Electronic States in n-Type GaAs Delta-Doped Quantum Wells Under Hydrostatic Pressure

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The calculation of the electronic energy levels of n-type δ-doped quantum wells in a *GaAs* matrix is presented. The effects of hydrostatic pressure on the band structure are taken into account specially when the host material becomes an indirect gap one. The results suggest that under the applied pressure regime the *GaAs* can support two-dimensional conduction channels associated to the delta-doping, with carrier densities exceeding $10^{13}\,\mathrm{cm}^{-2}$

Keywords: GaAs; Delta-doping; Hydrostatic pressure

I. INTRODUCTION

Ultrathin semiconducting layers with exceptional quality can be obtained with the use of modern crystal growth techniques. Impurity seeding is achieved up to the atomic layer scale (δ-doping). The localization of ionized impurities in a very thin layer gives rise to a very intense electric field which -in turns- causes a bending of the energy bands and the occurrence of a particular V-shaped potential. Work on δ-doped structures was primarily in n-type, on Si and III-V semiconducting materials (see, for instance, [1–8]). However, there is also an early report on this kind of system grown on $Al_xGa_{1-x}As$ alloy [9]. In all cases, the main application sought for these systems is the fabrication of high electron mobility transistors provided the formation of a high density two-dimensional electron gas.

The GaAs-based delta-doped systems are among the most studied both experimentally and from the theoretical point of view. It is known that for the n-type GaAs delta wells, the upper limit for the two-dimensional density of ionized impurities is of about $10^{13}\,\mathrm{cm}^{-2}$ (see for instance [10] and references therein). This is a saturation limit and above it no additional increase in the electron concentration, N_{2D}, is achieved.

The aim of the present work is to present the calculation of the electron energy levels of n-type delta-doped quantum wells in the conduction band of GaAs, including the effect of hydrostatic pressure. This is done with the use of the local-density Thomas-Fermi approximation [10, 11]. Such approach has proven to be a simple and accurate alternative to self-consistent electronic calculation in the two-dimensional electron gas (2DEG) of delta-doped structures. Details of the model can be found in Refs. [11, 12]. Particular attention will be paid to the effect of the transition from direct to indirect gap as a result of the increasing applied pressure (see Table I). To illustrate the situation, the figure 1 shows, in schematic form, the relative position of the Γ and X minima in the GaAs conduction band and the corresponding delta-doped quantum wells for a doping density of $10^{13}\,\mathrm{cm}^{-2}$. It can be observed that the ground electronic energy level in the system moves from the Brillouin zone center (at $P = 0$) to locate at the X-point (the transition from direct to indirect energy gap occurs when P goes above 36.69 kbar).

P(kbar)	0	40	80	120
$E_\Gamma(eV)$	1.5189	1.9626	2.2856	2.4880
$E_X(eV)$	1.9809	1.9249	1.8689	1.8129

Table I. Γ and X energy gaps in *GaAs* for different values of the hydrostatic pressure. Energies are measured from the top valence band edge.

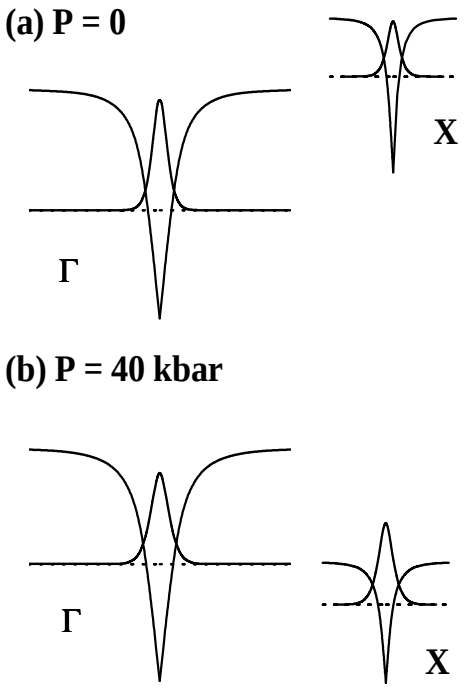

FIG. 1: Schematic view of the relative disposition of the conduction band minima Γ and X of GaAs, together with the corresponding delta-doped quantum wells formed for a two-dimensional ionized impurity density of $10^{13}\,\mathrm{cm}^{-2}$. (a) represents the situation in which no hydrostatic pressure is applied to the system. (b) corresponds to the case where the pressure is of 40 kbar. For illustration, both the first energy levels $E_0(\Gamma)$ and $E_0(X)$, and their squared wavefunctions, are shown as well.

The inclusion of the effects of the hydrostatic pressure is done by introducing a pressure dependence for each of the basic input parameters. That is, the position of the Γ and X

minima with respect to the top of the valence band, the corresponding electronic effective masses, and the dielectric constant [13].

II. RESULTS AND DISCUSSION

$N_{2D} = 5 \times 10^{12}$ cm^{-2}			
	Energy levels (eV)		
P(kbar)	$E_0(\Gamma)$	$E_1(\Gamma)$	$E_0(X)$
0	1.4098	1.4767	1.9685
20	1.6563	1.7197	1.9417
40	1.8706	1.9312	1.9145
60	2.0533	2.1137	1.8872
80	2.2049	2.2613	1.8598
100	2.3252	2.3801	1.8322
120	2.4152	2.4685	1.8045

Table II. Pressure-dependent energy levels in a δ-doped *GaAs* quantum well with a two-dimensional doping concentration $N_{2D} = 5 \times 10^{12}$ cm^{-2}. Both Γ and X states are reported. Energies are measured from the top of the valence band.

Tables II to V show the results of the calculation for the ground and first excited energy levels in n-delta-doped GaAs quantum wells considering the effects of the applied hydrostatic pressure. In each case, the formation of the quantum well is assumed for both the Γ and X minima of the conduction band. The idea is to study the conditions for which the ground state in the system will move away from being located at the Brillouin zone center. In order to give a homogeneous picture, the levels are reported considering the zero of the energy scale located at the valence band top edge.

$N_{2D} = 10^{13}$ cm^{-2}				
	Energy levels (eV)			
P(kbar)	$E_0(\Gamma)$	$E_1(\Gamma)$	$E_0(X)$	$E_1(X)$
0	1.3199	1.4323	1.9572	1.9798
20	1.5739	1.6808	1.9313	-
40	1.7941	1.8967	1.9049	-
60	1.9816	2.0806	1.8781	-
80	2.1371	2.2331	1.8511	-
100	2.2611	2.3545	1.8239	-
120	2.3538	2.4450	1.7966	-

Table III. The same as in Table II but with a two-dimensional doping concentration of 10^{13} cm^{-2}.

For two-dimensional densities of 5×10^{12} cm^{-2} (Table II) and 10^{13} cm^{-2} (Table III), it is clearly seen that even for pressures above the Γ-X crossover, the ground state stays at $\mathbf{k} = 0$. More specifically, the ground energy level starts locating at X only for pressures around 60 kbar. The reason for this to happen is that even at $P = 40$ kbar, the changes in the Γ band parameters are not large enough as to cause a significant modification of the quantum well features (energy position of its edge, depth, and average width) in this point of the Brillouin zone.

$N_{2D} = 5 \times 10^{13}$ cm^{-2}				
	Energy levels (eV)			
P(kbar)	$E_0(\Gamma)$	$E_1(\Gamma)$	$E_0(X)$	$E_1(X)$
0	-	-	1.8768	1.9647
20	-	-	1.8573	1.9420
40	-	-	1.8357	1.9146
60	-	-	1.8128	1.8880
80	-	-	1.7888	1.8616
100	1.8322	2.1454	1.7640	1.8343
120	1.9430	2.2505	1.7385	1.8076

Table IV. The same as in Tables II and III for a two-dimensional doping concentration of 5×10^{13} cm^{-2}.

The two mentioned are admissible values for the ionized impurity density in GaAs, according to the above referred studies. It should be noticed that in all the previous literature on the subject the formation of the delta quantum well at Γ for atmospheric pressure is taken for granted. Here, we go beyond and calculate the spectrum of the delta-doped quantum wells assuming the possibility of having densities of 5×10^{13} cm^{-2} (Table IV) and 10^{14} cm^{-2} (Table V). The results for the ground level at the Γ minimum are only reported in the cases where they arise from a physically meaningful situation within the model. In this sense, even with the increase with pressure of the effective mass, and the decrease of the dielectric constant, the electrical environment in the material -reflected in the effective Bohr radius- will not allow for the formation of a delta well with such characteristics [14] (obviously, situations where the quantum well bottom turns out to be below the valence band top can not be accepted). This is equivalent to say that the system saturates and that those values of N_{2D} -for the given pressures- become unrealistic for they do not reflects in higher 2DEG densities.

$N_{2D} = 10^{14}$ cm^{-2}				
	Energy levels (eV)			
P(kbar)	$E_0(\Gamma)$	$E_1(\Gamma)$	$E_0(X)$	$E_1(X)$
0	-	-	1.7865	1.9401
20	-	-	1.7738	1.9197
40	-	-	1.7575	1.8968
60	-	-	1.7386	1.8730
80	-	-	1.7178	1.8468
100	-	-	1.6956	1.8219
120	-	-	1.6722	1.7948

Table V. The same as in Tables II to IV for a value of the two-dimensional doping concentration of 10^{14} cm^{-2}.

However, such inconvenient is not present in the case of the X minimum. The higher values of the electron effective mass conditions the shape of the quantum well potential profile to be wider and not too deep for concentrations well above $10^{13}\,\mathrm{cm}^{-2}$. In addition, the ground level of the system always locates at this point. The effective Bohr radius is smaller (at very high pressures it approaches the lattice constant), and it has been already shown that in such a case carrier concentrations can reach the order of $10^{14}\,\mathrm{cm}^{-2}$ [15, 16]. Therefore, there is the possibility of having high-density electronic channels.

III. CONCLUSIONS

The output of the present calculation indicates that the application of hydrostatic pressure to GaAs makes possible to attain high density two-dimensional conduction channels associated to the X minimum in the conduction band of that material. This is a desirable feature that can lead, for instance, to higher electron mobilities. The results of our work suggest that it is worth to perform some experimental study in this direction aiming to determine whether such X-associated conduction channels can be present; if not at normal pressure, at least for the case of an applied one.

IV. ACKNOWLEDGEMENTS

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[1] E. F. Schubert, A. Fischer, and K. Ploog, IEEE Trans. Electron Devices **ED-33** (1986) 625.
[2] H. P. Zeidl, T. Wegehaupt, I. Eisele, H. Resinger, G. Tempel, and F. Koch, Appl. Phys. Lett. **50** (1987) 1164.
[3] R. L. Headrick, B. E. Weir, A. F. J. Levi, D. J. Eaglesham, and L. C. Feldman, Appl. Phys. Lett. **57** (1990) 2779.
[4] W. -X. Ni, G. V. Hansson, J. -E. Sundgren, L. Hultman, L. R. Wallenberg, J. -Y Yao, L. C. Markert, and J. E. Greene, Phys. Rev. B **46** (1992) 7551.
[5] H. -J. Gossmann, C. S. Rafferty, A. M. Vredenberg, H. S. Luftman, F. C. Unterwald, D. J. Eaglesham, D. C. Jacobson, T. Boone, and J. M. Poate, Appl. Phys. Lett. **64** (1994) 312; H. -J. Gossmann, and F. C. Unterwald, Phys. Rev. B **47** (1993) 12618.
[6] B. E. Weir, L. C. Feldman, D. Monroe, H.-J. Gossmann, R. L. Headrick, and T. R. Hart, Appl. Phys. Lett. **65** (1994) 737.
[7] L. M. R. Scolfaro, D. Beliaev, P. Enderlein and J. R. Leite, Phys. Rev. B. **50** (1994) 8699.
[8] Y. Wang, R. J. Hamers and E. Kaxiras, Phys. Rev. Lett. **74** (1995) 403.
[9] E. F. Schubert, C. W. Tu, R. F. Kopf, J. M. Kuo, and L. M. Lunardi, Appl. Phys. Lett. **54** (1989) 2592.
[10] L. M. Gaggero-Sager and R. Pérez-Alvarez, J. Appl. Phys. **78** (1995) 4566.
[11] L. Ioriatti, Phys. Rev. B **41** (1990) 8340.
[12] L. M. Gaggero-Sager, M. E. Mora-Ramos and D. A. Contreras-Solorio, Phys. Rev. B **57** (1998) 6286.
[13] See C. A. Duque, N. Porras-Montenegro, Z. Barticevic, M. Pacheco, and L. E. Oliveira, Microelectronics Journal **36**, 231 (2005), and references therein.
[14] L. M. Gaggero-Sager, M. E. Mora-Ramos, and M. A. Olivares-Robles, Microelect. J. **36** (2005) 413.
[15] A. Aleksov, A. Vescan, M. Kunze, P. Gluche, W. Ebert, E. Kohn, A. Bergmaier, and G. Dollinger, Diam. Relat. Mater. **8** (1999) 941.
[16] M. E. Mora-Ramos, Diam. Relat. Mat. **17** (2003) 33.