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Study of the electronic properties of GaAs-based atomic layer doped field effect transistor (ALD-FET) under the influence of hydrostatic pressure

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Based on a Thomas–Fermi envelope function scheme we perform the calculation of the electronic structure of a GaAs atomic layer doped field effect transistors (ALD-FET). We calculate the electronic structure for the device as a function of the involved parameters, in particular we study the effects of the hydrostatic pressure onto the electronic level structure in order to investigate the formation of high conductivity electron channels in such devices. We consider the pressure-induced Γ–X crossover within the conduction band as a possible effect causing the enhancement of the associated two-dimensional carrier densities.

1 Introduction Doping techniques with atomic precision make possible the fabrication of very thin impurity layers within a semiconducting host material. In practice, impurities occupy just a few atomic monolayers in the crystal and they usually distribute following a Gaussian pattern. In first place, one can speak about δ-doped systems if the doping layer width is less than 25 Å. Secondly, one can also refers to the relation between the spatial extension of the wave function and the thickness of the doping profile. In this case, it must be fulfilled that the wave function extension is greater than the width of the doping profile. The first aspect essentially depends upon the growth technique, while the second is mostly associated to the amount of impurities that ionize. Then, it is possible to deal with δ-doped quantum wells if the number of ionized impurities is such that the average electronic orbits overlap thus creating a two-dimensional gas of electrons or holes, according to the donor or acceptor character of the impurity atoms. The combined effect of the electrostatic potentials corresponding to both the doped layer and the electron gas renormalizes the energy band profiles, with the appearance of a confining potential function. In principle, the density of impurities should be equals to the density of carriers. However, this relations does not holds for all values of impurity densities. There always exists certain value of this quantity for which the carrier density ceases to vary. This is mainly due to compensation effects, and it is said that the system is in its saturation limit. Of course, both the limit of δ-doped quantum well creation and the limit of saturation strongly depend on the host material and the type of dopant used. In 1980 Wood et al. [1] began to study the δ-doped systems. The basic technique consists of interrupting the growth process, decreasing its operating temperature. They envisaged that the application of this kind of doping in the fabrication of Field Effect Transistors (FET's) would substantially improve properties like the extrinsic transconductance. Some years later Schubert and Ploog [2] first presented the δ-FET. Among the advantages reported there are the high value of the breakdown gate voltage, the high extrinsic transconductance and the large carrier density.

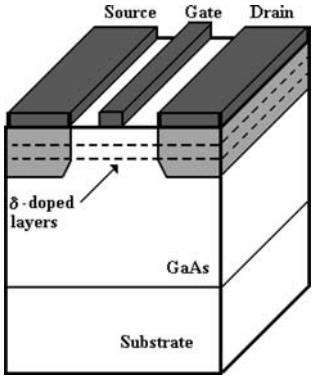

Figure 1 Schematical representation of an ALD-FET in GaAs.

Yamaguchi and coworkers [3] proposed a way to improve the performance of the δ-FET's. It relies in putting a potential barrier in the conduction band, generated through p-type δ-doping, and located a certain distance away from de donor layer. They named this device as Atomic Layer Doped Field Effect Transistor (ALD-FET). The aim of this barrier is to eliminate – as much as possible – the punchthrough between source and drain. Later on, Nakagawa et al. [4] showed that, in fact, the punchthrough is suppressed by the inclusion of the barrier and that the transconductance keeps high. This indicates that such a device is promising as a short-channel FET. It is worth mentioning that the reported ALD-FET transconductance is not larger than the δ-FET one. Nevertheless, the suppression of the punchthrough effect substantially improves the performance of the ALD-FET in comparison with the δ-FET.

The application of hydrostatic pressure to δ-doped quantum wells could positively modify their transport properties by virtue of its influence onto the conduction band electronic structure [5]. This mechanism could also serve to achieve a high density of charge carriers [6]. The systems to consider are diverse: single and double δ-doped quantum wells, electronic devices with δ-doped channels, and so on. Although the study of the pressure effect in this class of systems is relatively new, there are already some experimental reports on the subject [7, 8].

In this work we analyze the electronic structure of the n-type δ-doped quantum-well for an ALD-FET in a GaAs matrix. This device is obtained upon growing two δ-doped quantum-wells (DDQW) which are placed between the source and the drain terminals in a normal field effect transistor, the closest one to the metal–semiconductor interface is n-type and the farther is of p-type (see Fig. 1). We construct a simple model that allow us to study the effect caused by the p-type well on the electronic structure of the n-type well as well as to take into account the influence of the hydrostatic pressure on the electronic structure.

2 Theoretical framework The system we are interested on is formed by a metal–semiconductor contact characterized by the well known Schottky barrier potential. Located in its neighborhood there is a n-type DDQW, typically at 300 Å from the metal semiconductor interface and then a p-type DDQW is grown at an appropriated relative distance $d - d_{\mathrm{p}}$ from the n-type one. This relative distance turns out to be an important element because it represents the confining tool for the electronic states of the n-type DDQW. The general form of the model potential for the conduction band of this device is [9]

$$V(z) = \frac{4\pi}{\varepsilon_{\mathrm{s}}} N_{\mathrm{d}} (z-l)^2 \, \theta(l-z) + \left(V_{\mathrm{n}}(z) + V_{\mathrm{p}}(z)\right) \theta(l_{\mathrm{d}} - z) \,. \tag{1}$$

All quantities in this expression are given in effective atomic units. The first part of the potential function describes the Schottky barrier potential, and uses the so-called depletion approximation with its typical parabolic dependence. Here we find the static dielectric constant, ε_{s}, as well as the characteristic depletion region width, l, which is a function of V_{c} – the Schottky barrier height –, and the background impurity concentration (N_{d})

$$l = \sqrt{\frac{\varepsilon_{\mathrm{s}} V_{\mathrm{c}}}{4\pi N_{\mathrm{d}}}} \,. \tag{2}$$

The second part of the potential model contains the contribution of the two δ-doped quantum-wells. $V_{\mathrm{n}}(z)$ and $V_{\mathrm{p}}(z)$ are, respectively, the self-consistent potential of the n-type well and the one describing the p-type one. Both functions are derived within the local density Thomas–Fermi approximation [10, 11]. The $V_{\mathrm{n}}(z)$ potential is given by

$$V_{\mathrm{n}}(z) = -\frac{\alpha_{\mathrm{n}}^2}{(\alpha_{\mathrm{n}}|z| + z_{0\mathrm{n}})^4} - \frac{\alpha_{\mathrm{n}}}{(\alpha|z| + z_{0\mathrm{n}})^2} \times c\left[1 + \frac{a(\alpha_{\mathrm{n}}|z| + z_{0\mathrm{n}})^2}{\alpha_{\mathrm{n}}} \ln\left(1 + \frac{b\alpha_{\mathrm{n}}}{(\alpha_{\mathrm{n}}|z| + z_{0\mathrm{n}})^2}\right)\right] \tag{3}$$

and represents the combination of Hartree, exchange and correlation contributions in the electron gas [12]. The parameters involved are $\alpha_{\mathrm{n}} = 2/15\pi$, $z_0 = (\alpha_{\mathrm{n}}^3/\pi N_{2\mathrm{d}})^{1/5}$, $a = 0.7734\alpha_{\mathrm{n}}/21$, $b = 21\alpha_{\mathrm{n}}^{-1}$ and $c = 2/\pi$. $N_{2\mathrm{d}}$ is the effective two-dimensional impurity density for the n-type DDQW. Additionally, the potential energy function $V_{\mathrm{p}}(z)$ is derived within the so-called Thomas–Fermi–Dirac approach in which Hartree and exchange contributions for the hole gas are included [13]. It is given by

$$V_{\mathrm{p}}(z) = \frac{\alpha_{\mathrm{p}}^2}{\left(\alpha_{\mathrm{p}}|z - d_{\mathrm{p}}| + z_{0\mathrm{p}}\right)^4} - \frac{2\varsigma^2(w) m_{\mathrm{a}}}{\pi^2} \times \left[1 - \sqrt{1 + \frac{\pi^2}{\varsigma^2(w) m_{\mathrm{a}}} \frac{\alpha_{\mathrm{p}}^2}{\left(\alpha_{\mathrm{p}}|z - d_{\mathrm{p}}| + z_{0\mathrm{p}}\right)^4}}\right], \tag{4}$$

where

$$\alpha_{\mathrm{p}} = \frac{2}{15\pi}\left[1+\left(\frac{m_{\mathrm{lh}}}{m_{\mathrm{hh}}}\right)^{3/2}\right]. \tag{5}$$

Here, the parameters m_{hh} and m_{lh} are the heavy ($0.51m_0$, where m_0 is the free electron mass) and light ($0.082m_0$) hole masses respectively, and d_{p} is the position of the p-type DDQW. In this expression $z_{0\mathrm{p}}$ is

$$z_{0\mathrm{p}} = \left(\frac{\alpha_{\mathrm{p}}^3}{\pi P_{2\mathrm{d}}}\right)^{1/5}. \tag{6}$$

Furthermore, we have

$$\varsigma(w) = 2^{-1/3} + (1-w^2)\left[w^2(\mathrm{d}w+e) + f(4w^3+3w^2+2w+1)\right], \tag{7}$$

with $w = m_{\mathrm{lh}}/m_{\mathrm{hh}}$, $d = 0.679$, $e = -0.0686$, and $f = -0.0811$.

We are here reporting the calculation of the electronic structure for the GaAs ALD-FET and the proposed model permit us to vary a great amount of parameters involved in the device design. For instance, the contact voltage V_{c}, the two dimensional impurity densities of n- and p-type DDWQs, $N_{2\mathrm{d}}$ and $P_{2\mathrm{d}}$, respectively. At the same time, this model also gives us the possibility to investigate the effect of the relative distance between the two DDQW onto the electronic level structure of the n-type DDQW.

To analyze the effects of the hydrostatic pressure (P) on the electronic structure of the system, we choose a typical configuration of the device; that is, we fix the device parameters and consider the pressure dependence for each of the basic input parameters. They are the position of the Γ and X conduction band minima with respect to the top of the valence band, the corresponding effective masses $m_{\Gamma}(P)$ and $m_{\mathrm{X}}(P)$, as well as the dielectric constant $\varepsilon_{\mathrm{s}}(P)$. In fixing the different lengths of the system, we have assumed that their values are kept, absorbing within the modification of the lattice constant by pressure. We analyze the obtained electronic structure and compare it with the case of $P = 0$. The dependencies of the input parameters with P used in the calculation are directly taken from the table listed in Ref. [14]

3 Results and discussion In the calculation of the energy level structure the background impurity density is kept fixed at $N_{\mathrm{d}} = 1.0\times10^{18}$ cm^{-3}. This is an experimentally achieved value and is compatible with depletion region widths, l_{d}, that do not exceed the value of 300 Å, for the usual range of contact potentials of experimental interest; $100\ \mathrm{meV} < V_{\mathrm{c}} < 900\ \mathrm{meV}$. Actually, when $V_{\mathrm{c}} = 900$ meV, we obtain for such concentration the value $l_{\mathrm{d}} = 238$ Å. This ensures the presence of a confined electron gas in the n-type δ-doped QW. The other parameters to be fixed are the two-dimensional impurity densities of both types: $N_{2\mathrm{d}} = 7.5\times10^{12}$ cm^{-2}, which generates a n-type potential well with depth equals to 278.9 meV (at the two-dimensional Brillouin zone center); and $P_{2\mathrm{d}} = 5.0\times10^{13}$ cm^{-2}.

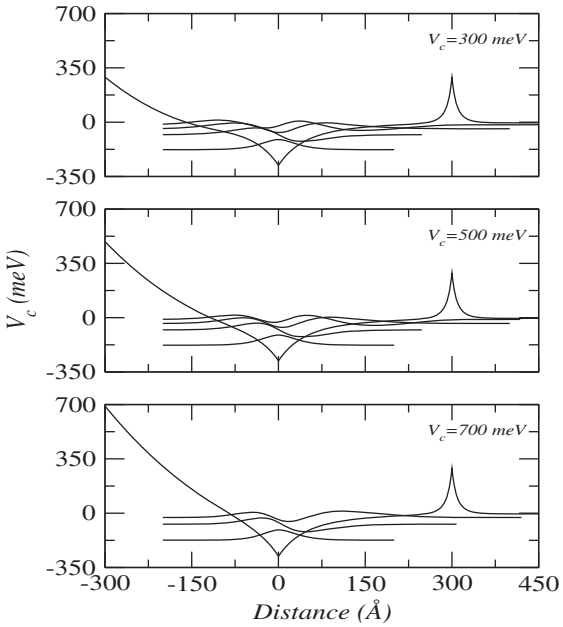

Figure 2 Wave function as a function of the contact potential (V_{c}) for a GaAs ALD-FET. Here the relative distance between wells is fixed to 300 Å and $P = 0$.

Results for the single electron states for a GaAs ALD-FET are shown in Fig. 2 in which the interwell distance is kept constant at $d_{\mathrm{p}} - d = 300$ Å and the contact potential V_{c} varies within the range of experimental interest. We are presenting the behavior of the energy level structure and the corresponding wave functions for $V_{\mathrm{c}} = 300$ meV, 500 meV and, 700 meV. The number of levels in the well tends to decrease for larger values of V_{c}. In addition, Fig. 3 presents the outcome of the energy spectrum calculation with fixed $V_{\mathrm{c}} = 500$ meV and three different values of the relative interwell distance. For $d_{\mathrm{p}} - d = 300, 400$ Å the number of discrete energy levels is four. However, when the relative distance is of 200 Å the highest level escapes from the well keeping only three confined states. This example helps to show that the interwell distance is a parameter that can significantly influence the level structure in the n-type δ-doped well. The energy spectrum observed in Figs. 2 and 3 indicate that modifying input parameters like the contact voltage and the distance between the δ-doped wells can result in significant changes in properties such as the carrier mobility between the device's source and drain.

The previous analysis allows us to select the most appropriate configuration, regarding an optimum value of the interwell distance for a given range of contact potentials. Here we choose a distance of 300 Å. Once the selection for both V_{c} and $d_{\mathrm{p}} - d$ is made, we explore the influence of hydrostatic pressure. It is known that the GaAs becomes an indirect gap material for pressure values very close to

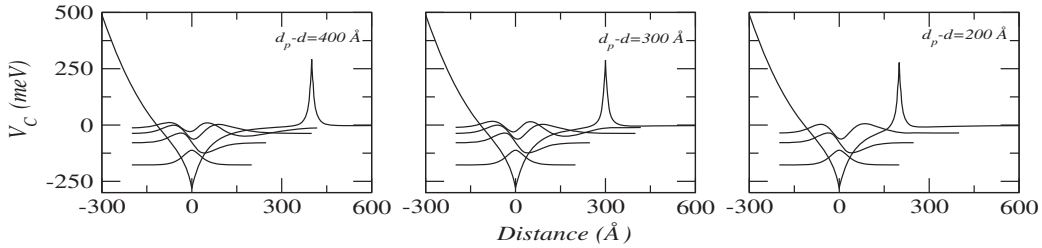

Figure 3 Single electron states in a GaAs ALD-FET as a function of the relative distance between the n- and p-type DDQWs ($d_p - d$) for $P = 0$.

40 kbar and above. In this situation, the conduction band minimum is found at the X-point of the Brillouin zone. As it has been previously shown, for that pressure range the comparison between the DDQW energy level spectra calculated at the Γ-point and at the X-point yields that, for all the values of the impurity densities, the ground state of the n-type δ-doped QW is located precisely at the X-point [6]. If one assumes that the two-dimensional electron gas forms at that specific Brillouin zone position, it immediately follows that the electron system undergoes a transition to a heavier carrier situation. Thus, potential function profile modifies accordingly. In general, it becomes shallower and wider, as can be seen from Fig. 4. Only for high enough pressure values a sufficiently deep well is attained. The number of levels is reducedand, most importantly, the saturation condition is reached for larger values of N_{2d} due to the increase of the effective Bohr radius. All this suggests that a two-dimensional channel with higher conductivities can be associated to the X-point for those values of P.

In Fig. 5 the energy levels in the conduction band are presented for both situations, regarding the position of the true ground state for electrons in the device. That is, when the hydrostatic pressure is below or above the crossover value for which the system becomes of indirect gap. The curves show energy values measured from the correspond

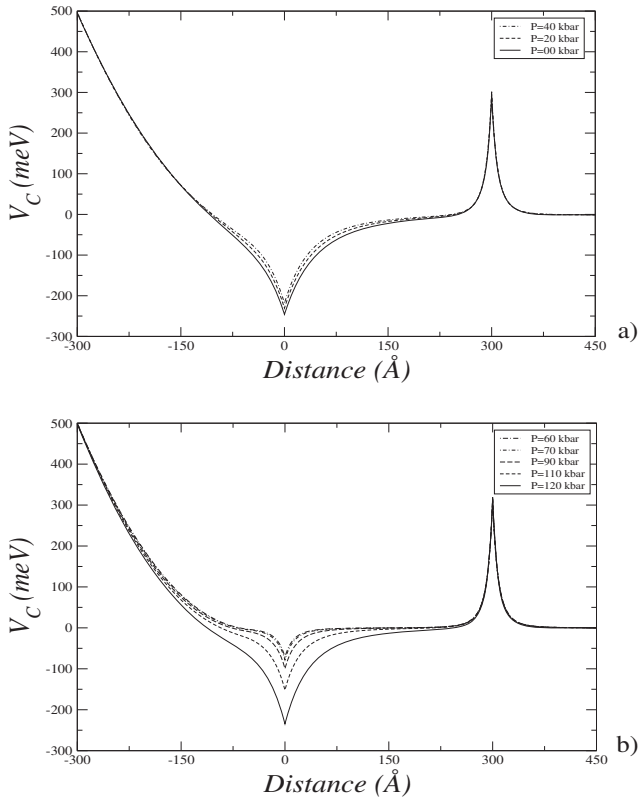

Figure 4 N-type potential well profile in the ALD-FET for different values of the hydrostatic pressure. a) Ground state is located at the Γ-point. b) Ground state is located at the X-point.

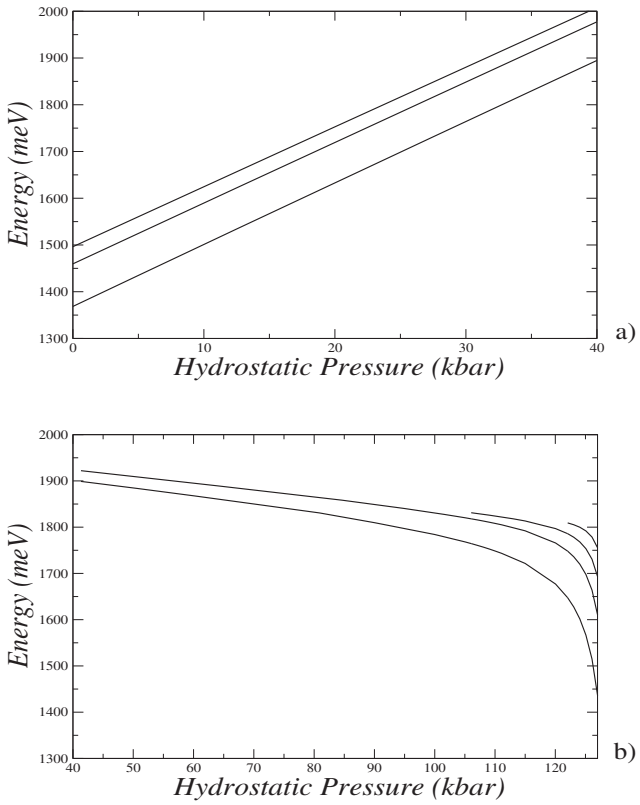

Figure 5 Energy levels in the ALD-FET as functions of the hydrostatic pressure. a) The ground state is located at the Γ-point. b) The ground state is located at the Γ-point.

ing conduction band edge. However, the best picture is obtained when the energy levels refer to the top of the valence band. In Fig. 5(a) $P < 40$ kbar and the conduction band minimum is at Γ. For $P = 0$ we obtain $E_0 = 1368.5$ meV, $E_1 = 1459.57$ meV, and $E_2 = 1496.32$ meV. Well depth is 246 meV. These levels increase linearly and, for a pressure value $P = 35$ kbar the corresponding levels are: $E_0 = 1829.51$ meV, $E_1 = 1913.02$ meV, and $E_2 = 1994.14$ meV, while the quantum well depth is 221 meV. The smaller potential well depth is directly related to the increasing in the effective mass with pressure at that point. Figure 5(b) contains the dependence of the quantum well energy levels upon pressure for beyond the Γ–X crossover of 40 kbar. This is a very interesting region in which it can be seen that the system binds only two levels in the pressure range 40 kbar $< P <$ 105 kbar. An additional level is present for a pressure value of 106 kbar, with the following energy states: $E_0 = 1764.68$ meV, $E_1 = 1818.05$ meV, and $E_2 = 1831.15$ meV, always decreasing, according to the behavior of the X-related band gap. Finally, one finds that for $P = 122$ kbar a fourth energy level is bound: $E_0 = 1647.41$ meV, $E_1 = 1748.14$ meV, $E_2 = 1785.91$ meV, and $E_3 = 1809.22$ meV. Another interesting fact is that a nonlinear dependence of the energy levels upon pressure begins to show above $P = 110$ kbar.

4 Conclusions We present results for the electronic level structure of GaAs-based ALD-FET as a function of the hydrostatic pressure. For $0 < P < 40$ kbar well's shape does not significantly change, and the energy levels increase linearly with P. In the case when $P \geq 40$ kbar, within the indirect gap regime, the potential shape is greatly modified allowing the appearance of additional bound states for high enough pressure values, while their behavior as a function of the pressure is clearly non-linear above $P = 110$ kbar. A rather similar behavior has been previously found in the case of GaAs δ-doped field effect transistors [15].

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