Table I). The interface corrugation has been found to affect only slightly the exciton binding energy. We explain this fact by the strong coupling of the electron and hole states in neighboring regions and the small size of the 1D channel (d=32 Å) which cannot localize the exciton as a whole. The calculated results for perfect faceted QW's are in contrast with the experimental data.[7-9] We ascribe the significant redshift of the heavy-hole exciton peak obtained in the luminescence experiments to be due to exciton localization by monolayer fluctuations in the 1D channels. From Fig. 3 these will be 7 meV per monolayer of 1.7 Å in the [311] direction for electrons in a quantum well with an effective width of 45 Å.

In summary we have developed a method of realistic calculations of electron states in structures with complex geometries and applied this technique in order to investigate the influence of interface corrugation on electron and exciton states in QW's. It has been found that in the case of the GaAs/AlAs heteropair the corrugation has a surprisingly small effect on the electron states at the bottom of the first miniband and even in the limiting case of a chain of rhombic clusters does not destroy the in-plane transport perpendicular to facets. The excitation binding energy is only slightly renormalized by the potential of corrugation. Its influence is negligible in thicker QW's. We expect the effect to be more pronounced for interface faceting of larger size due to the possibility to localize the exciton in a single 1D-channel region.

Our model calculations can be improved by including the conduction-band nonparabolicity in bulk semiconductors as well as by considering hole states in the framework of the Luttinger Hamiltonian approximation. We have also neglected the presence of indirect minima in conduction bands of bulk materials. It was found experimentally that samples with widths above 43 Å show a type I band structure.[21] We confirm this conclusion because in our effective-mass calculations for $a > 37$ Å the lowest Γ electron state in a corrugated QW occurs below the X point in AlAs.

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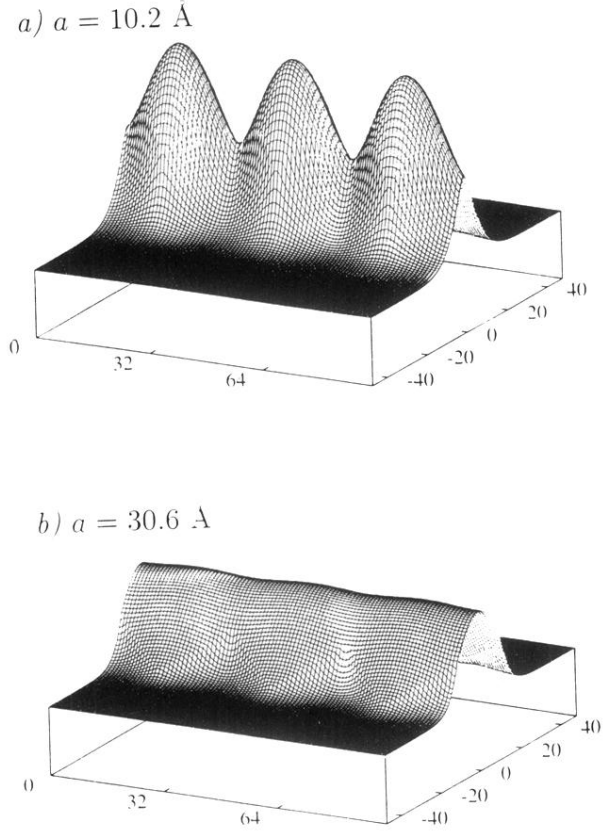

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