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Thomas–Fermi–Dirac theory of the hole gas of a double p-type δ-doped GaAs quantum wells

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Abstract

We present the hole subband structure of two coupled p-type δ-doped GaAs quantum wells as a function of the impurity concentration and the distance l between them, including exchange effects. We present an analytical expression for the Hartree–Fock potential as a function of these two magnitudes, by using the Thomas–Fermi–Dirac approximation. The numerical results for a double Be-δ-doped GaAs quantum well show that many body effects are important when the concentration is low and the energy levels are degenerate for $l \geqslant 100$ Å and an impurity concentration of 5×10^{12} cm^{-2}, while without exchange effects the energy levels are degenerated for $l \geqslant 150$ Å and the same impurity concentration. We present an expression for the relative electronic mobility, that is, we calculate the ratio of the electronic mobility of a double δ-doped quantum well and that of a simple δ-doped quantum well. The theoretical results agree quite well with the experimental data available.

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1. Introduction

The Thomas–Fermi–Dirac (TFD) theory is the generalisation of the Thomas–Fermi approximation when the many body effects are considered through an exchange potential. This theory is known in the literature and has been applied to free atoms [1]. Briefly, it does not lead to a self-consistent (SC) solution in which the electron density $n(\mathbf{r})$ either tends to zero at infinity for the neutral atom, nor indeed a solution of finite radius in which the boundary density is zero. Rather, when used for neutral atoms, there is inevitably a discontinuity in $n(\mathbf{r})$ at the boundary of the atom which is manifestly unsatisfactory [1]. If we were to use the same theory, to describe the conduction band bending of a semiconductor quantum system caused by an electric charge in some region of the space, exactly the same thing would happen. However, when the

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charge in question involves holes, things are completely different, because the effective masses are negative and this avoids the algebraic origin of these problems [1]. As we will see further on, in this case, the solution which is obtained is SC and satisfactory.

Several papers have been published where double and triple δ-doped GaAs structures were investigated in order to obtain higher conductivity for field effect transistor (FET) applications [2–6]. On the other hand there are only a few papers with theoretical results about this kind of systems [7,8].

The present work is intended to provide a procedure for the calculation of the energy levels in double p-type δ-doped quantum wells along the lines of the TFD theory.

δ-Doped GaAs:Si/$Al_{0.33}Ga_{0.67}As$ double heterostructures have been grown [6] and it has been observed that increasing the optical power density the band bending due to surface trap states is essentially removed. Photoluminescence (PL) spectroscopy and electric-field-induced Raman scattering have been used to study the effect of photoexcitation on the surface electric field due to surface trap states. Upon variation of the optical power density over four orders of magnitude a continuous reduction of the surface electric field is found for increasing continuous wave illumination. This is evidently due to recombination of electrons at the doping layer with photogenerated holes localized at the topmost heterointerface. For the highest power densities of 103 W/cm^2 the electric field at that interface becomes almost zero indicating that band bending due to surface trap states is removed.

A double δ-doped (DDD) heterostructure employing symmetric graded InGaAs quantum wells as the active channel grown by low-pressure metalorganic chemical vapor deposition (LP-MOCVD) has been fabricated [3]. It was found that symmetrically graded InGaAs pseudomorphic structure manifests significantly improved electron mobility as high as 5300 (26 000) cm^2/V s at 300 (77) K due to superior confinement and to the lower interface roughness scattering at GaAs/InGaAs heterointerfaces.

A double n-type Si δ-doped GaAs system has been grown [4] and the electron transport properties were studied as function of the impurity concentration and the distance between the layers. It was found that a maximum in the conductivity appears for a thickness around 200 Å which exceeds by 20% at 77 K the conductivity of a single δ-doped (SDD) layer with the same concentration. Due to low sheet concentration the advantage of the high mobility of the SDD layer is not so useful for practical FET application as an increase in the conductivity of the DDD structures.

A theoretical study of transport properties in two coupled δ layers was reported in [8]. The quantum mobility was calculated numerically for Si δ-doped GaAs systems and the effect of coupling the two δ layers was investigated. It was found that the electron mobility increased from two to five times over that of a SDD case. It is clear that there are differences when compared to the experimental results of [4], and some further study is needed.

In Section 2 we present the TFD approximation for the inhomogeneous hole gas of two p-type δ-doped quantum wells. Results are presented in Section 3. Conclusions are presented in Section 4.

2. The Thomas–Fermi–Dirac approximation

The energy functional in our particular case is given by [9]

$$E_{\mathrm{TFD}} = \frac{3}{10m_{\mathrm{ed}}}\int n(z)[3\pi^2\hbar^3 n(z)]^{2/3}\,\mathrm{d}z - \frac{e^2\pi}{\varepsilon_r}\int\int n(z')n(z)|z-z'|\,\mathrm{d}z\,\mathrm{d}z' - \varsigma(w)\frac{3a_0^*}{2\pi}(3\pi^2)^{1/3}R_y^* \times \int n(z)^{4/3}\,\mathrm{d}z + \frac{2\pi e^2}{\epsilon_r}\left\{p_{2\mathrm{D}}^1\int n(z)|z+l/2|\,\mathrm{d}z + p_{2\mathrm{D}}^2\int n(z)|z-l/2|\,\mathrm{d}z\right\} \tag{1}$$

where $n(z)$ is the concentration of holes, $p_{2\mathrm{D}}^1(p_{2\mathrm{D}}^2)$ is the two-dimensional impurity concentration of the first (second) δ-doped quantum well, $m_{\mathrm{ed}} = m_{hh}[1+(m_{lh}/m_{hh})^{3/2}]^{2/3} \equiv m_{hh}m_a$,

$$\varsigma(w) = 2^{-1/3} + (1 - w^2)[w^2(aw + b) + c(4w^3 + 3w^2 + 2w + 1)]$$

(with $a = 0.679$, $b = -0.0686$, $c = 1/4 + 3\pi^2/64 - 2^{-1/3} \approx -0.0811$, and $w = \sqrt{m_{lh}/m_{hh}}$), $R_y^* = e^2/(2\varepsilon_r a_0^*)$ and $a_0^* = \varepsilon_r \hbar^2/(e^2 m_{hh})$ [10].

The variational principle leads to $\delta(E_{\mathrm{TFD}} - \mu N) = 0$ with $N = \int n(z)\,\mathrm{d}z$ and μ is the Lagrange multiplier. Calculating the variational by the standard procedure we find (taking $n_{au}(\mathbf{r}) = (a_0^*)^3 n(\mathbf{r})$)

$$\mu = \left[\frac{3\pi^2 n_{au}(\mathbf{r})}{m_a^{3/2}}\right]^{2/3} R_y^* + V_H - \varsigma(w)\frac{2}{\pi}(3\pi^2)^{1/3} n_{au}(\mathbf{r})^{1/3} R_y^* \tag{2}$$

Thus,

$$n_{au}(\mathbf{r}) = m_a^3 \frac{1}{3\pi^5}\left[\varsigma(w) - \sqrt{\varsigma^2(w) + \pi^2 \frac{\mu^* - V_H^*(\mathbf{r})}{m_a}}\right]^3 \tag{3}$$

In this case, using Eq. (3), we can calculate the exchange potential as a function of the Hartree potential. It was found in this case [10]

$$V_x(\mathbf{r}) = -\varsigma(w)\frac{2}{\pi}(3\pi^2)^{1/3} n_{au}(\mathbf{r})^{1/3} R_y^* \tag{4}$$

and substituting (3) in (4) ($V_H^*(\mathbf{r}) = V_H(\mathbf{r})/R_y^*$, $\mu^* = \mu/R_y^*$), we obtain

$$V_x^*(\mathbf{r}) = -\frac{2\varsigma(w) m_a}{\pi^2}\left[\varsigma(w) - \sqrt{\varsigma^2(w) + \pi^2 \frac{\mu^* - V_H^*(\mathbf{r})}{m_a}}\right] \tag{5}$$

where $V_x^*(\mathbf{r}) = V_x(\mathbf{r})/R_y^*$. That is, we are supposing that the presence of the exchange modifies the level structure and the charge density, but we discard changes in the form of the Hartree potential due to the presence of the exchange.

If we assume that the impurity concentration is the same in both wells, the system is symmetric with respect to the central point, the potential is an even function and we can restrict ourselves to any half-space. Then, for $z \leqslant 0$

$$\frac{\mathrm{d}^2 V_H^*(\mathbf{r})}{\mathrm{d}z_{au}^2} = -m_a^3 \frac{8}{3\pi^4}\left[\varsigma(w) - \sqrt{\varsigma^2(w) + \pi^2 \frac{\mu^* - V_H^*(\mathbf{r})}{m_a}}\right]^3 + \frac{4\pi e^2}{\epsilon_r} p_{2\mathrm{D}}^1 \delta(z + l/2) \tag{6}$$

For this type of equations, a solution of the form $1/f^4(z)$, where $f(z)$ must be a linear function of z, was proposed in [7]. Due to the presence of the δ function, the specific form in this case is

$$V_H^*(z) - \mu^* = -\frac{\alpha^2}{(\alpha|z + l/2| + z_0)^4} \tag{7}$$

where $\alpha = 2m_a^{3/2}/15\pi$ and $z_0 = (\alpha^3/\pi p_{2\mathrm{D}}^{au})^{1/5}$.

Thus, the charge density will be

$$n_{au}(\mathbf{r}) = \frac{m_a^3}{3\pi^5}\left[\varsigma(w) - \sqrt{\varsigma^2(w) + \frac{\pi^2}{m_a}\frac{\alpha^2}{(\alpha|z + l/2| + z_0)^4}}\right]^3 \tag{8}$$

Then the total potential, $V(z) = V_H(z) + V_x(z)$, is

$$V^*(z) = -\frac{\alpha^2}{(\alpha|z+l/2|+z_0)^4} - \frac{2\varsigma^2(w)m_a}{\pi^2}\left[1 - \sqrt{1 + \frac{\pi^2}{\varsigma^2(w)m_a}\frac{\alpha^2}{(\alpha|z+l/2|+z_0)^4}}\right] \tag{9}$$

Eq. (9) summarizes the proposed model for the total potential of p δ-doped quantum wells. One of its advantages is that of avoiding carrying out long SC calculations. With this potential it is possible to solve in a simpler way than in a full SC calculation, two uncoupled Schrödinger-like equations with corresponding ladders of hole subbands. The eigenvalues and eigenfunctions thus obtained are the eigenvalues and eigenfunctions in the Hartree–Fock approximation. They constitute the starting point for LDOS and mobility calculations.

Based on this approximation to the SC solutions of the electronic structure and the wave functions, we study the electron transport properties of the system. In the calculation, only the scattering by ionized acceptors in the doped layers is considered, because it is the most important scattering mechanism at low temperature. We consider the Coulomb scattering potential due to ionized impurities, distributed randomly in the doped layer. As pointed before, the issue is to know if the mobility of the DDD is higher than that of the SDD. If the experimental conditions are the same, we have using the Fermi gold rule (the bands are parabolic)

$$\mu_{\mathrm{rel}}^{\delta} = \frac{\mu_{\mathrm{DDD}}}{\mu_{\mathrm{SDD}}} = \frac{\int\int \rho_{\mathrm{e}}^{\delta}(z')\rho_{\mathrm{imp}}^{\delta}(z)|z-z'|\,\mathrm{d}z\,\mathrm{d}z'}{\int\int \rho_{\mathrm{e}}^{2\delta}(z')\rho_{\mathrm{imp}}^{2\delta}(z)|z-z'|\,\mathrm{d}z\,\mathrm{d}z'}, \tag{10}$$

where $\rho_{\mathrm{e}}^{\delta}(z')$ ($\rho_{\mathrm{e}}^{2\delta}(z')$) is the electron density in the SDD (DDD) and $\rho_{\mathrm{imp}}^{\delta}(z)$ ($\rho_{\mathrm{imp}}^{2\delta}(z)$) is the impurity density in the SDD (DDD). The former expression can be put in the following form

$$\mu_{\mathrm{rel}}^{\delta} = \frac{\sum_{i=1}^{n}\int\int |F_{\mathrm{e}}^{\delta}(z')|^2(k_{\mathrm{F}}^{\delta} - E_i^{\delta})p_{2\mathrm{D}}\delta(z)|z-z'|\,\mathrm{d}z\,\mathrm{d}z'}{\sum_{i=1}^{n}\int\int |F_{\mathrm{e}}^{2\delta}(z')|^2(k_{\mathrm{F}}^{2\delta} - E_i^{2\delta})p_{2\mathrm{D}}(\delta(z+l/2)+\delta(z-l/2))|z-z'|\,\mathrm{d}z\,\mathrm{d}z'} \tag{11}$$

$$\mu_{\mathrm{rel}}^{\delta} = \frac{\sum_{i=1}^{n}\int |F_{\mathrm{e}}^{\delta}(z')|^2(k_{\mathrm{F}}^{\delta} - E_i^{\delta})|z'|\,\mathrm{d}z'}{\sum_{i=1}^{n}\int |F_{\mathrm{e}}^{2\delta}(z')|^2(k_{\mathrm{F}}^{2\delta} - E_i^{2\delta})(|z'-l/2|+|z'+l/2|)\,\mathrm{d}z'} \tag{12}$$

where $F_{\mathrm{e}}^{\delta}(z')$, k_{F}^{δ} and E_i^{δ} ($F_{\mathrm{e}}^{2\delta}(z')$, $k_{\mathrm{F}}^{2\delta}$ and $E_i^{2\delta}$) are the envelope function, the Fermi level and the ith level respectively of the SDD (of the DDD). The important thing is to find the optimum distance parameter in order to obtain the maximum mobility.

The former expressions are valid for $T = 0$ K. In [11] the variation with the temperature of the Fermi level and some of the eigenvalues measured from the band bottom, has been shown. According to these results this kind of systems is slightly modified when the temperature is equal or less than 6 meV (≈77 K). However, the levels change significantly for higher temperatures. Therefore, for temperatures less than 6 meV the electronic structure of the system can be taken as that corresponding to 0 K. The thermal effect can be seen as a charge redistribution. Under these assumptions the mobility expression would be

$$\mu_{\mathrm{rel}}^{\delta} = \frac{\sum_{i=1}^{n}\int |F_{\mathrm{e}}^{\delta}(z')|^2 k_{\mathrm{B}}T\ln\left[1+\exp\left(\frac{k_{\mathrm{F}}^{\delta}-E_i^{\delta}}{k_{\mathrm{B}}T}\right)\right]|z'|\,\mathrm{d}z'}{\sum_{i=1}^{n}\int |F_{\mathrm{e}}^{2\delta}(z')|^2 k_{\mathrm{B}}T\ln\left[1+\exp\left(\frac{k_{\mathrm{F}}^{2\delta}-E_i^{2\delta}}{k_{\mathrm{B}}T}\right)\right](|z'-l/2|+|z'+l/2|)\,\mathrm{d}z'} \tag{13}$$

3. Results and discussion

We shall use our simple formulas to analyze different experimental situations concerning single and double delta doped quantum wells. The assumptions in our theoretical scheme will not fully cover all the

range of characteristics of the different experiments, but our scheme provides a simple and reasonable basis for the different experimental setups. The following input parameters: $m^*_{hh} = 0.52m_0$, $m^*_{lh} = 0.087m_0$, $\epsilon_r = 12.5$, $\zeta(w) = 0.6476$, and 2×10^{12} cm^2 $< p_{2D} < 1 \times 10^{14}$ cm^{-2} are typically used for GaAs, where m_0 is the free electron mass, and they will be employed in our calculations.

In Fig. 1a and b we present the potential profile and eigenfunctions, normalized to 1, for two different values of the distance between the impurity planes, $l = 50$ Å and $l = 100$ Å, respectively. Notice the kink at $z = 0$ due to the approximations made. This has no relevance for the outputs since the peak is in a depleted region.

In Fig. 2a and b we show the dependence of the first energy levels versus the distance between the impurity planes for two typical hole concentrations found in experiments, $p_{2D} = 1 \times 10^{12}$ and 1×10^{13} cm^{-2}, including exchange effects. The trends are similar for both concentrations. As expected the exchange effects are significant when the concentration is lower and as we can see Fig. 2 reveals that when we consider exchange effects the first energy level becomes degenerate for distances around 200 and 75 Å for the concentrations mentioned above. A similar thing happens for the other levels, depending on the concentration and on which level is observed. On the other hand when we omit the many body effects the first

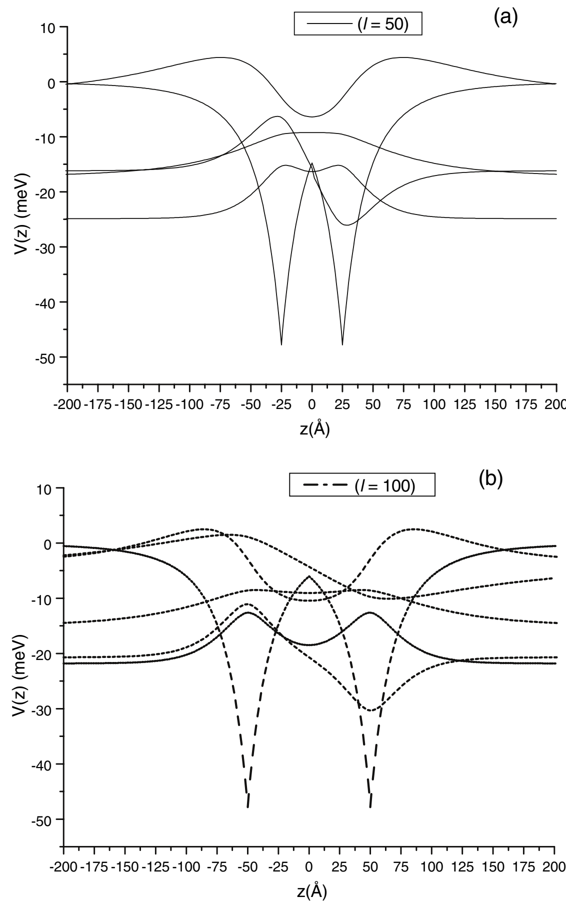

Fig. 1. Potential profiles and eigenfunctions, normalized to 1, for a double Be-δ-doped GaAs quantum well for different values of the distance between the planes: (a) $l = 50$ Å, (b) $l = 100$ Å, and for a given impurity density ($p_{2D} = 1 \times 10^{13}$ cm^{-2}). $V(z)$ is in meV, z in Å.

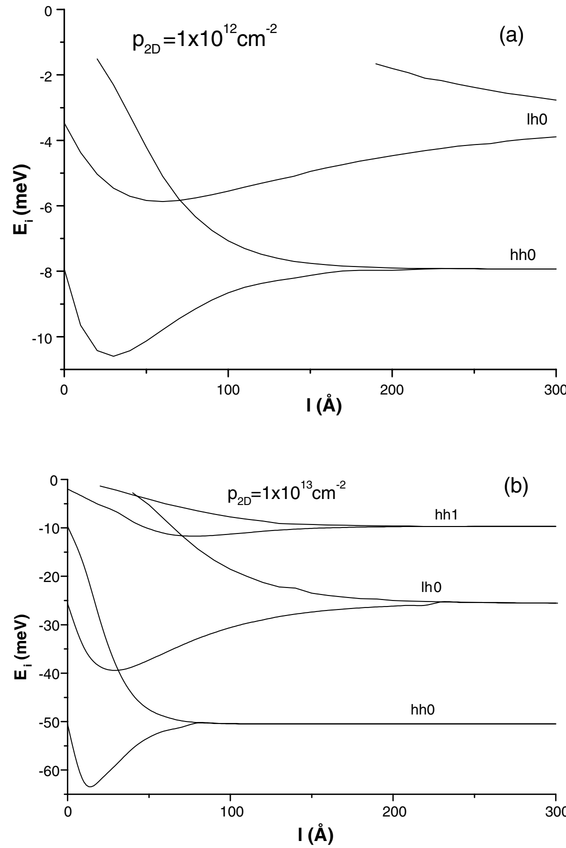

Fig. 2. Energy levels (in meV) of a double Be-δ-doped GaAs quantum well for (a) $p_{2D} = 1 \times 10^{12}$ cm^{-2} and (b) $p_{2D} = 1 \times 10^{13}$ cm^{-2}, versus the distance between the planes (in Å) considering exchange effects.

energy levels become degenerate for distances around 260 and 100 Å for the same concentrations as before. Beyond these distance values the wells can be considered as isolated. This distance diminishes as the concentration grows, and its value for the first level is lower than for the other ones.

Wagner et al. [12] have grown $Al_{1-x}Ga_xAs/GaAs/Al_{1-x}Ga_xAs$ quantum wells and doped the GaAs layer with Be with an intended dopand density of 8×10^{12} cm^{-2}. They measured the doping spike width by secondary ion mass spectroscopy and it was found to be less than 10 nm. Recombination between different hole subbands was assigned to the two emission peaks observed. They found a subband separation of 36 meV. Although our calculations ($l = 0$) refers to a simpler system, we find an energy difference between the first and second hh levels of 37 meV.

Damen et al. [13] have grown Be δ-doped GaAs quantum wells with p-doping density in the range from 6×10^{12} to 2×10^{14} cm^{-2}. They observed that only two levels exist and the Fermi energy is close to the last one, for an impurity concentration of 6×10^{12} cm^{-2}. Besides the energy difference between the Fermi and basic levels is approximately 22 meV. In our calculations ($l = 0$) the difference between the Fermi and basic levels is about 26 meV.

Richards et al. [14] have studied the PL spectroscopy for a quasi-two-dimensional hole gas formed by a Be-δ-doped GaAs quantum well system. They obtained also theoretical results for subband energies, by means of a SC calculation, for an impurity density of 8×10^{12} cm^{-2} and with a dopand spread of 2 nm. Their

SC calculations give a value of approximately 15.1 meV for the difference $E_{hh0} - E_{lh0}$. According to the PL spectroscopy measurements the difference is $\simeq$19 meV. In our calculations ($l = 0$) the spacing level is 20 meV approximately. For 3×10^{12} cm^{-2} the PL result is $E_{hh0} - E_{lh0} \simeq 11$ meV, whereas in our calculations ($l = 0$) for the same impurity concentration we obtain a difference of 14 meV approximately.

Sipahi et al. [15] studied PL spectroscopy in p-type Be δ-doped GaAs layers for 3×10^{12} cm^{-2} (8×10^{12} cm^{-2}), obtaining two peaks around 1.499 and 1.487 eV (1.498 and 1.481 eV). Then $E_{hh0} - E_{lh0} \simeq 12$ meV ($E_{hh0} - E_{lh0} \simeq 17$ meV). Within the TFD approximation we obtained ($l = 0$) $E_{hh0} - E_{lh0} \simeq 10.2$ meV ($E_{hh0} - E_{lh0} \simeq 19.7$ meV).

Gilinsky et al. [16] showed the PL spectrum in p-type Be δ-doped GaAs layers for 4×10^{12}, 1.8×10^{13} and 3.6×10^{13} cm^{-2}, obtaining $E_{hh0} - E_{lh0} \simeq 8$, 20 and 30 meV respectively. Through the TFD approximation ($l = 0$) we obtain $E_{hh0} - E_{lh0} \simeq 12.5$, 35 and 55 meV. The discrepancy, as we can see for the higher impurity concentrations, can be due to the impurity spreading.

Gurtovoi et al. [4] have grown a double n-type Si δ-doped GaAs system and studied the electron transport properties as a function of the impurity concentration and the distance between the layers. They observed a maximum of the mobility for a thickness around 200 Å which exceeds by 20% at 77 K the conductivity of a SDD layer with the same concentration. The mobility of the SDD layer is the highest of all studied samples, but due to low sheet concentration the advantage of high mobility is not so useful for practical FET applications as an increase in the conductivity of the DDD structures. For a 100 Å separation they observed a mobility lower by a 25% than in the SDD case. Even when we study p-type δ-doped quantum wells, qualitative differences are not expected with respect to n-type quantum wells of [4]. By using Eq. (13) we obtain the mobility of Fig. 3, for $T = 0$ K and $T = 6$ meV (~77 K), where we can see a maximum in the mobility for a thickness around 200 Å, in reasonable agreement with the experiment. Nevertheless in our results this is lower than in the SDD. The minimum is obtained for a separation of 50 Å, but for a separation of 100 Å ($T = 6$ meV) the mobility is 25% lower than that of the SDD. There are not, to our knowledge, equivalent studies like this one for double p-type δ-doped wells. We think that there must not be important qualitative differences between both situations, and because of this we have applied our scheme for double p-type δ-doped wells directly. The agreement with experimental results is good, thus lending support to this hypothesis.

Sheih el al. [5] obtained a decrease of the mobility for a 50 Å separation in a DDD with respect to that of a SDD, in agreement with our calculations.

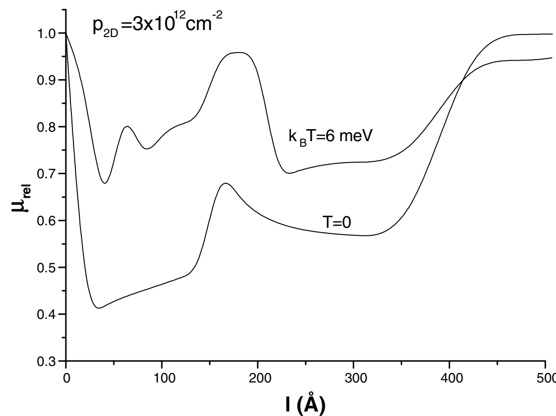

Fig. 3. Mobility of a double Be-δ-doped GaAs quantum well for $p_{2D} = 3\times10^{12}$ cm^{-2} and $T = 0$ ($T = 77$ K).

4. Conclusions

We have studied here the hole subband of two coupled p-type δ-doped GaAs quantum wells, as a function of the impurity concentration and the distance between them, including exchange effects. We have used the TFD approximation and we have obtained an analytical expression for the Hartree–Fock potential as a function of the former two magnitudes. We have applied this formula to different calculations covering several of the samples experimentally grown and the corresponding experimental data. The two Be-δ-doped GaAs quantum wells considering exchange effects reveals that when the concentration is lower its importance is greater. Comparing our results with and without many body effects we found that the double delta doped quantum well behaves as two single and non-coupled wells for distances around 100 ($p_{2D} = 1 \times 10^{12}$ cm^{-2}) and 75 Å ($p_{2D} = 1 \times 10^{13}$ cm^{-2}) with exchange, and around 150 and 100 Å without exchange for the same concentration. Thus the exchange effects are important in the treatment of the two Be-δ-delta doped GaAs quantum wells. There is not much experimental work on double δ wells in the literature. This could be due to the fact that the samples are grown with a considerable distance between the wells, and then the two δ-doped quantum wells behave as two single and non-coupled wells, and because at such distances the diffusion effects are very important. This could lead, probably, to observe no qualitative differences in the absorption peaks respect to isolated Be-δ-doped GaAs quantum wells.

We have presented an expression to calculate the relative electronic mobility. In this way it is possible to compare in a reasonable way the mobilities of the SDD and DDD quantum wells having similar material, doping, etc., experimental characteristics. The difference between these systems lies in the interaction between the δ-doped layers of impurities and the electron gas. It is very important, face to possible applications, to know which system has the higher mobility. Using this kind of expression it is very easy to study the range of parameters governing this problem and to get the best choice of them. The generalization of the expression to other kind of systems with similar features is immediate. The agreement with the experimental data available shows the usefulness of the expression here obtained.

As a final conclusion of the present work, it is possible to say that TFD calculations for the hole subband in double Be-δ-doped GaAs quantum wells provide a rather simple way of obtaining valuable information, in comparison with other approaches. If more sophisticated calculations are needed, the potential here obtained can be used as a starting potential for self-consistency.

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