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2006 J. Phys.: Condens. Matter 18 8715

(http://iopscience.iop.org/0953-8984/18/39/004)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **18** (2006) 8715–8721 doi:10.1088/0953-8984/18/39/004

Can one-dimensional electron gas be generated in vicinal steps of GaAs?

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Received 22 July 2006, in final form 17 August 2006
Published 11 September 2006
Online at stacks.iop.org/JPhysCM/18/8715

Abstract

In this work we study the electronic structure of doped multi-quantum wires formed by steps in the vicinal surfaces of GaAs. It is verified that multi one-dimensional electronic systems can exist, which contrasts with a previous conclusion in the case of a single wire where it was demonstrated that the presence of residual acceptors inhibited the formation of such a type of structure. The effects of dopant diffusion, residual density of acceptors and exchange–correlations contributions have been addressed by the self-consistent solution of the Schrödinger equation treated in the effective mass approximation.

1. Introduction

The extraordinary advance in the modern techniques of epitaxial growth allows a huge number of possibilities concerning the ways of quantum confinement of charge carriers. A particular situation occurs when the carriers are furnished by defined doped atomic planes (planar doping) of the host semiconductor material [1–3]. In the metallic doping regime, the latter generate a self-consistent potential which confines the carriers, giving rise to discrete energy levels in the direction perpendicular to the doping directions while the electron liquid is free in the doping plane. Contrarily to modulation doped quantum wells, where in general only one subband is occupied, such space charge layers can give rise to various subbands which present distinct transport mobilities along the doping layer due to different spatial superposition with the dopants.

An interesting proposal has been suggested which combines the epitaxial growth in vicinal planes (terraces) and the planar doping technique with the aim of obtaining quasi-one-dimensional doped systems [4, 5]. The results do not lead to conclusive experimental realizations of such a type of structures; nevertheless, they present clear evidences of a substantial Si incorporation in Ga sites in the vicinities of the steps that delimit vicinal planes, for example, in the ones originated from the (100) plane in GaAs crystals, as illustrated in figure 1.

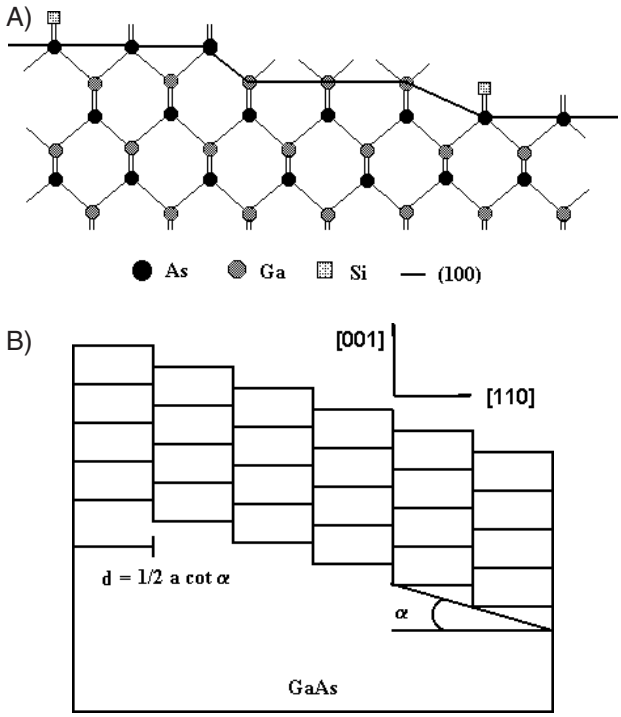

Figure 1. Formation of quantum wires in the (100) GaAs face, with incorporation of Si in the place of Ga and the epitaxial growth after planar doping. (A) Transversal section with Si incorporation in the vicinities of the steps which delimit the vicinal planes in the (100) plane of Ga. (B) Schematic representation of the vicinal planes as a function of the angle α and of the crystal lattice parameter a.

Aiming to mimic the experimental situation just described, recent calculations were conducted on isolated cylindrical GaAs n-type doped quantum wires based on the semiclassical Thomas–Fermi approximation, as well as on the density functional theory in the local density approximation (LDA) [6]. As a result, it has been demonstrated that the presence of residual acceptors in the host material (GaAs) would prevent the formation of such kind of wires.

Contrarily to what has been previously demonstrated [6], in this work we show that the experimental realization of vicinal doped quantum wires may be achieved if instead of isolated quantum wires one contemplates the formation of multi-quantum wires. It is verified that the formation of quasi-one-dimensional electron liquids relies on an appropriate distance between the contiguous wires. Explicitly, such a distance should be less than the typical depletion layer of usual planar doping structures, which is of the order of 1000 Å. In other words, this corresponds to a estimate of how large the width of the steps of the ladder should be. Moreover, it is verified also that there is a threshold doping density for the formation of the doped wires.

In order to perform the calculations we resort to the self-consistent solution of the Schrödinger equation. In it, subjects like the effects of dopant diffusion and the role of the residual density of acceptors are addressed. Our investigations are conducted considering the dopants to be distributed in the form of a cylinder, as shown in figure 2. In the next section we present the theoretical model and the basic equations which solve the electronic structure.

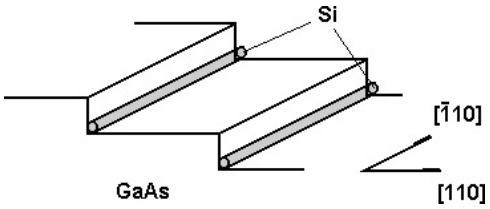

Figure 2. Schematic representation of the multi-quantum wires considered in this work.

2. Theoretical model

The theoretical model proposed in this work is based on the following assumptions: (a) the donor distribution is considered to be radial; (b) the wires are considered infinite, which means that edge effects are not taken in account; (c) we assume parabolic bands and the effective mass approximation. Based on such assumptions the electronic density $n(\mathbf{r})$ and the effective potential $V_{\mathrm{ef}}(\mathbf{r})$ will depend only on the radial coordinate. In the following, we present the theoretical grounds of our calculations. They are similar to the case of isolated quantum wires [6] except for a crucial consideration that will differentiate the two cases as will be explained bellow.

The equations are self-consistently solved. As a first step, one has to know the total potential,

$$V(r) = V_{\mathrm{H}}(r) + V_{\mathrm{xc}}, \tag{1}$$

where V_{xc} takes into account the exchange and correlation effects in the frame of the local density approximation (LDA). The parameterization used to estimate many-body effects is the one suggested by Hedin and Lundqvist for the case of a homogeneous electron gas [7]. The Hartree potential, V_{H}, is obtained via the solution of the Poisson equation:

$$\nabla^2 V_{\mathrm{H}} = 8\pi[n_{\mathrm{D}}(\mathbf{r}) - n(\mathbf{r}) - n_{\mathrm{A}}(\mathbf{r})] \tag{2}$$

where the electronic density $n(\mathbf{r}) = \sum_i N_i |\psi_i(\mathbf{r})|^2$ is obtained through the solution of the Schrödinger equation with N_i and ψ_i being the linear electron density and the wavefunction of the ith subband. The wavefunction may be written as

$$\psi_{j,m}(r,\theta,z) = R_{j,m}(r)\frac{\mathrm{e}^{\mathrm{i}m\theta}}{\sqrt{2\pi}}\frac{\mathrm{e}^{-\mathrm{i}k_z z}}{\sqrt{L}} \tag{3}$$

where k_z denotes the wavevector along the z-axis and j and m are the principal and magnetic quantum numbers, respectively. As regards $R_{j,m}(r)$, it should satisfy the radial equation given by

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right) R_{j,m}(r) - \left[V(r) + \frac{m^2}{r^2}\right] R_{j,m}(r) = E_{j,m} R_{j,m}(r). \tag{4}$$

Now we will stress the difference between considering an isolated quantum wire and multi-quantum wires. This comes basically from the boundary conditions imposed on the problem. In the isolated case, [6] had propagated the potential until the derivative of it was zero. This condition was reached by pinning its value at the acceptor level of the bulk material. Nevertheless, in the case of multi-wires, the space between the wires is sufficiently small (200–300 Å) which, from the bulk point of view, means that the system can be analysed as a planar doped sheetin the scale of the depletion layer, as shown in figure 3. The value of the depletion

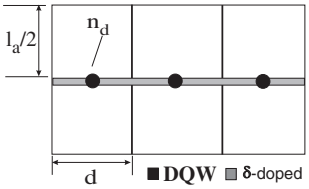

Figure 3. Idealized representation of isolated doped multi-quantum wires (DQW) that in the scale of the depletion layer, l_a, may be considered a planar sheet for $d \ll l_a$.

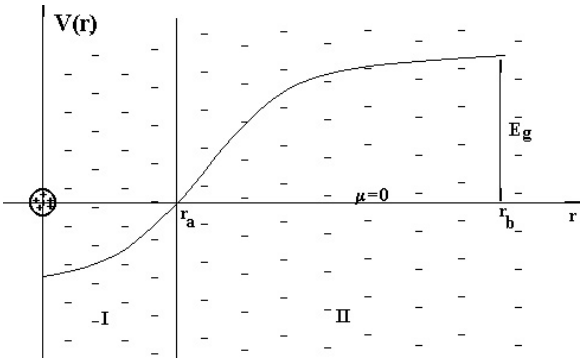

Figure 4. Effective potential of cylindrical quantum wires considering the incorporation of acceptors uniformly distributed in the bulk of the GaAs. $\mu = 0$ corresponds to the Fermi energy.

layer may be deduced from the knowledge of the electric force (by means of the Gauss law) and the work to take an electron from r_a to r_b in region II of figure 4. The estimated value is given by

$$l_a \simeq \sqrt{\frac{E_g}{\pi n_a}}, \tag{5}$$

where E_g is the gap of the host material (GaAs) and n_a is the three-dimensional acceptor density. Considering that each acceptor will take one electron from the electron gas, we have that $n_a l_a$ will furnish the number of depleted electrons per unit of area. Therefore, the number of depleted electrons per wire, per unit length, N^{dep}, may be written as a function of the distance d of the wires as

$$N^{dep} \simeq \sqrt{\frac{E_g n_a}{\pi}} d. \tag{6}$$

From the previous equation one can see that there is a linear dependence with the distance between the wires. This shows that when d increases, the case of an isolated wire is recovered, which means that the potential energy of the donors cannot supplant the potential energy of the acceptors with the result that the isolated wire will be complete depleted. From the Gauss law, the boundary condition to the equation (2) obtained in $r = r_a$, the region I in the figure 4, is given by

$$V(r_a) = 0 \qquad \text{and} \qquad \frac{dV}{dr}(r_a) = \frac{4}{r_a} N^{dep}. \tag{7}$$

Table 1. Percentage of depleted electrons for wires of $r_{DQW} = 50$ Å, linear densities, $\lambda = 0.78 \times 10^6$, 3.9×10^6 and 7.8×10^6 cm^{-1}, distance between the wires, $d = 200$ Å and a homogeneous acceptor density, $n_a = 10^{15}$ cm^{-3}.

Donors cm^{-1}	0.78×10^6	3.9×10^6	7.8×10^6
N^{dep} (%)	72	14	7

3. Results and discussion

Considering the multi-quantum-wire system previously sketched, figure 5 shows the electronic structure of three types of wire calculated in the Hartree (H) and LDA approximations. In the scale of the depletion layer, much bigger than the wires' separation, the superlattice of wires is equivalent to a single planar doped structure, which can lead to the formation of an one-dimensional electron liquid even with the incorporation of an uniform density of acceptors. This may be understood as a consequence of the electrostatic competition between the 'two-dimensional' structure formed by the superlattice and the three-dimensional structure formed by the volumetric distribution of the acceptors. Based on such a model, figures 5(a)–(c) present the results for doped quantum wires (DQW) with radius $r_{DQW} = 50$ Å and linear densities $\lambda = 0.78 \times 10^6$, 3.9×10^6 and 7.8×10^6 cm^{-1}, respectively. Moreover, they are immersed in a homogeneous acceptor density with $n_a = 10^{15}$ cm^{-3} and inter-wire separations of 200 Å. With such parameters, tunnelling between the wires can be neglected due to the fact that the electronic density decreases quickly as a function of the radial coordinate, r, above 200 Å (see the insets of figure 5). The figures also show the probability densities, the calculated energy per subband, E_{mk} (horizontal dotted lines), and the number of electrons per subband, n_{mk}. For the latter quantity, one can observe in figure 5(b) and (c) that there is a considerable number of electrons in higher subbands where there may even occur an inversion of population, as the second subband of figure 5(c) shows. Allied to this, such carriers are not in the same region of the dopants, which will increase their mobilities. It is interesting to note that the number of the electrons depleted from the system increases rapidly with the decrease of doping. Such a fact is represented in table 1. This represents one of the theoretical limits to obtaining doped multi-quantum wires: below 10^{18} donors cm^{-3} the background of acceptors will considerably affect the electron occupation. As a final comment, we have found that the estimated value of the depletion layer is around 5×10^4 Å, and that for d bigger than 400 Å the wires are completely depleted, which recovers the isolated wire case [6].

4. Conclusions

In summary, we have shown that it is possible to obtain quasi-one-dimensional electron liquids through the growth of multi-quantum wires on the corners of terraces of GaAs ladder structures via silicon planar doping. Nevertheless, such realization is only possible if there is a compromise between the size of the steps, the density of acceptors throughout the structure, and the density of donors. For example, for steps larger than 1000 Å, the wires will be completely depleted. The importance of such structures is that they may be used for the realization of a quantum-wire intersubband laser through the jumping of the electrons from one energy subband to another via the action of an electric field. The basic principle of such a device is based on a conventional quantum-well cascade laser. However, the optically active region does not consist of coupled quantum-wells anymore, but now consists of coupled quantum-wires. The advantage of quantum-wire intersubband structures is a theoretically predicted decrease

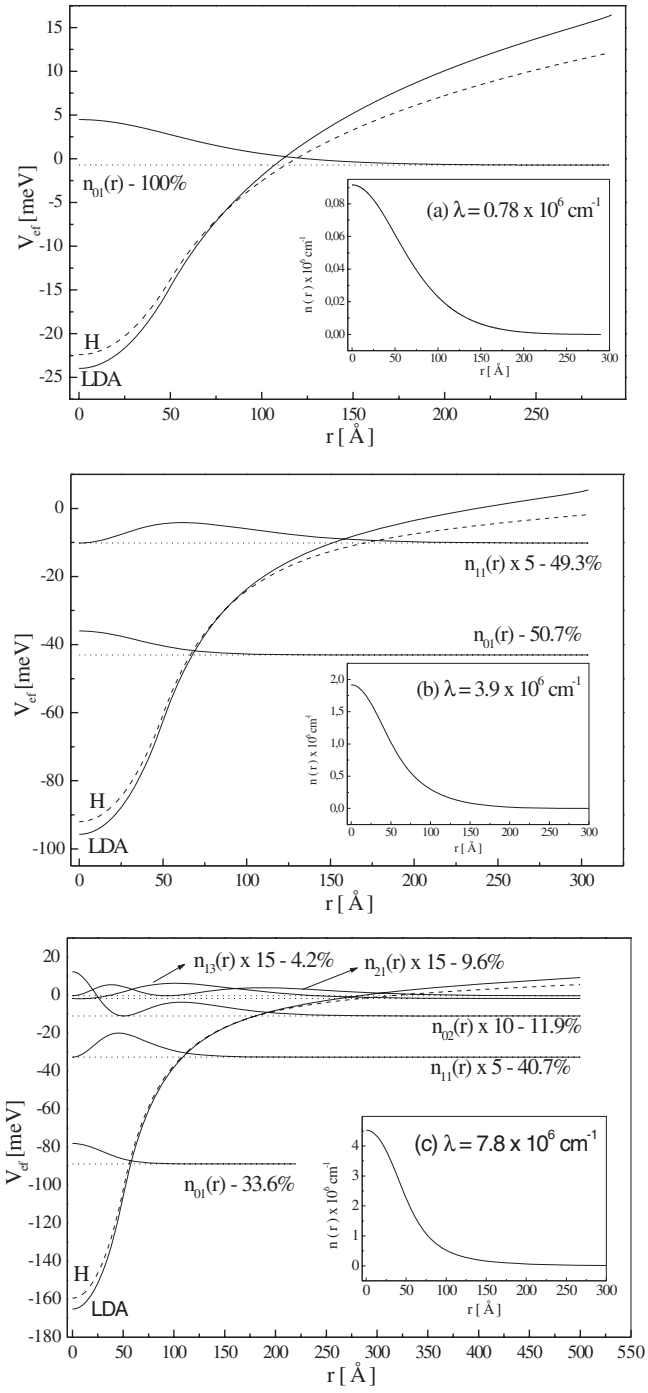

Figure 5. Electronic structure data for the unitary cell of cylindrical quantum wires 200 Å apart. The figure shows the effective potentials in the Hartree (H) and LDA approximations. The electronic densities per unit length (insets), the energy levels (horizontal dots), the probability densities per subband and the electronic occupation per subband, n_{mk}, are presented for wires with $r_{\mathrm{DQW}} = 50$ Å, $n_{\mathrm{a}} = 10^{15}$ acceptors cm^{-3} and linear densities (a) $\lambda = 0.78 \times 10^6$ donors cm^{-1}, (b) 3.9×10^6 donors cm^{-1} and (c) 7.8×10^6 donors cm^{-1} respectively.

of non-radiative losses compared to quantum-well structures [8] and a possible reduction of the threshold current [9]. Also interesting to note from the results is that the higher energy subbands possess higher population density compared to the usual delta doped superlattices [10] and that such subbands are not in the same region of the dopants which would furnish samples of higher mobilities.

Acknowledgments

The authors would like to thank Professor L Ioriatti for calling their attention to the problem and for earlier discussions. They are also grateful for the financial support of the Brazilian funding research agencies FAPEMIG and CNPQ.

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