

# Thomas-Fermi approximation in two $p$ -type delta-doped quantum wells in GaAs and Si

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Thomas-Fermi calculations of the hole subband structure in two coupled  $p$ -type  $\delta$ -doped GaAs and Si quantum wells are carried out as a function of the impurity concentration and the distance  $l$  between them. A simple formula is obtained for the potential as a function of these two magnitudes by both types of systems. The numerical results for a double Be- $\delta$ -doped GaAs (double B- $\delta$ -doped Si) quantum well show that the energy levels degenerate for  $l \geq 300 \text{ \AA}$  ( $l \geq 200 \text{ \AA}$ ) for an impurity concentration of  $1 \times 10^{13} \text{ cm}^{-2}$ .

*Keywords:* Thomas-Fermi;  $\delta$ -doped quantum wells

Presentamos cálculos de la estructura de subbandas de huecos, utilizando la aproximación de Thomas-Fermi para dos pozos cuánticos  $\delta$ -dopados tipo  $p$  en GaAs y Si, como función de la concentración de impurezas y de la distancia  $l$  entre ambos para los dos tipos de sistemas. Los resultados numéricos muestran que para un pozo doble de Be- $\delta$ -dopado GaAs (pozo doble de B- $\delta$ -dopado Si) con una concentración de  $1 \times 10^{13} \text{ cm}^{-2}$  los niveles están degenerados para  $l \geq 300 \text{ \AA}$  ( $l \geq 200 \text{ \AA}$ ).

*Descriptores:* Thomas-Fermi; pozos cuánticos  $\delta$ -dopados

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## 1. Introduction

In recent years, as a natural development of the increasing precision of modern MBE growth techniques, the doping of semiconductors down to atomic resolution ( $\delta$ -doping) has become possible. The emphasis was initially on  $n$ -type structures, and these initial works have succeeded in studying the subband spectra and mobilities of these systems through electrical and optical measurements (see Refs. 1–6) and references therein).

On the other hand,  $p$ -type delta-doped GaAs quantum wells can be made with Be, Si-acceptor and C layers [7–10]. These systems have potential technological applications ( $\delta$ -FET [2, 11, 12], ALD-FET [13], etc.). From a fundamental point of view they are suitable systems for the study of the physics at extremely high carrier densities. The  $p$ - $\delta$ -doped Si quantum well is only beginning to be investigated. The B  $\delta$ -doped Si quantum well, for example, features a situation where the interesting extremum of the band structure is localized at the  $\Gamma$  point of the Brillouin zone, for the valence band. This situation is the same as the one that occurs in the  $p$ -type  $\delta$ -doped GaAs quantum well. In Refs. 14–16 self-consistent (SC) calculations of the electronic states in these systems have been reported. More recently, other systems begin to be calculated and/or measured [17, 18].

The use of the Thomas-Fermi (TF) approximation to calculate the energy spectrum in  $\delta$ -doped quantum wells was presented for the first time by Ioriatti [19] in  $n$ -type sys-

tems, and in Ref. 20 for  $p$ -type structures. Those works turned to be of great importance because for the first time a self-consistent, analytically expressed potential was presented, providing a very useful tool for the theoretical and experimental study of those kinds of systems. Those potentials arise in the framework of a quasiclassical approximation as the Thomas-Fermi equation results to be, and it comes directly from the simultaneous solution of both the Poisson and Schrödinger equation.

The present work is intended to provide a procedure for the calculation of the energy levels in double  $p$ -type  $\delta$ -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 it shall be seen in this paper, it gives very good results in some cases. Eventually the results of these calculations may be used as good starting potential and energy levels in more sophisticated SC calculations.

## 2. 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 [21]

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

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,

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

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

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

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 [22]

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

$$= \frac{[3\pi^2 \hbar^3 n(r)]^{5/3} \left[1 + \left(\frac{m_{lh}}{m_{hh}}\right)^{3/2}\right]^{-2/3}}{10\pi^2 m_{hh} \hbar^3}. \quad (4)$$

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

The kinetic energy functional is

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

The potential energy associated to the interaction between the electron gas and the two plane of impurities is described by the following functional of the density:

$$V_{en} = \int n(r) V_N(r) dr$$

$$= \frac{2\pi e^2}{\epsilon_r} \left\{ p_{2D}^1 \int n(z) \left|z + \frac{l}{2}\right| dz + p_{2D}^2 \int n(z) \left|z - \frac{l}{2}\right| dz \right\}, \quad (6)$$

where  $p_{2D}^1$  and  $p_{2D}^2$  are respectively the impurity concentration in wells 1 and 2.  $l$  is the distance between the wells, and the energy functional which corresponds to the electron-electron interaction is

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

Here, it is assumed that the electrons are in an homogeneous medium of dielectric constant  $\epsilon_r$  (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 (if the term corresponding to the energy associated to electron self-interaction is neglected) as

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

Therefore, the TF energy-density functional is given by

$$E_{TF} = \frac{3 \left[1 + \left(\frac{m_{lh}}{m_{hh}}\right)^{3/2}\right]^{-2/3}}{10m_{hh}} \int n(z) [3\pi^2 \hbar^3 n(z)]^{2/3} dz$$

$$+ \frac{2\pi e^2}{\epsilon_r} \left\{ p_{2D}^1 \int n(z) \left|z + \frac{l}{2}\right| dz + p_{2D}^2 \int n(z) \left|z - \frac{l}{2}\right| dz \right\}$$

$$- \frac{\pi e^2}{\epsilon_r} \int \int n(z) n(z') |z - z'| dz dz'. \quad (9)$$

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

$$\mu = \frac{\left[1 + \left(\frac{m_{lh}}{m_{hh}}\right)^{3/2}\right]^{-2/3}}{m_{hh}} [3\pi^2 \hbar^3 n(z)]^{2/3}$$

$$+ \frac{2\pi e^2}{\epsilon_r} \left\{ p_{2D}^1 \left|z + \frac{l}{2}\right| + p_{2D}^2 \left|z - \frac{l}{2}\right| \right\}$$

$$- \frac{2\pi e^2}{\epsilon_r} \int n(z) |z - z'| dz. \quad (10)$$

The spatial band bending is described by a Poisson equation,

$$\frac{d^2 V(z)}{dz^2} = -\frac{4\pi e^2}{\epsilon_r} n(z)$$

$$+ \frac{4\pi e^2}{\epsilon_r} \left\{ p_{2D}^1 \delta\left(z + \frac{l}{2}\right) + p_{2D}^2 \delta\left(z - \frac{l}{2}\right) \right\}; \quad (11)$$

then

$$V(z) = \frac{2\pi e^2}{\epsilon_r} \left[ p_{2D}^1 \left|z + \frac{l}{2}\right| + p_{2D}^2 \left|z - \frac{l}{2}\right| \right]$$

$$- \frac{2\pi e^2}{\epsilon_r} \int n(z') |z - z'| dz'. \quad (12)$$

So, it is possible to write

$$\mu = \frac{\left[1 + \left(\frac{m_{lh}}{m_{hh}}\right)^{3/2}\right]^{-2/3}}{m_{hh}} [3\pi^2 \hbar^3 n(z)]^{2/3} + V(z), \quad (13)$$

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

$$\frac{d^2 V(z)}{dz^2} = -\frac{4e^2 m_{hh}^{3/2} \left[1 + \left(\frac{m_{lh}}{m_{hh}}\right)^{3/2}\right]}{3\pi \hbar^3} [\mu - V(z)]^{3/2}$$

$$+ \frac{4\pi e^2}{\epsilon_r} \left\{ p_{2D}^1 \delta\left(z + \frac{l}{2}\right) + p_{2D}^2 \delta\left(z - \frac{l}{2}\right) \right\}. \quad (14)$$

If we assume 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 the half. Then, for  $z \geq 0$

$$\frac{d^2V(z)}{dz^2} = -\frac{4e^2 m_{\text{hh}}^{3/2} \left[ 1 + \left( \frac{m_{\text{lh}}}{m_{\text{hh}}} \right)^{3/2} \right]}{\epsilon_r 3\pi\hbar^3} [\mu - V(z)]^{3/2} + \frac{4\pi e^2}{\epsilon_r} p_{2D}^1 \delta \left( z + \frac{l}{2} \right) \quad (15)$$

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

$$V(z) - \mu = -\frac{\alpha^2}{(\alpha |z + l/2| + z_0)^4} \quad (16)$$

and the substitution in (15) gives

$$\alpha = \frac{e^2 m_{\text{hh}}^{3/2} \left[ 1 + \left( \frac{m_{\text{lh}}}{m_{\text{hh}}} \right)^{3/2} \right]}{\epsilon_r 15\pi\hbar^3}. \quad (17)$$

If the system is required to be neutral, it can easily be obtained that

$$z_0 = \left( \frac{2\epsilon_r \alpha^3}{\pi e^2 n_{2D}} \right)^{1/5}. \quad (18)$$

Expressions (16–18) summarize the results of the model. With the TF potential  $V(z)$  (16), a Schrödinger wave equation is numerically solved in order to look for the energy levels and wave functions in the well.

### 3. Results and discussion

We take the origin for the energies at the top of the valence band. It has been verified many times that the chemical potential  $\mu$  is very close to this band [14, 16], *i.e.*, is almost zero, and we assume that.

#### 3.1. Double Be- $\delta$ -doped GaAs quantum well

We have in mind a double Be- $\delta$ -doped GaAs quantum well. For numerical calculation we use typical GaAs values, *i.e.*  $m_{\text{hh}}^* = 0.62 m_0$ ;  $m_{\text{lh}}^* = 0.087 m_0$  and  $\epsilon_r = 12.5$ ,  $m_0$  being the free electron mass.

In Fig. 1 we present the potential profile for two different values of the distance between the impurity planes by double Be  $\delta$ -doped GaAs quantum well. 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 Figs. 2a, 2b and 2c we depict the dependence of the first energy levels against the distance between the impurity planes for  $p_{2D} = 5 \times 10^{12} \text{ cm}^{-2}$ ,  $1 \times 10^{13} \text{ cm}^{-2}$  and  $5 \times 10^{13} \text{ cm}^{-2}$ . The trends are similar for all the studied con-

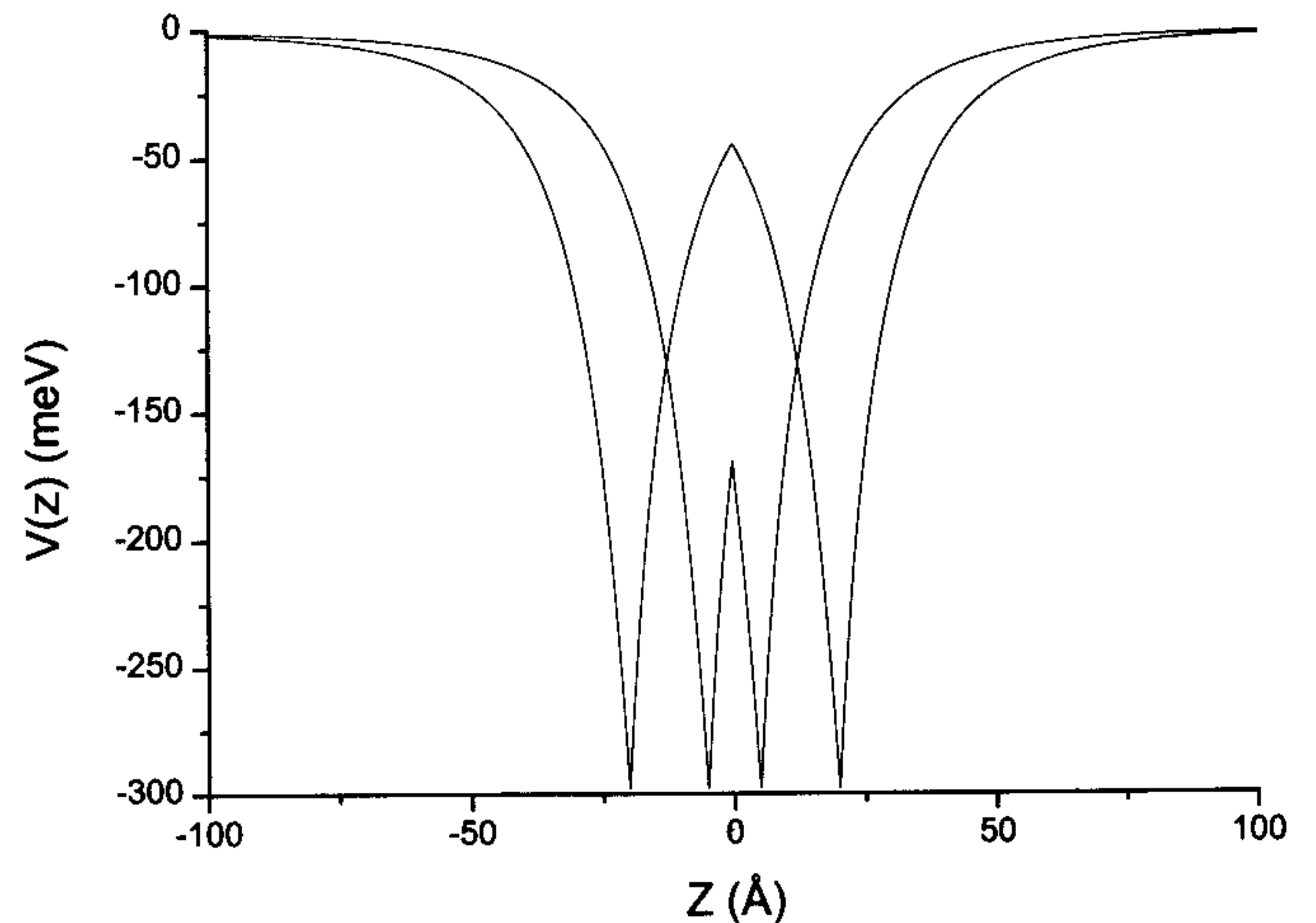


FIGURE 1. Potential profiles for a double Be- $\delta$ -doped GaAs quantum well for  $l = 10, 40 \text{ \AA}$  and  $p_{2D} = 5 \times 10^{13} \text{ cm}^{-2}$ .  $V(z)$  is in meV;  $z$  in  $\text{\AA}$ .

centrations. As expected, the first energy levels become degenerate for distances about 50–150  $\text{\AA}$ , depending on the concentration and on which level is observed. Above this value the wells can be considered isolated. This distance diminishes as the concentration grows, and its value for the first level is less than for the other ones.

A similar situation is treated in Ref. 23. These authors consider an inverse parabolic AlGaAs/GaAs quantum well within the semi-empirical tight-binding model. When the well potential has a similar form as in our Fig. 1, the authors of [23] obtained the same type of behavior for the hole energies as in our Fig. 2a.

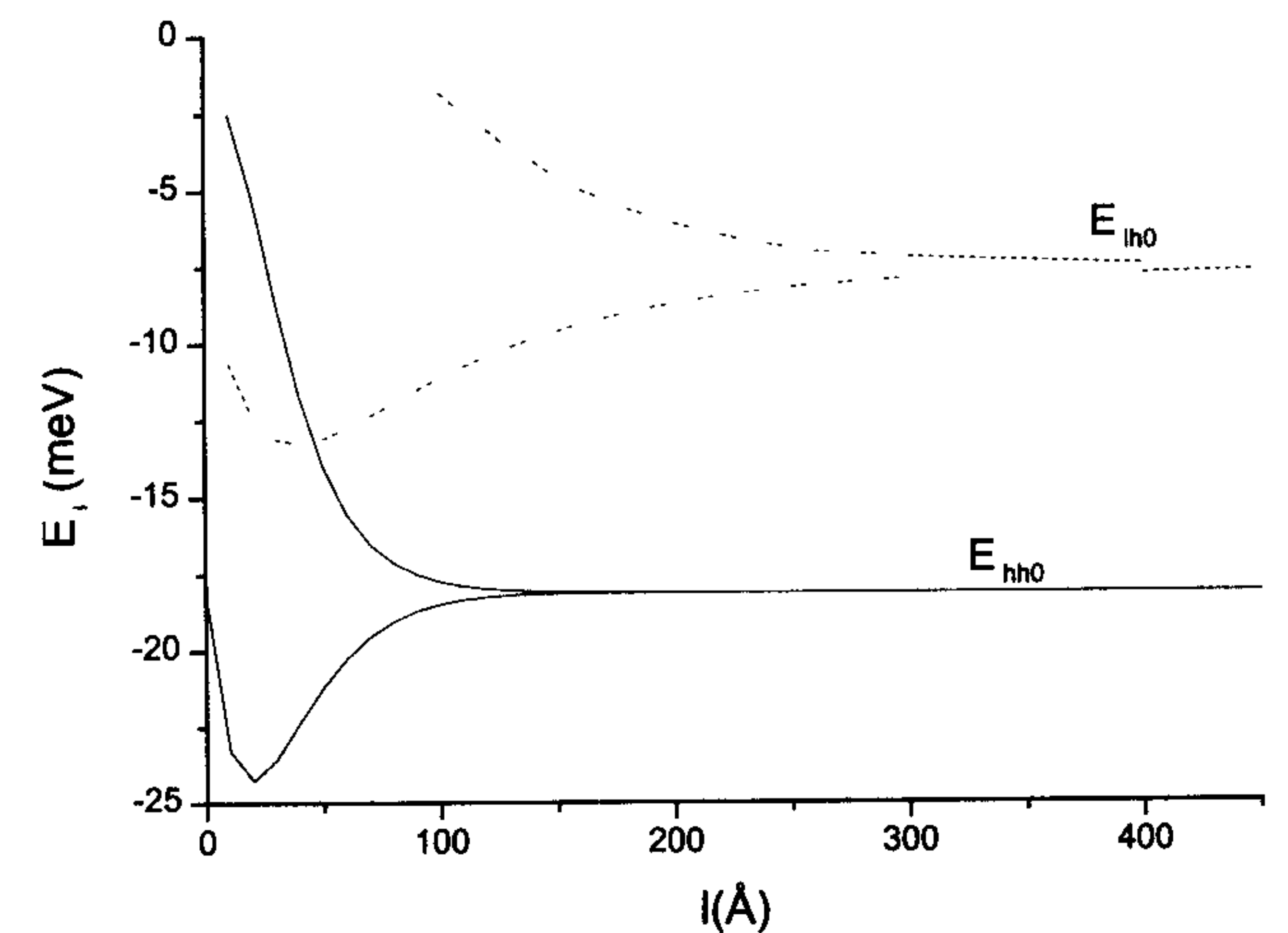
#### 3.2. Double B- $\delta$ -doped Si quantum well

We use the following input parameters:  $m_{\text{hh}}^* = 0.52 m_0$ ,  $m_{\text{lh}}^* = 0.16 m_0$ ,  $m_0$  being the free electron mass,  $\epsilon_r = 11.7$ . In Fig. 3 we present the potential profile for three different values of the distance between the impurity planes by double B  $\delta$ -doped Si quantum well. The form is similar to the one obtained in the double Be  $\delta$ -doped GaAs presented in Fig. 2.

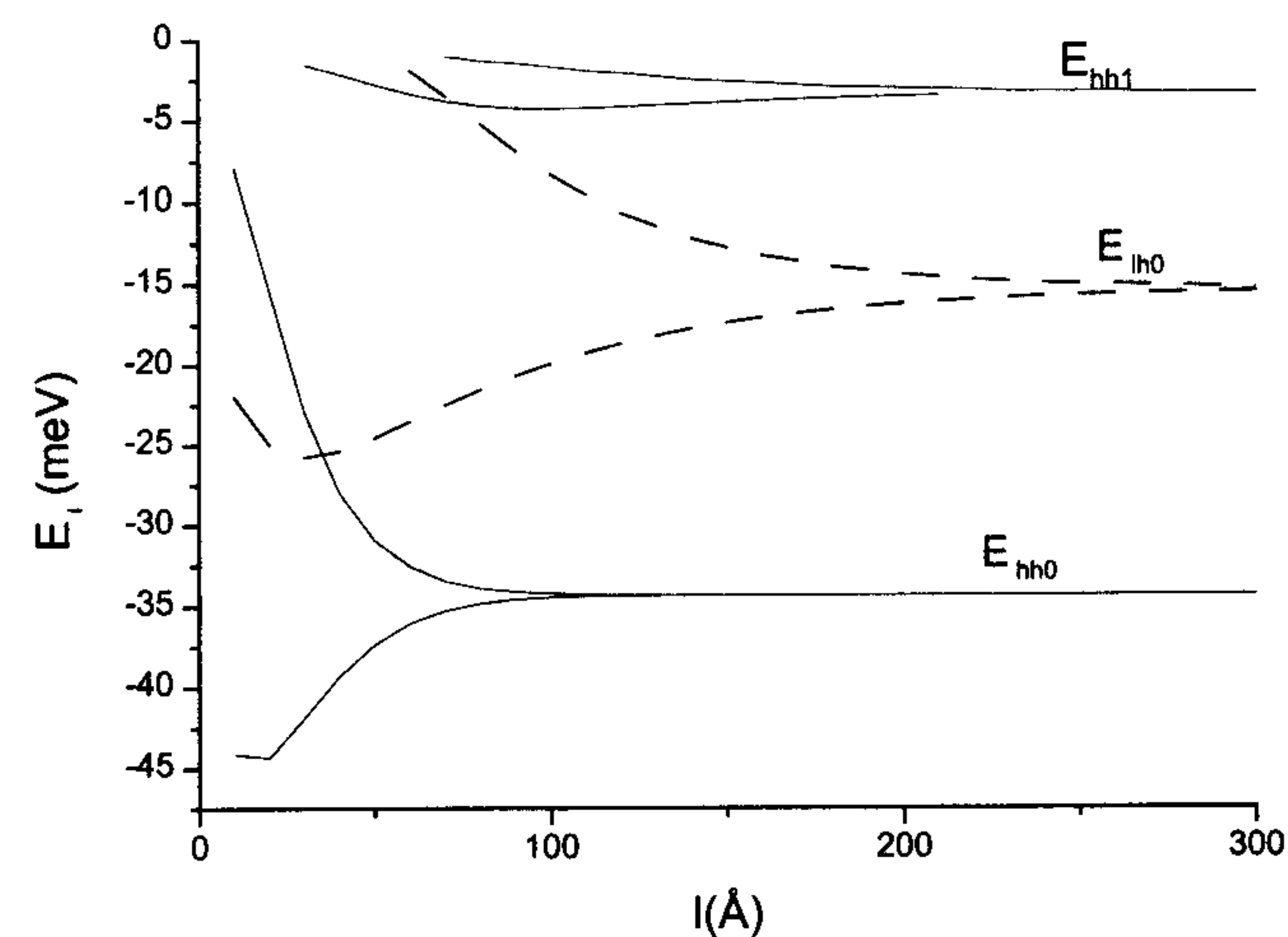
In Figs. 4a and 4b we depict the dependence of the first energy levels against the distance between the impurity planes for  $p_{2D} = 5 \times 10^{12} \text{ cm}^{-2}$  and  $1 \times 10^{13} \text{ cm}^{-2}$ .

For higher concentrations it is necessary to consider the splitt-off valence band [24]. The behavior is similar to the Be  $\delta$ -doped GaAs quantum well, *i.e.*, the confinement diminishes when the distance grows. In this case, for distances greater than 200  $\text{\AA}$  all the levels can be considered degenerate and the wells behave as isolated, except for the lowest concentration studied for which the ground level extends 300  $\text{\AA}$ .

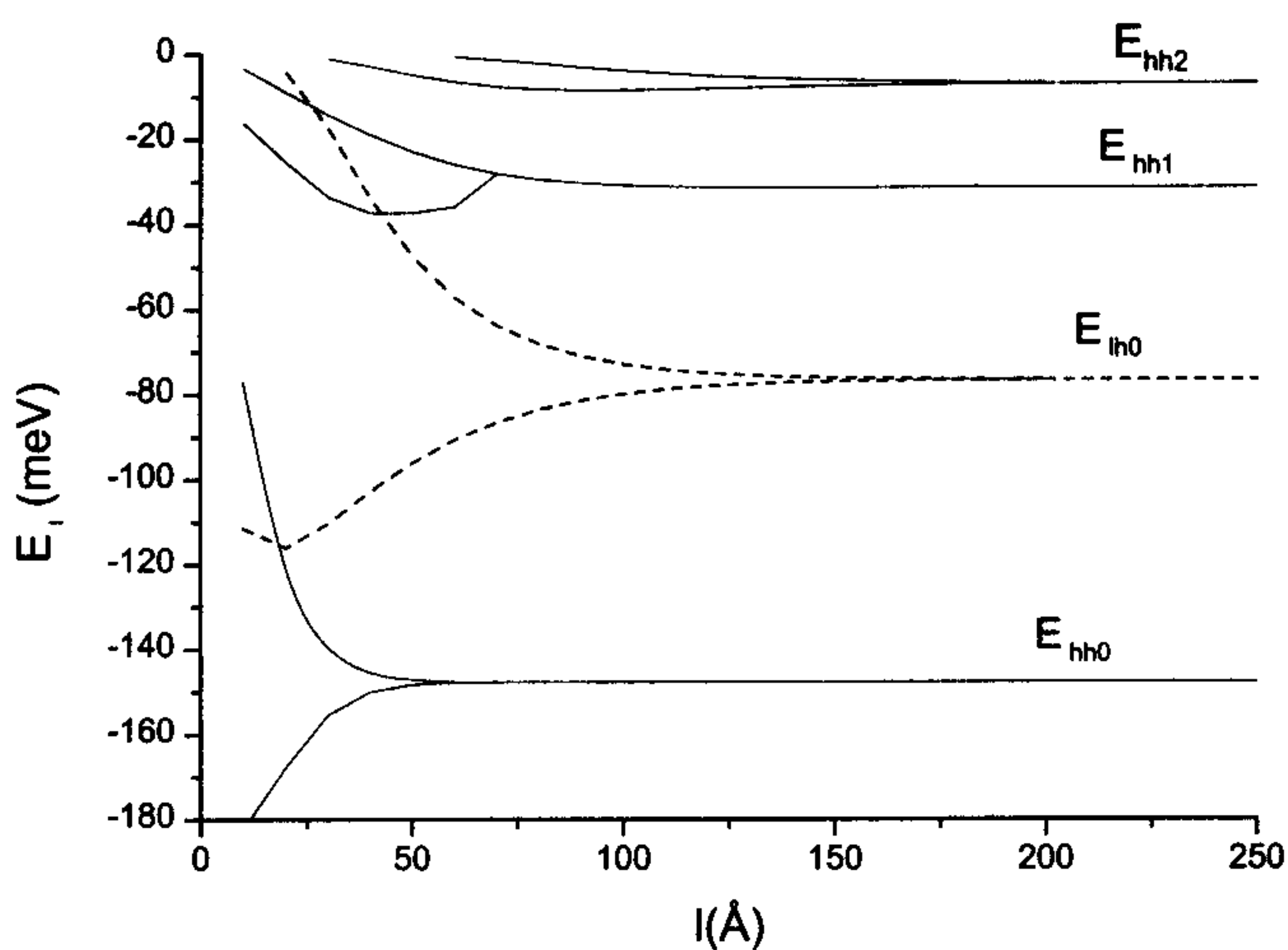
Wang *et al.* [25] report a selfconsistent calculation for  $p_{2D} = 2 \times 10^{12} \text{ cm}^{-2}$  and  $l = 200 \text{ \AA}$ , taking into account the heavy hole band only. Their value for the ground energy level ( $\sim 11 \text{ meV}$ ) considering that they only take into account the heavy holes, the result is very close to our value (16.5 meV).



(a)



(b)



(c)

FIGURE 2. Energy levels (in meV) of a double Be- $\delta$ -doped GaAs quantum well for (a)  $p_{2D} = 5 \times 10^{12} \text{ cm}^{-2}$ ; (b)  $p_{2D} = 1 \times 10^{13} \text{ cm}^{-2}$  and (c)  $p_{2D} = 5 \times 10^{13} \text{ cm}^{-2}$  vs. the distance between the planes (in Å).

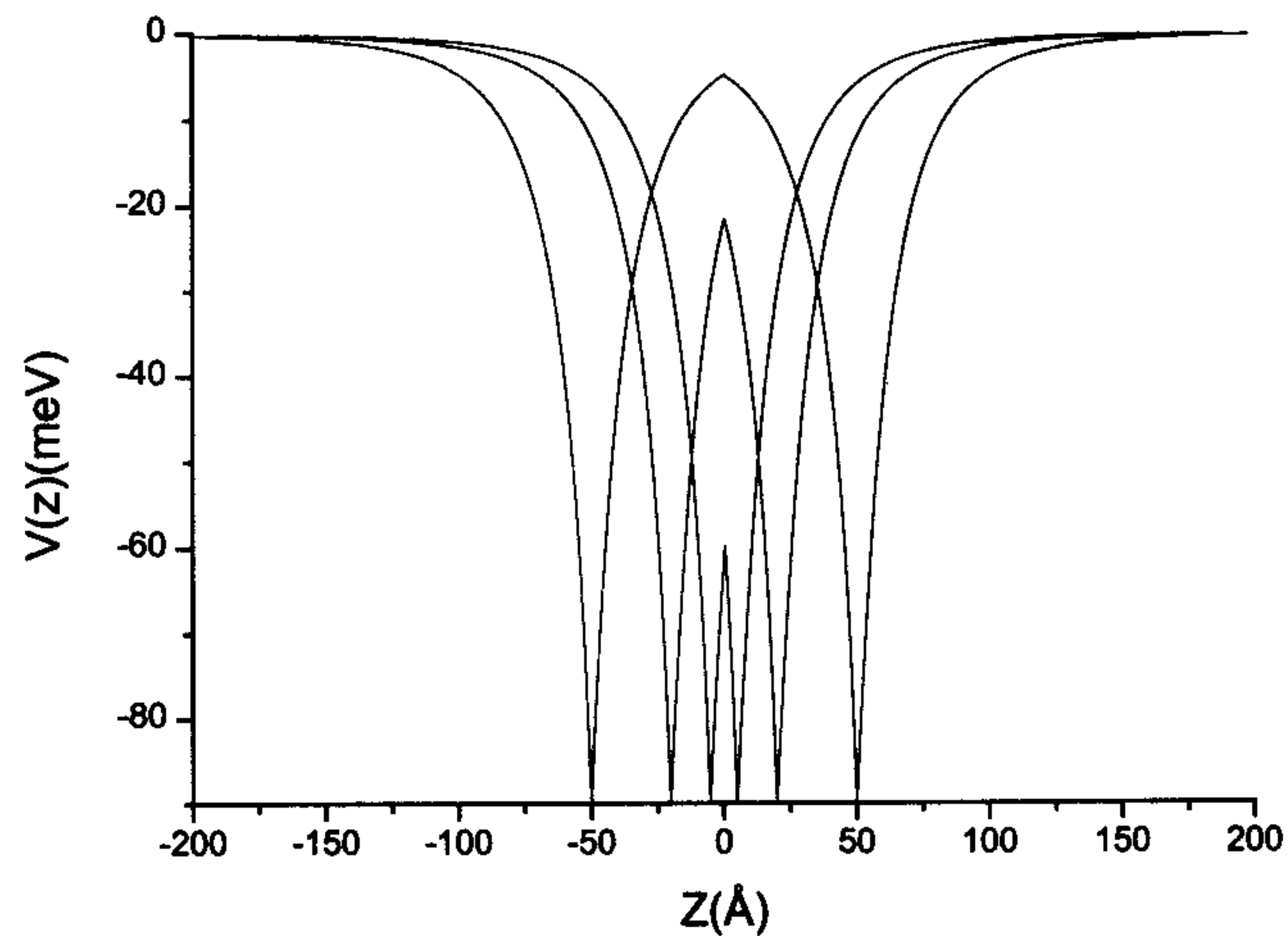
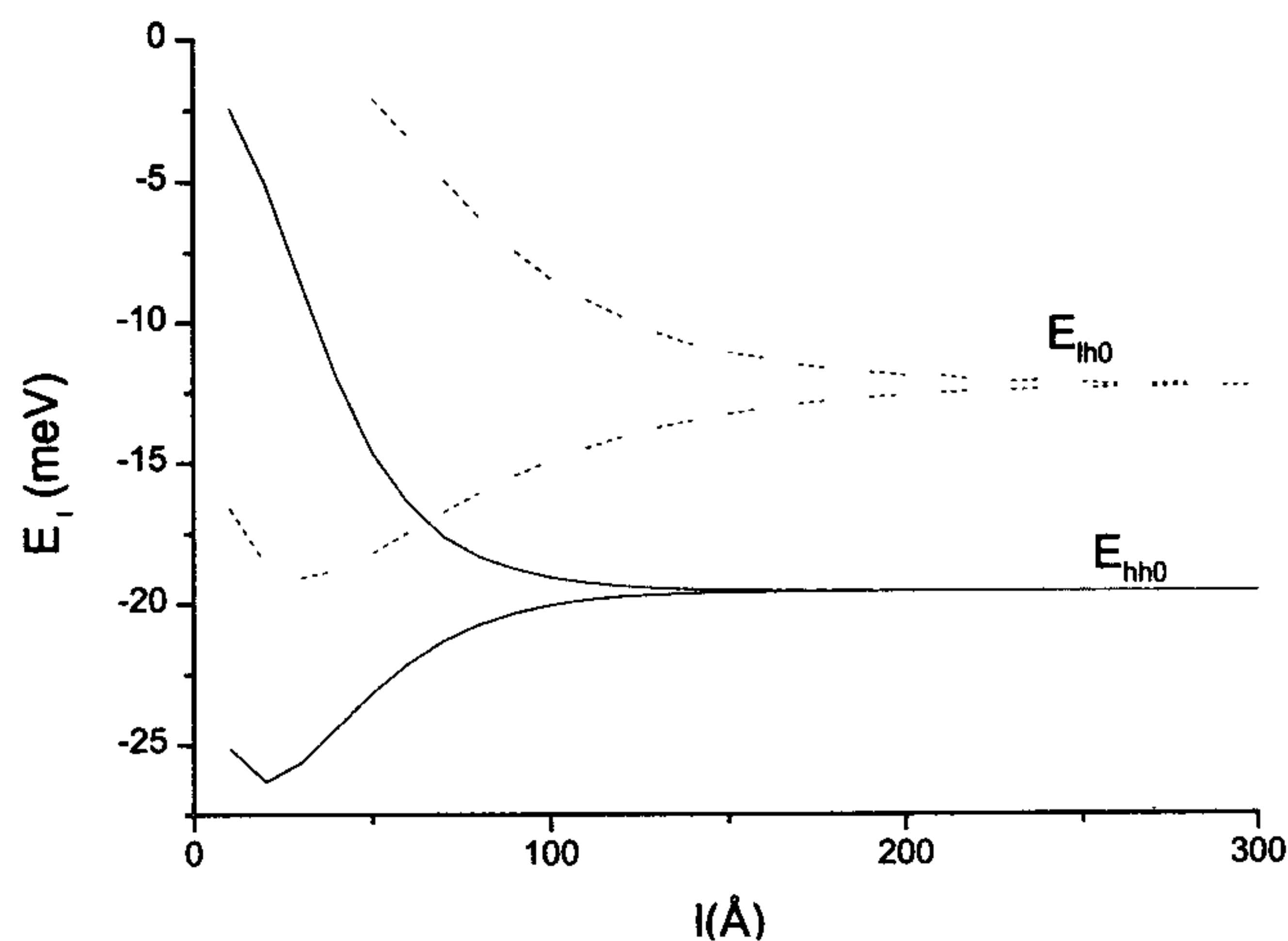
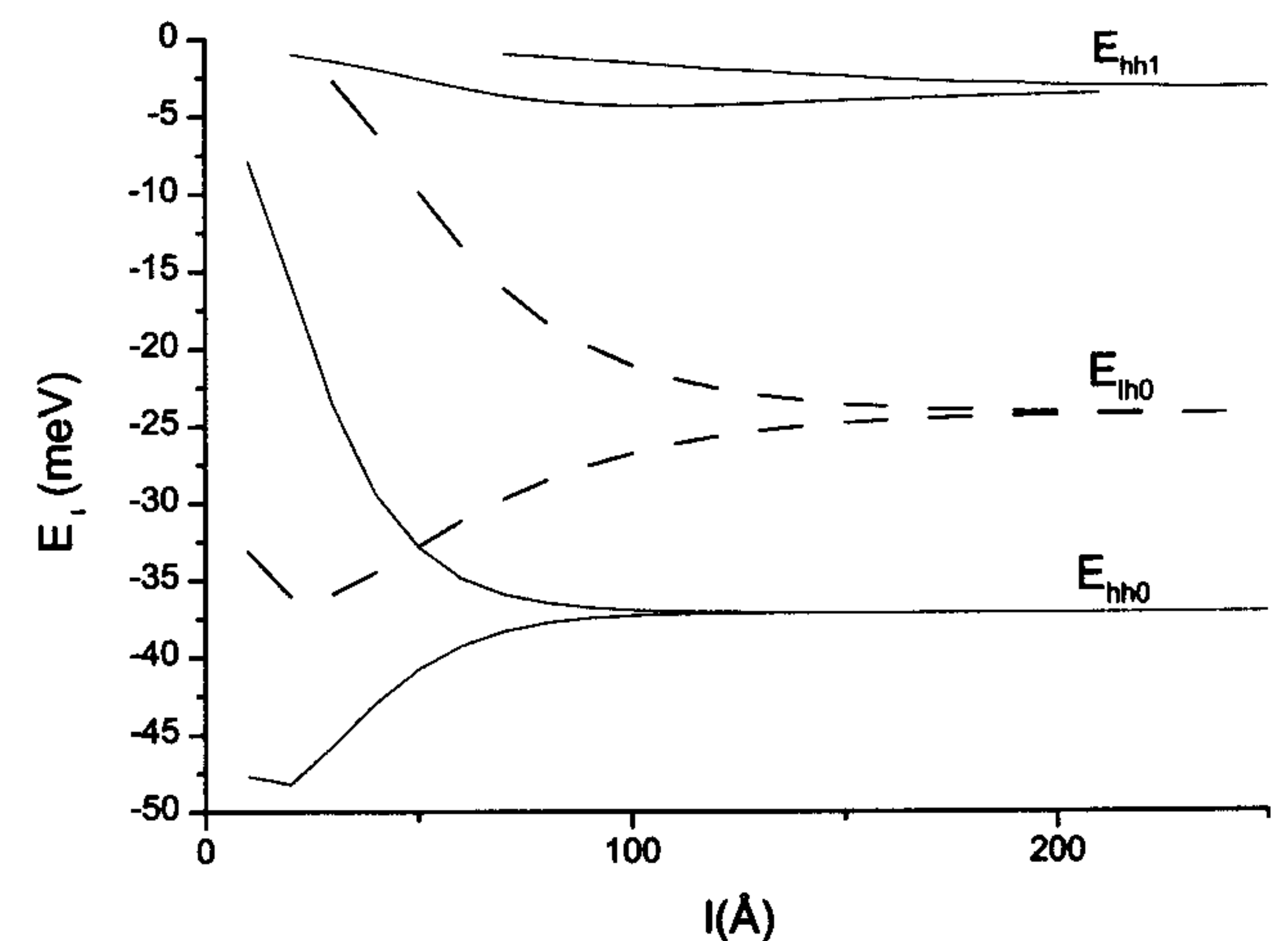


FIGURE 3. Potential profiles for a double B- $\delta$ -doped Si quantum well for  $l = 10, 40, 100 \text{ Å}$  and  $p_{2D} = 1 \times 10^{13} \text{ cm}^{-2}$ .  $V(z)$  is in meV;  $z$  in Å.



(a)



(b)

FIGURE 4. Energy levels (in meV) of a double B- $\delta$ -doped Si quantum well for (a)  $p_{2D} = 5 \times 10^{12} \text{ cm}^{-2}$  and (b)  $p_{2D} = 1 \times 10^{13} \text{ cm}^{-2}$  vs. the distance between the planes (in Å).

## 4. Conclusions

The double delta-doped quantum well behaves as two single and non coupled delta-doped quantum wells for distances about or greater than some hundreds of Å. This distance diminishes when the impurity concentration grows. For the same concentration, this distance is lower for the B  $\delta$ -doped Si compared to the case of double Be  $\delta$ -doped GaAs. On the other hand, when the distance between impurity layers is very little the system behaves as a single well (see Figs. 1 and 3). On growing the distance between the layers, the well is broadened and the levels approach the values for single isolated wells. This behavior is reached firstly by the lower levels than by the upper ones (see Figs. 2a, 2b, 2c, 4a and 4b).

As a final conclusion of the present work, it is possible to say that TF calculations for the hole energy levels in double *p*-type  $\delta$ -doped quantum wells are plausible and quite accurate, and provide a rather simple way of obtaining valuable information of the subband structure in those systems, in comparison with other approaches. If more sophisticated calculations are desired, the results here presented can be useful as a starting point for selfconsistency.

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1. G.H. Döhler, *Surf Sci.* **73** (1978) 97.
2. E.F. Schubert, A. Fischer, and K. Ploog, *IEEE Transactions on Electron Devices* **ED-33** (1986) 625.
3. H.P. Zeidl, *Appl. Phys. Lett.* **50** (1987) 1164.
4. B. Méndez and F. Domínguez-Adame, *Phys. Rev. B* **49** (1994) 11471.
5. F. Domínguez-Adame, E. Maciá, and B. Méndez, *Phys. Letters A* **194** (1994) 184.
6. L.M.R. Scolfaro, D. Beliaev, P. Enderlein, and J.R. Leite, *Phys. Rev. B* **50** (1994) 8699.
7. M. Hirai *et al.*, *J. Crystal Growth* **150** (1995) 209.
8. D.A. Woolf, *J. Crystal Growth* **150** (1995) 197.
9. T. Iida, *J. Crystal Growth* **150** (1995) 236.
10. N.Y. Li, H.K. Dong, C.W. Tu, and M. Geva, *J. of Crystal Growth* **150** (1995) 246.
11. L.M. Gaggero-Sager and R. Pérez-Alvarez, *J. Appl. Phys.* **74** (1995) 4566.
12. L.M. Gaggero-Sager and M.E. Mora-Ramos, *Materials Science and Engineering B* **47** (1997) 279.
13. K. Nakagawa, A.A. van Gorkum, and Y. Shiraki, *Appl. Phys. Lett.* **57** (1989) 1869.
14. L.M. Gaggero-Sager and R. Pérez-Alvarez, *Phys. Stat. Sol. (b)* **197** (1996) 105.
15. G.M. Sipahi, P. Enderlein, L.M.R. Scolfaro, and J.R. Leite, *Phys. Rev. B* **53** (1996) 9930.
16. L.M. Gaggero-Sager and R. Pérez-Alvarez, *J. Appl. Phys.* **79** (1996) 3351.
17. W-ch Wang *et al.*, *Superlattices and Microstructures* **26** (1999) 23.
18. R.T. Hsu, *Superlattices and Microstructures* **24** (1999) 175.
19. L. Ioriatti, *Phys. Rev. B* **41** (1990) 8340.
20. L.M. Gaggero-Sager, M.E. Mora-Ramos, and D.A. Contreras-Solorio, *Phys. Rev. B* **57** (1998) 6286.
21. S. Lundqvist and N.H. March, *Theory of the Inhomogeneous Electron Gas*, (Plenum, New York, 1983).
22. S.J. Vlaev and L.M. Gaggero-Sager, *Phys. Rev. B* **58** (1998) 1142.
23. S. Vlaev, V.R. Velasco, and F. García-Moliner, *Phys. Rev. B* **51** (1995) 7321.
24. L.M. Gaggero-Sager and M.E. Mora-Ramos, *Solid-State Electronics* **44** (2000) 175.
25. Shui Jinn Wang, San Lein Wu, Fang Yuh Yeh, and Ching Yuan Cheng, *Jpn. J. Appl. Phys.* **B33** (1994) 2429.