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J. Phys.: Condens. Matter 5 (1993) 9069–9076. Printed in the UK

On the theory of GaAs-based quantum wells with external δ-doping

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Received 11 August 1993

Abstract. The electron gas confined in GaAs/$Al_xGa_{1-x}As$ quantum wells δ-doped in the barriers has been self-consistently studied in an effective-mass model. In agreement with experimental evidence, our calculations show how the limitations in 2D electron density found in modulation-doped structures can be overcome with the delta-doping technique. The role of different structural parameters of these systems in the practical outcome is also discussed.

1. Introduction

The modulation-doping technique has been widely used in the fabrication of high-mobility electronic devices. Si-doped GaAs/$Al_xGa_{1-x}As$ heterostructures constitute one of the most widely known examples of application of modulation-doping, which allows one, on the one hand, to reduce impurity scattering and, on the other hand, to confine in the GaAs channel a high-density quasi-two-dimensional electron gas (2DEG). Nonetheless, due to structural limitations [1] (3D solubility limit of Si in $Al_xGa_{1-x}As$, Si impurity levels) the areal density in the GaAs channel N_{GaAs} takes values lower than 1×10^{12} cm^{-2} in single heterojunctions and somewhat higher (not exceeding 2×10^{12} cm^{-2}) in quantum wells. This density limit has been surpassed in barrier-delta-doped heterostructures. As measurements in this kind of system indicate [2, 3], N_{GaAs} is nearly doubled with respect to the densities obtained in modulation-doped heterostructures. Mobilities in these systems are still rather high, so transistors with very high transconductances can be made from such structures.

The references on these systems appear to be so far experimental. Cunningham *et al* [2] report the growth of barrier-δ-doped single heterojunctions. They find areal electron densities larger than 1×10^{12} cm^{-2} and room temperature mobilities over 8000 cm^2 V^{-1} s^{-1}. Kuo *et al* [3] study barrier-δ-doped quantum wells, where they find areal electron densities N_{GaAs} of 4×10^{12} cm^{-2} in the GaAs channel.

To optimize these structures it is desirable to have most of the carriers in the GaAs channel, where the impurity scattering is lower, forming only one 2DEG of the highest possible areal density. It is not possible to know *a priori* the carrier density in the δ channels, and whether these will be formed, although logically the higher the impurity density and the narrower the spacer layer between the delta layers and the GaAs quantum well, the larger the electron population in the δ channels. The purpose of this paper is to show in what situations the electron density in the GaAs well is higher, and to clarify why the N_{GaAs} limits found in modulation-doped structures are overcome in delta-doped systems.

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2. Model and calculations

The configuration studied is as follows: we consider a GaAs quantum well of width L_W with $Al_xGa_{1-x}As$ barriers symmetrically delta-doped at a distance L_S from the quantum well (figure 1). The impurity areal density is N_D; for this system Si is used as dopant. We shall study cases in which N_D is sufficiently high to allow us to assume that the positive charge is uniformly distributed in the growth plane xy. In practice this means $N_D \geqslant 1\times10^{11}$ cm^{-2} [4]. In the growth direction z the impurity distribution can be modelled by a Gaussian, the width of which at half maximum will be fixed and equal to 20 Å for this calculation. Although in the first delta-doped structures grown the width of the doped zone varied considerably from sample to sample and happened to be a parameter that was hardly controlled, the impurity distributions grown recently are rather narrow; it has been shown that Si segregation occurs when the substrate temperature T_S during growth is high ($T_S > 530$ °C) [5, 6]. Now the impurity distribution width is well controlled and the width chosen here is a typically representative value. In any case, as shown in [7], this parameter does not appreciably affect the spectrum when it varies within the range of current experimental interest (at most 40 Å).

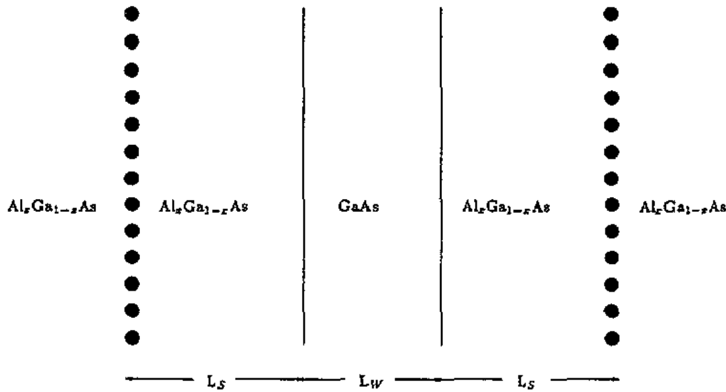

Figure 1. Schematic view of a barrier-δ-doped GaAs/$Al_xGa_{1-x}As$ quantum well. L_W is the GaAs quantum well width; L_S is the spacer layer.

For most of the wells investigated we have fixed the width as $L_W = 80$ Å. To show how the areal electron density depends on the width of the well we present also an example of a wider well with $L_W = 120$ Å. For the wells with $x = 0.3$ and wider than 200 Å two quasi-2D electron gases are formed close to the interface [8–10], while the practical interest lies in having only one 2DEG around the centre of the quantum well where impurity and interface roughness scattering are lowest.

The aluminium fraction in the barriers x will also be fixed. As our goal is to achieve the highest possible population in the GaAs channel, we seek the highest possible barrier without entering the indirect-gap regime, so we can match effective-mass models at the interfaces. We shall vary the impurity density N_D and the spacer layer L_S to evaluate the resulting changes in the electron density distributions.

The Fermi level is not known *a priori* in these systems; nevertheless, the total areal electron density is known and is equal to the impurity density introduced, so from this value and imposing charge neutrality,

$$N_S = -\frac{1}{e}\int_{-\infty}^{+\infty} dz\ \rho_e(z) = 2N_D$$

where

$$\rho_e(z) = -e \sum_{j\kappa} f(E_F - E_j(\kappa)) |\psi_{j\kappa}(r)|^2$$

is the local electron density, E_F is self-consistently determined. This is the fundamental difference with regard to modulation-doped quantum wells, in which E_F is fixed and determined with respect to the bottom of the conduction band (CB) far from the region with band bending, and determined by the impurity ionization energies. The problem of the position of E_F in $GaAs/Al_xGa_{1-x}As$ modulation-doped structures has been widely discussed [10–13]. Assuming that there are no acceptors, for $T = 0$ K and for $x = 0.3$, it is justified to fix it at half the ionization energy of DX impurity levels down from the bottom of the CB in the flat-band region. Thus for MDQWs E_F is fixed and N_{GaAs} is self-consistently calculated for different structural parameters of the wells (L_S and L_W). In contrast, in δ-doped structures it is the total population that is *a priori* known and then charge distribution, fraction of depletion of the δ-layers and E_F are calculated self-consistently from it [7, 14].

The presence of carriers in the structure considerably alters the potential, and the eigenenergies and eigenstates of the problem, so it has to be solved self-consistently in the customary Schrödinger–Poisson scheme. We use an effective-mass one-band model associated with the CB minimum in the Γ point for both materials. We have taken into account the effective-mass difference in solving the Schrödinger equation for the envelope functions; this can be done by combining the transfer matrix and surface Green function matching techniques as explained in [15, 16] and done in [7]. In terms of the wavefunctions it amounts to imposing continuity of the wavefunction ψ and of ψ'/m^* at the interfaces. As usual in this kind of calculation we consider exchange and correlation effects within the *local density functional approximation.* We have used the Hedin–Lundqvist parametrization [17]. We regard the solution as self-consistent when the mean square deviation of the potential evaluated at all the points used in the integration in two consecutive cycles of the calculation is less than 0.1 meV.

3. Results and comments

To carry out the calculation, we have taken the gap as $E_g = (1155x + 370x^2)$ meV [18] and the barrier height as $V = 0.6\ \Delta E_g$ [19]. For the effective masses we use the formula $m^* = (0.0665 + 0.0835x)m_0$ [20], where m_0 is the free-electron mass.

The results for four wells with L_W = 80 Å, x=0.3, and different values of N_D and L_S are shown in figures 2 to 5. In figures 2 and 3, $N_D = (1+1) \times 10^{12}$ cm^{-2}, that is, each delta-doped layer has a density of 1×10^{12} cm^{-2}, so the total electron density of the system is twice the areal density of a delta layer. The spacer layers are of 50 and 70 Å respectively. The potential profiles are very similar; the difference between these two cases is in the Fermi level position: for L_S = 50 Å it is at 38.7 meV from the bottom of the CB in the bulk zone, whilst in the L_S = 70 Å case it is at only 9.7 meV. This is the main difference compared with modulation-doped quantum wells, in which E_F is fixed beforehand by the impurities, and is always at the same distance from the bottom of the CB in the bulk. Therefore, although the potential shapes shown in figures 2 and 3 are apparently similar to the ones obtained with modulation doping, the statistical treatment is different, analogous in any case to the one followed in δ-doped structures [7, 14].

As the systems shown in figures 2 and 3 have the same areal electron density and only one occupied subband, their envelope functions are practically equal, and the distances from the bottom of the subband E_1 to the Fermi level are almost the same. In this case

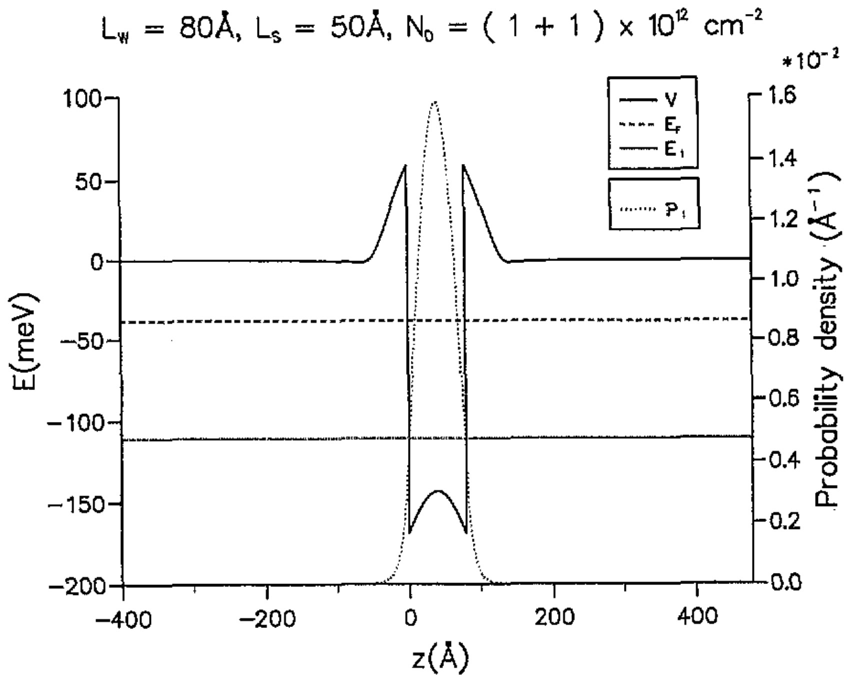

Figure 2. Self-consistent potential (V), probability density P of the state E_1 and Fermi level E_F for the structure with the parameters shown in the figure. In this and in the following figures $x = 0.3$.

the delta-doped layers are depleted: all the electrons from the Si impurities have ended up in the GaAs channel and the positive charges are not sufficiently attractive to retain some electronic population trapped in the self-consistent δ-like wells seen in the next two cases.

Figures 4 and 5 show two systems with densities twice those of the former cases: $N_D = (2+2) \times 10^{12}$ cm^{-2}. In both cases there are five occupied subbands, and the delta-doped zones result in δ-like wells with an appreciable population. The ground subband is characteristic of the structural quantum well (of GaAs): its probability density is highly localized in the GaAs channel. The four upper subbands are bunched up in pairs of very close energies and they correspond to symmetric/antisymmetric states of the δ wells, coupled through the GaAs quantum well. In fact, the distance between the levels 2 and 3 on the one hand and 4 and 5 on the other hand are very similar. This indicates that they come from the same isolated δ well levels split apart by the coupling. This picture is confirmed by the difference between the cases with L_S= 50 and 70 Å: if the spacer layer is wider, the coupling is smaller and the difference in energies between the symmetric and antisymmetric levels is also smaller; moreover, the probability densities outside the GaAs well are very alike. Inside the GaAs well they must be different in any case because they have opposite symmetry.

The probability densities of the subbands 2 to 5 are much larger in the δ wells than in the GaAs channels in both systems. The higher the bottom of the subband energy is, the farther away from the GaAs well the probability maximum is, i.e., the less confined the electrons are.

Note the difference between (i) the coupled δ wells of the structure studied here and (ii) those one would have in the absence of the intermediate GaAs well. The ground state E_1 of case (i) has no parallel in (ii). It is nearly all concentrated in the GaAs channel—except for

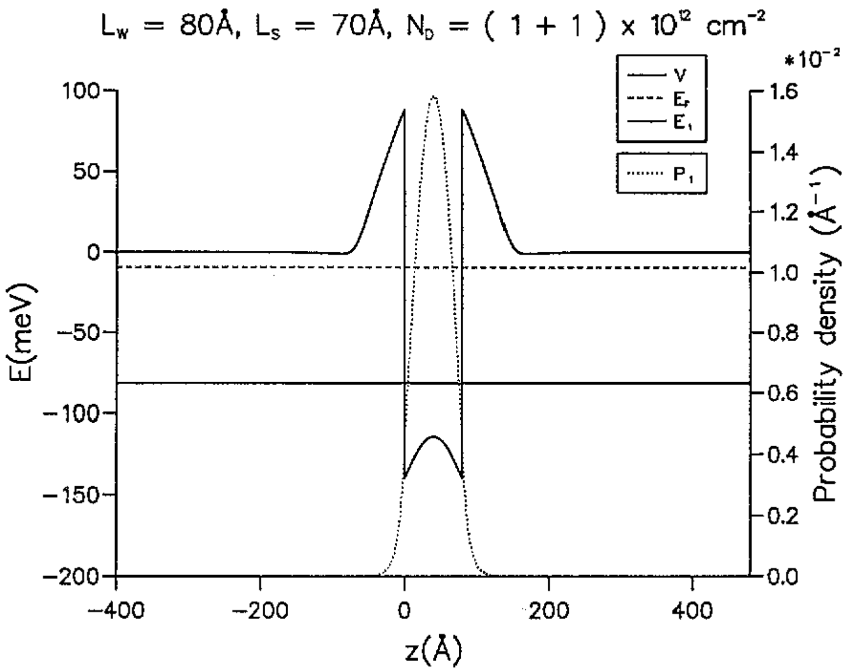

Figure 3. As figure 2, but with a different L_S.

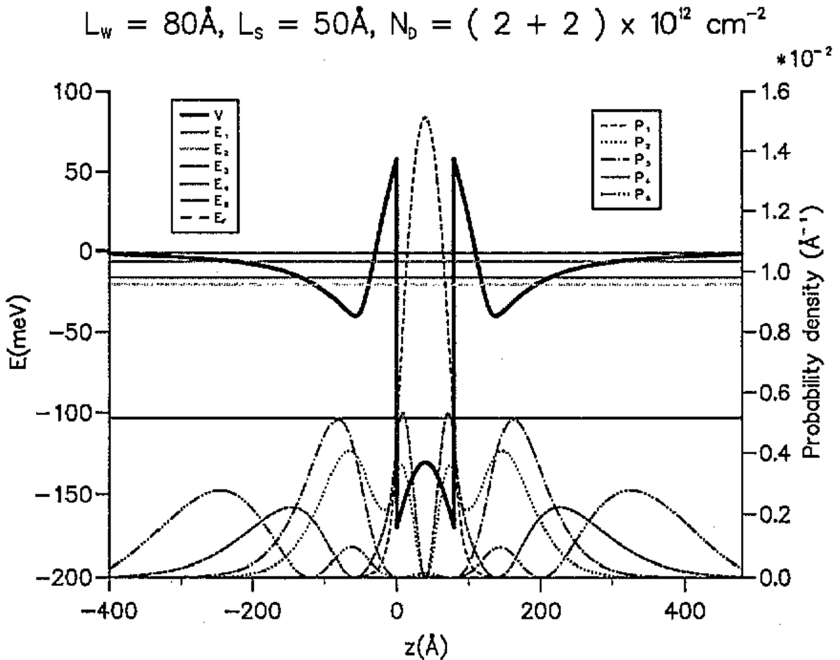

Figure 4. Self-consistent potential (V), probability densities of each subband (P_i) and subband ground levels for the values of the parameters shown in the figure.

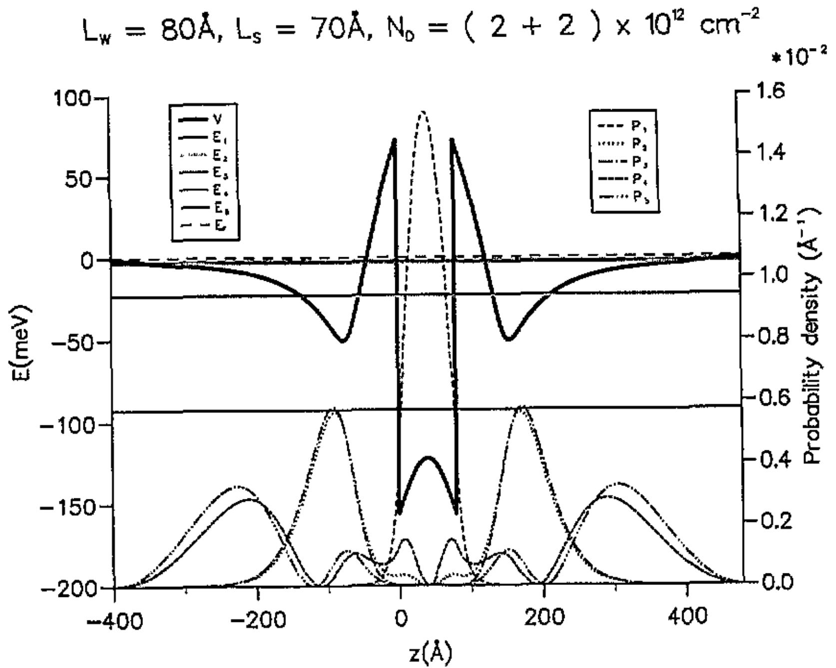

Figure 5. As figure 4, but with a different L_S.

the small amplitude of the evanescent tails of the wavefunction outside—due to the attraction of the GaAs well. The states E_2 and E_3 of case (i) would correspond to the first two states of case (ii). In this case the lower/upper state of this pair is symmetric/antisymmetric, whereas in case (i) the lower state, E_2, is the first one above the ground state, E_1, in the spectrum of the entire δ–GaAs–δ structure and is therefore antisymmetric, while the next one, E_3, is symmetric. Both still have a significant amplitude in the central part due to the attraction of the well, but their symmetry pattern is distinctly that of the entire structure. When changing impurity areal density in a δ layer from 1 to 2 $\times 10^{12}$ cm^{-2} one can smoothly pass from figures 2 and 3 to the figures 4 and 5. One can see from table 1 that the areal electron density inside the GaAs QW (N_{GaAs}, defined as the integral of $-\rho_e(z)/e$ from 0 to L_W) does not change very much when the δ layers are not fully depleted. So to optimize the structure one should approach this areal electron density without populating the δ wells. Thus, for a given L_W, L_S, one should choose N_D slightly lower than half the areal electron density achieved in the GaAs channel N_{GaAs} for the structures with partial depletion of the δ layers. We have done this for the case L_W = 80 Å, L_S = 70 Å, taking N_D as 1.1 $\times 10^{12}$ cm^{-2}. For this structure we get N_{GaAs} = 2.03 $\times 10^{12}$ cm^{-2} and only one occupied subband, with $E_F - E_1$ = 79.2 meV. Increasing N_D further, the outside-the-well minimum of the potential gets deeper and the number of subbands increases; for N_D=1.5 $\times 10^{12}$ cm^{-2}, the well already has three occupied subbands with the energies −85.8, −11.4 and −11.0 meV measured from the bottom of the CB in the flat potential region. The outside-the-well minimum of the potential is equal in this case to −29.8 meV, measured from the same CB energy. Nevertheless, the areal density in the GaAs channel hardly varies: N_{GaAs} is 2.20 $\times 10^{12}$ cm^{-2}.

Table 1 gives the Fermi level and energy eigenvalues for the systems of figures 2 to 5. In the last case E_2 and E_3 are so close that they are indistinguishable in the corresponding

Table 1. N_{GaAs}: areal electron density inside the GaAs well; E_F: Fermi level; E_i: ith subband energy at κ=0 for the systems shown in the table heading with the notation $L_W/L_S/(N_D + N_D)$. All the energies are in meV measured from the bottom of the CB in the $Al_xGa_{(1-x)}As$ bulk; densities are in 10^{12} cm^{-2} and lengths in Å.

	80/50/(1+1)	80/70/(1+1)	80/50/(2+2)	80/70/(2+2)	120/70/(2+2)
N_{GaAs} (10^{12} cm^{-2})	1.85	1.85	2.74	2.38	2.61
E_F (meV)	− 38.7	− 9.7	− 0.6	− 0.03	− 1.39
					− 2.73
			− 1.0	− 2.0	− 2.91
			− 6.3	− 3.2	−19.72
E_i (meV)			− 16.1	−22.8	−20.87
			− 20.6	−23.6	−28.61
	−110.7	−81.7	−103.2	−92.5	−77.61

figure (figure 5) and likewise for E_4 and E_5. A reduction of L_S from 70 to 50 Å suffices to separate these energy levels so they can be distinguished in figure 4. Also, as commented on above, in the results for figures 2 and 3 there is no difference in the value for $E_F - E_1$.

The areal electron density in the GaAs channels N_{GaAs} for all the systems is also given in table 1. In the structures with $N_D = (1+1) \times 10^{12}$ cm^{-2}, N_{GaAs} is 92.5% of the total electron density; by looking at the potential profiles it is clear that the electron density in the barriers N_x is due to the wavefunction penetration in the barriers and not to the possible population of the δ quantum wells. If one were to choose between these two structures to build an electronic device, one would prefer the one with the wider spacer layer ($L_S = 70$ Å); with the same areal electron density in the GaAs channel, the impurity scattering is lower because the doping zone is farther away from the quasi-2D electron gas. As to the structures with $N_D = (2+2) \times 10^{12}$ cm^{-2}, the areal electron density in the barriers is about one third of the total density N_{GaAs} (32.5% if $L_S = 70$ Å and 40% if $L_S = 50$ Å). This is because the delta-doped zones form δ wells with an appreciable population, as we have already seen in the description of the spectrum for these cases. The quasi-2D electron density in these cases is of almost 3×10^{12} cm^{-2}. In order to make a quantitative comparison between the δ-doping case and the MD one, we have also calculated the MDQW having $L_W = 80$ Å, $L_S = 70$ Å with a bulk impurity concentration of 10^{18} cm^{-3}. The resulting N_{GaAs} is 1.36 $\times 10^{12}$ cm^{-2}. By comparison, a δ-doped well with the same values of L_W and L_S and with $N_D = (1.1 + 1.1) \times 10^{12}$ cm^{-2} yields a higher value of $N_{GaAs} = 2.03 \times 10^{12}$ cm^{-2}, and for the δ-doped wells with $N_D = (2 + 2) \times 10^{12}$ cm^{-2}, N_{GaAs} is even higher (see table 1), but now there is also an appreciable population of the δ wells. This reflects the fundamental difference in the formation of the Fermi level in both kinds of structure. In order to decide theoretically which one is more suitable for practical purposes it would be necessary to study the mobility of the 2DEG, considering that there are two distinctly different electron populations in parallel.

Finally we have calculated a wider quantum well with $L_W = 120$ Å, $L_S = 70$ Å, impurity density $(2 + 2) \times 10^{12}$ cm^{-2}. The results are shown in table 1. An increase of L_W with the same value of L_S results, of course, in an increase of N_{GaAs}, but this is rather slight.

All the results shown in table I have been calculated considering exchange and correlation effects. The self-consistent potentials in a Hartree calculation are somewhat less attractive, so the subband energies at $\kappa = 0$, E_i, and the Fermi level E_F are closer to the bottom of the conduction band in the bulk. Nevertheless, the relative positions of the subband energies with respect to the Fermi energy—and consequently N_{GaAs}—do not change much. In fact, when the delta layers are fully depleted the difference between N_{GaAs}

as computed in the Hartree approximation and those with exchange and correlation effects taken into consideration is typically less than 1%. When the delta wells retain some electron population, one would expect N_{GaAs} to be somewhat smaller for the less attractive Hartree potential. Some sample calculations indicate that the differences in this case are typically not larger than 5%.

It has been suggested [2, 3] that the observed increase in electron population of the GaAs well comparing modulation-doped with δ-doped structures is due to a quantum-size effect. The present calculations provide a straightforward interpretation based simply on the fact that the position of the Fermi level is determined in a substantially different way, and the corresponding self-consistent calculation results in different level alignments with respect to E_F. In conclusion it seems rather more convenient in practice to avoid the population of δ-like wells, thus having a final self-consistent potential profile and probability density distribution similar to that of the modulation-doped quantum well but with a higher free-carrier population in the GaAs channel.

Acknowledgments

This work was partly supported by the Spanish CICYT under grant MAT91-0738. LC acknowledges the support of the Spanish Ministry of Education and Science for a study visit to the Mikolaja Kopernika Uniwersytet. RP-A also acknowledges the support of the Spanish MEC for a sabbatical stay in Madrid.

It is a pleasure to thank V R Velasco and H Rodríguez-Coppola for many interesting and useful discussions.

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