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Thomas-Fermi approximation in p-type δ-doped quantum wells of GaAs and Si

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Thomas-Fermi calculations of the hole subband structure in p-type δ-doped Si and GaAs quantum wells are carried out for different values of impurity concentration. Results are compared with previous self-consistent calculations and with some experimental reports, and very good agreement is found. In particular, the result of hole ground level from this model is exactly equal to the value reported for the experimental system with the smallest impurity spreading that has been achieved. [S0163-1829(98)04507-X]

I. INTRODUCTION

In recent years, as a natural development of the increasing precision of modern molecular-beam-epitaxy growth techniques, the doping of semiconductors down to atomic resolution (δ-doping) has become possible. Work on δ-doped structures was initially on n-type structures, and has allowed one to study the subband spectra and mobilities of these systems through electrical and optical measurements.[1–4]

p-type δ-doped GaAs quantum wells can be made with Be, Si-acceptor, and C layers.[5–8] They are suitable systems for the study of the physics at extremely high carrier densities, and for potential technological applications (δ-FET,[2,9,10] ALD-FET,[11] etc.).

Another system of this kind, which is only beginning to be investigated, is the p-δ-doped Si quantum well. For instance, the B-δ-doped Si quantum well features a situation where the interesting extremum of the band structure is localized at the Γ point of the Brillouin zone, for the valence band. This situation is the same as the one that occurs in the p-type δ-doped GaAs quantum well, and is exploited in recent self-consistent (SC) calculations of the electronic states in both systems.[12–14]

The use of the Thomas-Fermi (TF) approximation to calculate the energy spectrum in n-type δ-doped quantum wells was presented for the first time by Ioriatti.[15] That work turned out to be of great importance because for a self-consistent, analytically expressed, potential was presented, providing a very useful tool for the theoretical and experimental study of those kinds of systems. This potential arises in the framework of a quasiclassical approximation as the Thomas-Fermi equation results to be, and it directly comes from the simultaneous solution of both the Poisson and Schrödinger equations.

The present work is intended to provide a procedure for the calculation of the energy levels in p-type δ-doped quantum wells along the lines of the TF approximation, for both Si and GaAs. This reveals to be a simpler way, alternative to the self-consistent calculations and, as shall be seen in this paper, it gives very good results in some cases.

II. MODEL

Here and henceforth we assume to be in the low-temperature limit. In an ideal, uniform electron gas, the number of electrons per unit volume is

$$n=\frac{2}{(2\pi)^3}\,\frac{4\pi}{3}\,\frac{p_F^3}{\hbar^3}=\frac{1}{3\pi^2}\,\frac{p_F^3}{\hbar^3},\tag{1}$$

where p_F is the radius of the Fermi sphere in the momentum space. If we consider the gas as locally homogeneous, i.e., that the ideal gas approximation be valid at each point, then

$$n(\vec{r})=\frac{1}{3\pi^2}\,\frac{p_F^3(\vec{r})}{\hbar^3}.\tag{2}$$

The probability $I_r(\vec{p})d\vec{p}$, that the momentum of the electron has a value between p and $p+dp$, is

$$I_r(\vec{p})d\vec{p}=\frac{4\pi p^2dp}{4/3\pi p_F^3}\,\theta(p_F-p).\tag{3}$$

If the light-hole (lh) and heavy-hole (hh) bands are considered as independent bands, the kinetic energy for a single hole can be written as[16]

$$t=\frac{\left[1+\left(\frac{m_{\rm lh}}{m_{\rm hh}}\right)^{3/2}\right]^{-2/3}}{2\pi^2m_{\rm hh}\hbar^3}\int_0^{p_F}p^4dp$$
$$=\frac{[3\pi^2\hbar^3n(r)]^{5/3}\left[1+\left(\frac{m_{\rm lh}}{m_{\rm hh}}\right)^{3/2}\right]^{-2/3}}{10\pi^2m_{\rm hh}\hbar^3}.\tag{4}$$

In the above expression, $m_{\rm lh}$ and $m_{\rm hh}$ are, respectively, the effective band mass of the light holes and the effective band mass of the heavy holes.

The kinetic energy functional is

$$T=\int t\,d\vec{r}=\frac{3\left[1+\left(\frac{m_{\mathrm{lh}}}{m_{\mathrm{hh}}}\right)^{3/2}\right]^{-2/3}}{10m_{\mathrm{hh}}}\int n(z)[3\pi^2\hbar^3 n(z)]^{2/3}dz. \tag{5}$$

The potential energy associated with the interaction between the electron gas and the plane of impurities is described by the following functional of the density,

$$V_{en}=\int n(r)V_N(r)dr=\frac{2\pi e^2}{\epsilon_r}n_{\mathrm{2D}}\int n(z)|z|dz, \tag{6}$$

and the energy functional which corresponds to the electron-electron interaction is

$$V_{\mathrm{ee}}=\frac{e^2}{2\epsilon_r}\int\int\frac{n(\vec{r}\,')n(\vec{r})}{|\vec{r}-\vec{r}\,'|}d\vec{r}\,d\vec{r}\,'. \tag{7}$$

Here it is assumed that the electrons are in a homogeneous medium of dielectric constant ϵ_r (the so-called *hydrogenic model*).

Going over polar coordinates and taking the limit of infinite radius, the expression for the potential energy functional is written as (if the term corresponding to the energy associated to electron self-interaction is neglected)

$$V_{\mathrm{ee}}=\frac{\pi e^2}{\epsilon_r}\int\int n(z)n(z')|z-z'|dz\,dz'. \tag{8}$$

Therefore, the TF energy-density functional is given by

$$\begin{aligned}E_{\mathrm{TF}}=&\frac{3\left[1+\left(\frac{m_{\mathrm{lh}}}{m_{\mathrm{hh}}}\right)^{3/2}\right]^{-2/3}}{10m_{\mathrm{hh}}}\int n(z)[3\pi^2\hbar^3 n(z)]^{2/3}dz\\&+\frac{2\pi e^2}{\epsilon_r}n_{\mathrm{2D}}\int n(z)|z|dz\\&-\frac{\pi e^2}{\epsilon_r}\int\int n(z)n(z')|z-z'|dz\,dz'.\end{aligned} \tag{9}$$

As it is known from TF density-functional theory, the functional derivative of E_{TF} with respect to the density is identified with the chemical potential

$$\begin{aligned}\mu=&\frac{\left[1+\left(\frac{m_{\mathrm{lh}}}{m_{\mathrm{hh}}}\right)^{3/2}\right]^{-2/3}}{m_{\mathrm{hh}}}[3\pi^2\hbar^3 n(z)]^{2/3}+\frac{2\pi e^2}{\epsilon_r}n_{\mathrm{2D}}|z|\\&-\frac{2\pi e^2}{\epsilon_r}\int n(z)|z-z'|dz.\end{aligned} \tag{10}$$

The spatial band bending is described by a Poisson equation

$$\frac{d^2V(z)}{dz^2}=-\frac{4\pi e}{\epsilon_r}n(z)+\frac{4\pi e}{\epsilon_r}n_{\mathrm{2D}}\delta(z); \tag{11}$$

then

$$V(z)=\frac{2\pi e^2}{\epsilon_r}n_{\mathrm{2D}}|z|-\frac{2\pi e^2}{\epsilon_r}\int n(z')|z-z'|dz'. \tag{12}$$

So it is possible to write

$$\mu=\frac{1}{m_{\mathrm{hh}}}[3\pi^2\hbar^3 n(z)]^{2/3}+V(z), \tag{13}$$

and, with the use of Eq. (13) in Eq. (11), we finally arrive at the differential equation for $V(z)$:

$$\begin{aligned}\frac{d^2V(z)}{dz^2}=&-\frac{4e^2}{\epsilon_r}\frac{m_{\mathrm{hh}}^{3/2}\left[1+\left(\frac{m_{\mathrm{lh}}}{m_{\mathrm{hh}}}\right)^{3/2}\right]}{3\pi\hbar^3}[\mu-V(z)]^{3/2}\\&+\frac{4\pi e^2}{\epsilon_r}n_{\mathrm{2D}}\delta(z).\end{aligned} \tag{14}$$

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

$$V(z)-\mu=-\frac{\alpha^2}{(\alpha|z|+z_0)^4}, \tag{15}$$

and the substitution in Eq. (14) gives

$$\alpha=\frac{e^2}{\epsilon_r}\frac{m_{\mathrm{hh}}^{3/2}\left[1+\left(\frac{m_{\mathrm{lh}}}{m_{\mathrm{hh}}}\right)^{3/2}\right]}{15\pi\hbar^3}. \tag{16}$$

If the system is required to be neutral, it is obtained for z_0:

$$z_0=\left(\frac{2\epsilon_r^2\alpha^3}{\pi e n_{2D}}\right)^{1/5}. \tag{17}$$

Expressions (15)–(17) resume the results of the model. With the use of the TF potential $V(z)$ obtained above, a Schrödinger wave equation is numerically solved in order to look for the energy levels in the well.

III. RESULTS AND DISCUSSION

In our model, μ is assumed to be very close to the band. This is something that is verified when self-consistent calculations are performed for these systems. For that reason, we take the origin for the energies at the top of the valence band.[12,14]

A. B-δ-doped Si quantum well

In Table I, TF numerical results for the first energy levels of light and heavy holes in a B-δ-doped Si quantum well are presented as functions of the two-dimensional carrier concentration p_{2D} together with the results obtained via self-consistent calculation. We use the following input parameters: $m_{\mathrm{hh}}^*=0.52m_0$ and $m_{\mathrm{lh}}^*=0.16m_0$, m_0 being the free-electron mass, $\epsilon_r=11.7$, and $2\times10^{12}\ \mathrm{cm}^{-2}<p_{\mathrm{2D}}<1\times10^{14}\ \mathrm{cm}^{-2}$. This interval for p_{2D} includes its experimentally interesting values. The ground level (E_{hh0}) and first excited

TABLE I. Energy levels ($E_{\rm hh0}$,$E_{\rm hh1}$,$E_{\rm lh0}$) in meV obtained by means of the self-consistent (SC) and Thomas-Fermi (TF) calculations for a p-type B-δ-doped Si quantum well, as functions of the impurity concentration $p_{\rm 2D}$.

p2D (10^{12} cm^{-2})	$E_{\rm hh0}$ (SC)	$E_{\rm hh0}$ (TF)	$E_{\rm hh1}$ (SC)	$E_{\rm hh1}$ (TF)	$E_{\rm lh0}$ (SC)	$E_{\rm lh0}$ (TF)
2	8.1	8.3			3.5	4.9
3	11.9	12.1			5.9	7.4
4	15.7	15.9			8.5	9.8
5	19.5	19.5			11.1	12.3
6	23.3	23.1			13.7	14.7
7	27.0	26.7		1.9	16.3	17.1
8	30.6	30.2		2.4	18.7	19.5
9	34.2	33.7		2.9	21.1	21.8
10	37.7	37.1	1.1	3.4	23.4	24.2
20	71.0	70.0	6.6	9.6	46.6	47.3
30	102.5	101.0	13.5	16.8	69.1	69.7
40	132.8	130.9	21.0	24.6	91.2	91.5
50	162.2	159.9	28.9	32.8	112.8	113.0
60	190.9	188.3	37.1	41.3	134.1	134.1
70	219.1	216.1	45.6	50.0	155.1	155.0
80	246.7	243.4	54.2	58.7	175.9	175.6
90	273.9	270.3	63.0	67.7	196.5	196.0

TABLE II. Energy levels ($E_{\rm hh0}$,$E_{\rm hh1}$,$E_{\rm lh0}$) in meV obtained by means of the self-consistent (SC) and Thomas-Fermi (TF) calculations for a p-type Be-δ-doped GaAs quantum well, as functions of the impurity concentration $p_{\rm 2D}$.

p2D (10^{12} cm^{-2})	$E_{\rm hh0}$ (SC)	$E_{\rm hh0}$ (TF)	$E_{\rm hh1}$ (SC)	$E_{\rm hh1}$ (TF)	$E_{\rm lh0}$ (SC)	$E_{\rm lh0}$ (TF)
2	7.5	7.7			1.5	3.0
3	11.1	11.2			3.2	4.5
4	14.7	14.7			4.9	6.0
5	18.3	18.1			6.8	7.6
6	21.7	21.5			8.4	9.2
7	25.1	24.7		1.9	9.9	10.7
8	28.4	28.0		2.3	11.4	12.3
9	31.7	31.2	1.2	2.8	13.0	13.8
10	34.9	34.4	1.6	3.3	14.5	15.4
20	65.7	64.7	7.2	9.3	30.1	31.0
30	94.8	93.3	13.9	16.2	45.5	46.3
40	122.7	120.9	21.1	23.7	60.7	61.6
50	149.8	147.6	28.6	31.4	75.8	76.6
60	176.2	173.8	36.4	39.4	90.7	91.6
70	202.1	199.4	44.4	47.6	105.6	106.4
80	227.5	224.6	52.6	55.9	120.4	121.2
90	252.5	249.3	60.9	64.3	135.0	135.9

level ($E_{\rm hh1}$) are reported for the case of heavy holes, but for light holes only $E_{\rm lh0}$ is presented. This is because $E_{\rm lh1}$ for the light holes is so close to μ that it is out of experimental interest.

It is important to compare the results obtained by both TF and SC calculations. As expected, numerical coincidence is better for ground states. In the case of heavy holes, TF calculation gives the best agreement with SC calculation for lower values of $p_{\rm 2D}$. Differences greater than 1 meV are reported for $p_{\rm 2D}\geqslant 3\times 10^{13}$ cm^{-2}; but they remain below 4 meV. For light holes, TF results for the ground level show better coincidence with SC values for greater $p_{\rm 2D}$. Nevertheless, the largest difference observed is only of 1.5 meV for $p_{\rm 2D}=3\times 10^{12}$ cm^{-2}, and, for the greater values of the carrier concentration, very good coincidence is obtained.

Comparison of the energies of the first excited level for the heavy holes do not give so close an agreement between TF and SC. The best coincidence is again obtained for the greater values of $p_{\rm 2D}$. However, in the best case, both results differ by no more than 10%. It should be remembered that our values for the energy refer to the Fermi level. If another origin for the energy were chosen (for instance, the bottom of the well), the value of $E_{\rm hh1}$ would be larger, and so the relative difference between both results would be smaller. For the same reason, in Table I, SC results for $E_{\rm hh1}$ are reported starting from $p_{\rm 2D}=10^{13}$ cm^{-2}. SC values of first excited energy level below 1.0 meV are not realistic because the method itself allows an approximate precision of 0.1 meV.

Zhu *et al.*[17] made B-δ-doped Si with a Schottky barrier. They showed shifts of the conductance peaks in the spectra with a peak doping concentration of $p_{\rm 3D}\approx 2\times 10^{20}$ cm^{-3}, and doped thicknesses of 1.2 nm. The activation energy reported is 110 ± 20 meV. The difference between the basic level and the top of valence band, in our calculation, is of $\approx$86 meV for $p_{\rm 2D}=2.4\times 10^{13}$ cm^{-2}. Wang, Karunasiri, and Park[18] also obtained experimental intersubband absorption spectra in B-δ-doped Si multiple quantum wells. They measured ten periods of B-doped layers with a width of about 5 nm. They reported a transition energy of 125 meV for a doping density $p_{\rm 3D}\approx 0.7\times 10^{20}$ cm^{-3} ($p_{\rm 2D}\approx 3.5\times 10^{13}$ cm^{-2}). This is comparable to the transition energy of 116 meV obtained in our calculation for the transition between the ground level and the top of the valence band.

B. Be-δ-doped GaAs quantum well

Table II shows the same calculation in the case of a Be-δ-doped GaAs quantum well. Here the values $m^*_{\rm hh}=0.62m_0$, $m^*_{\rm lh}=0.087m_0$, and $\epsilon_r=12.5$ are used.

A similar discussion can be made here, concerning the comparison between our TF results for $E_{\rm hh0}$, $E_{\rm hh1}$, and $E_{\rm lh0}$, and those obtained via SC calculations. Values of $E_{\rm hh0}$ show better coincidence than in the p-δ-doped Si system for $p_{\rm 2D}\leqslant 10^{13}$cm^{-2}. The same can be said with respect to the values of $E_{\rm lh0}$, but for values of $p_{\rm 2D}<7\times 10^{12}$ cm^{-2}. For higher values of the concentration, coincidence between TF and SC calculations is almost the same for both systems. In the case of $E_{\rm hh1}$, that coincidence is better in the p-δ-doped GaAs quantum well, for the whole range of concentration considered.

Recently, Sipahi *et al.*[13] developed a method which allows one to calculate potential profiles, subband structures, and Fermi-level positions in p-type δ-doped quantum wells. Their numerical results are in very good agreement with photo luminescence experimental results for $E_{\rm hh0}-E_{\rm lh0}$, but the method and the model considered are quite complicated in comparison with our approach, though more complete.

Wagner Ruiz, and Ploog[19] grew $Al_{1-x}Ga_xAs$/GaAs/$Al_{1-x}Ga_xAs$ quantum wells in which they placed a Be-doping spike with an intended dopant density of 8×10^{12} cm^{-2} at the center of the GaAs layer.

The width of the doping spike measured by secondary-ion mass spectroscopy was found to be less than 10 nm. The two emission peaks observed were assigned to recombination involving two different hole subbands. If the energy difference between the two subbands is just given by the peak energy difference, a subband separation of 36 meV was found. Although our calculation refers to a simpler system, namely (i) strict δ doping without considering the spread of the dopands, and (ii) the δ well in a GaAs matrix, not inside a quantum well, we find an energy difference between the first and second hh levels of 25.6 meV, which gives a plausible approximation.

Richards *et al.*[20] studied the subband structure of a quasi-two-dimensional hole gas formed at a single Be-δ-doped layer in GaAs by means of photoluminescence spectroscopy. They also performed self-consistent subband energies calculations. For an 8×10^{12} cm^{-2} acceptor concentration, with a dopant spread of 2 nm, their SC result for the difference $E_{\mathrm{hh}0}-E_{\mathrm{lh}0}$ is $\approx$15.1 meV. Our TF result for that difference is 15.7 meV and our previous SC result[14] is 17 meV. According to the photoluminescence spectroscopy experiments reported in that work, the spacing between both levels is $\approx$19 meV. Thus our numerical values are in quite well agreement with the experiment, even when, in our case, no dopant spread is considered.

More significant is the comparison with the data of Damen *et al.*,[21] because in that experiment the δ well approximation is more closely resembled as the dopant spread is only between 9 and 25 A. These authors have grown Be-δ-doped GaAs with a p-doping density in the range from 6×10^{12} to 2×10^{14} cm^{-2}. They observed that in this system there are two levels for $p_{2D}=6\times10^{12}$ cm^{-2}. The Fermi level is close to the last level. The difference between the Fermi level and the basic level is $\approx$ 21.5 meV. For densities up to 6×10^{12} cm^{-2}, several more hole levels are claimed to be observed without further specification. In our calculation it is impossible to observe levels higher than the Fermi level, but the difference between the Fermi level and ground level is about 21.5 meV.

As a final conclusion of the present work, it is possible to say that TF calculations for the hole energy levels in p-type δ-doped quantum wells of Si and GaAs are plausible and very accurate, and provide a rather simple way to obtain valuable information of the subband structure in those systems, in comparison with other approaches.

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