Thomas-Fermi approximation in a tight-binding calculation of δ-doped quantum wells in GaAs

S. Vlaev and L. M. Gaggero-Sager*
Escuela de Física, Universidad Autónoma de Zacatecas, Zacatecas 98068, ZAC., Mexico
(Received 29 December 1997; revised manuscript received 27 February 1998)

We present a tight-binding calculation of the electronic structure of δ-doped quantum wells in GaAs. A self-consistent potential obtained in the Thomas-Fermi approximation is considered as an external potential in our tight-binding model. A spin-dependent sp^3s^* basis is used and nearest neighbors are considered to treat GaAs bulk crystals doped with Si or Be. We change the semiempirical Hamiltonian matrix of the (001) direction in each atomic layer, adding the value of the self-consistent external potential in this layer to all diagonal elements of the matrix. The inhomogeneous δ-doped finite region is matched with two semi-infinite homogeneous GaAs barriers within the framework of the surface Green-function matching method. We compare the tight-binding results with the results obtained in the envelope-function approximation and with the experimental data available for the Si- and Be-doped GaAs.
[S0163-1829(98)04323-9]

The doping of semiconductors down to atomic resolution (δ doping) has become possible recently due to the development of the modern crystal growth techniques. Two types of δ-doped structures (n type[1–4] and p type[5–9]) have been investigated experimentally and theoretically to understand their subband spectra. These structures allow one to study the physics of the doping at extremely high carrier densities, and have potential technological applications [δ-FET (Ref. 10, etc.]. The Thomas-Fermi approximation applied to δ-doped quantum wells permits one to obtain an analytical self-consistent potential.[1,5] Previous theoretical works about these systems have been done mainly in the envelope-function approximation (EFA).

In the literature, to our knowledge, there is no tight-binding consideration of δ-doped systems. We believe that a semiempirical tight-binding calculation (with its advantages and disadvantages) could complete the theoretical results we have at the present for these systems, and could also enrich the interpretations of the existing experimental data. In the present work we propose a way to treat δ-doped systems within the framework of a semiempirical tight-binding scheme.

A calculation of the energy spectrum of δ-doped quantum wells in the Thomas-Fermi (TF) approximation is presented in Refs. 1 and 5. The envelope-function approximation describes the band bending in δ-doped quantum wells by the solution of the Poisson's equation. One finds this solution with a carrier concentration obtained in the TF appoximation. Here and henceforth we assume to be in the low-temperature limit. As a result of self-consistent calculations for an ideal and uniform electron gas, one obtains

$$V(z)=\frac{\beta}{(\alpha|z|+z_0)^4}, \tag{1}$$

$$\alpha=\frac{e}{\epsilon_r}\frac{m_{ed}}{15\pi\hbar^3}, \tag{2}$$

where $\beta=-\alpha^2$ if the dopants are p type or $\beta=\alpha^2$ if the dopants are n type, m_{ed} is the density of states mass, which depends on the type of doping, ϵ_r is the GaAs dielectric function and

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

D_{2D} is the two-dimensional density of impurities in the δ-doped layer (n_{2D} for n-type dopant and p_{2D} for p-type dopant).

Semiempirical tight-binding calculations have been conducted recently[11,12] to treat the electronic, optical, and electro-optical properties of some quantum-well structures. To take into account an external constant electric field applied to a planar heterostructure in the growth direction, one has to add the value of the external potential to all diagonal elements of the Hamiltonian matrix in each atomic layer:[13]

$$TB_{ii}(n)=TB_{ii}(0)+neF. \tag{4}$$

We have used in Eq. (4) the discrete variable n, instead of the continuous variable z, to label the atomic layers in the growth direction. The zero of the external potential is in the atomic layer $n=0$, e is the electron charge, F is the magnitude of the constant electric field applied along to the growth direction, and TB_{ii} are the diagonal tight-binding parameters (i being the atomic orbitals index). We consider this approximation a reasonable one, at least as a first step, and will not change the nondiagonal tight-binding parameters. Equation (4) shows that we shift the energetic positions of all atomic orbitals in a given atomic layer n with the potential drop neF of the field potential. There is experimental evidence that justifies this shift, the Stark ladder phenomena in superlattices.[14] This kind of parametrization has given very good results for bulk GaAs when a constant electric field is applied along the growth (001) direction.[15] An energy shift of the projected density of states for each layer has been found in accordance with the electric-field potential drop.

 © 1998 The American Physical Society

TABLE I. The tight-binding parameters used in the present paper. The effective mass values obtained with these parameters applying the formulas of Boykin *et al.* (Ref. 18) are $m_e^* = 0.068m_0$, $m_{\rm hh}^* = 0.62m_0$, and $m_{\rm lh}^* = 0.081m_0$.

E_{sa}	E_{pa}	E_{sc}	E_{pc}	E_{s^*a}	E_{s^*c}	V_{xx}	V_{ss}
-8.3431	0.9252	-2.6569	3.5523	7.4249	6.6235	1.9546	-6.4513
V_{xy}	$V_{sa\,pc}$	$V_{sc\,pa}$	$V_{s^*a\,pc}$	$V_{pa\,s^*c}$	λ_c	λ_a	
4.2022	5.6800	7.7000	4.8500	3.0100	0.0580	0.1400	

In the present work we consider the potential $V(z)$ from Eq. (1) as an external potential applied to a finite region of the projected bulk in the growth direction. Similarly to Eq. (4), we have

$$TB_{ii}(n) = TB_{ii}(0) + V(n), \tag{5}$$

where $V(n)$ is the potential $V(z)$ from Eq. (1) written in discrete notation.

The tight-binding (TB) calculations in the present paper are made in spin-dependent sp^3s^* basis (nearest neighbors)[16] at the center of the two-dimensional Brillouin zone for the (001) growth direction of δ-doped GaAs. We have considered two different δ-doped quantum wells, n-type (Si-doped GaAs) and p-type (Be-doped GaAs). In both cases the size of the inhomogeneous doped region (the width of the δ-doped quantum well) is 500 ML. Outside this region $V(n)$ has practically zero values (with a precision of 10^{-5} eV) for all carrier concentrations considered in this paper. The finite inhomogeneous slab is matched with two homogeneous semi-infinite GaAs barriers within the framework of the surface Green function matching (SGFM) method.[12,15] An algorithm presented in Ref. 15 has been applied to calculate the Green function of the inhomogeneous part, while the usual transfer matrix approach[17] has been used to find the bulk Green functions of the barriers.

The tight-binding parameters we used in the present paper (see Table I) satisfy two conditions. They give good band-structure values at Γ point for zero temperature (0 K) taking into account the spin. These parameters also give the commonly accepted effective mass values $m_e^* = 0.068m_0$, $m_{\rm hh}^* = 0.62m_0$, and $m_{\rm lh}^* = 0.081m_0$ when the formulas of Boykin *et al.*[18] are applied. The values of the diagonal tight-binding parameters and the parameters V_{xx}, V_{ss} are the same as in the work of Priester *et al.*[16]

First we present the results for a Si δ-doped GaAs quantum well.

Table II presents numerical values of the ground (E_{C0}) and two excited (E_{C1} and E_{C2}) energy levels in a Si δ-doped GaAs quantum well for different two-dimensional carrier concentrations $n_{2\rm D}$. For each bound state, results of both calculations (EFA and TB) are shown. We have used as input parameters $m_{ed} = m^* = 0.068m_0$, m_0 being the free electron mass, $\epsilon_r = 12.5$, $n_{2\rm D}$ takes values in the interval $1 \times 10^{12}\ {\rm cm}^{-2} < n_{2\rm D} < 1 \times 10^{13}\ {\rm cm}^{-2}$, and tight-binding parameters showed in Table I. For $n_{2\rm D} = 1 \times 10^{12}\ {\rm cm}^{-2}$ we have not found a $C2$ bound state in the EFA calculation while a $C2$ bound state appears in the tight-binding calculation. The differences between TB and EFA results obey the following trends. For a given state the differences increase when the concentration increases. But these differences are always less than 5 meV. The agreement is very good.

Results are reported in Ref. 3 for the same system with $n_{2\rm D} = 3 \times 10^{12}\ {\rm cm}^{-2}$. We compare below the energy distances between the ground state $C0$ and the excited states $C1$, $C2$, $C3$ obtained from our TB calculations with the same distances presented in Ref. 3 (the values in parentheses). $E_{C1} - E_{C0} = 45(48)$ meV, $E_{C2} - E_{C0} = 59(62)$ meV, and $E_{C3} - E_{C0} = 67(69)$ meV.

A Si δ layer with a concentration $n_{2\rm D} = 6.8 \times 10^{12}\ {\rm cm}^{-2}$ is studied experimentally in Ref. 2 by infrared excitations. The parity-allowed transitions have energies $E_{C1} - E_{C0} = 82.4$ meV and $E_{C3} - E_{C0} = 126$ meV. Our TB calculations give for the same transitions values of 81 and 136 meV, respectively.

The photoluminescence spectrum is measured in Ref. 4 for a periodic Si-doped GaAs with period $d_s = 500$ Å and $n_{2\rm D} = 1 \times 10^{12}\ {\rm cm}^{-12}$. The distances between the peaks are 20 and 15 meV. From our TB calculations follows $E_{C1} - E_{C0} = 19$ meV and $E_{C2} - E_{C1} = 5$ meV.

Now we present the results for Be δ-doped GaAs quantum well.

Table III shows numerical values of the ground ($E_{\rm hh0}$) and two excited ($E_{\rm lh0}$ and $E_{\rm hh1}$) energy levels in a Be δ-doped GaAs quantum well for different two-dimensional

TABLE II. Energy levels (E_{C0}, E_{C1}, and E_{C2}) in meV obtained by means of the tight-binding (TB) and envelope-function approximation (EFA) calculations for an n-type Si δ-doped GaAs quantum well, as functions of the impurity concentration $n_{2\rm D}$ in units $10^{12}\ {\rm cm}^{-2}$.

n_{2D}	E_{C0} (TB)	E_{C0} (EFA)	E_{C1} (TB)	E_{C1} (EFA)	E_{C2} (TB)	E_{C2} (EFA)
1	-29	-27	-10	-8		
2	-51	-49	-18	-16	-8	-6
3	-72	-70	-27	-24	-13	-10
4	-92	-90	-36	-33	-17	-14
5	-110	-110	-45	-42	-22	-19
6	-129	-128	-54	-51	-27	-24
7	-147	-147	-64	-60	-32	-29
8	-164	-165	-73	-69	-38	-34
9	-181	-182	-82	-78	-43	-39
10	-198	-200	-91	-87	-49	-44

TABLE III. Energy levels (E_{hh0}, E_{hh1}, and E_{lh0}) in meV obtained by means of the tight-binding (TB) and envelope-function approximation (EFA) calculations for a p-type Be δ-doped GaAs quantum well, as functions of the impurity concentration p_{2D} in units 10^{12} cm^{-2}.

p_{2D}	E_{hh0} (TB)	E_{hh0} (EFA)	E_{hh1} (TB)	E_{hh1} (EFA)	E_{lh0} (TB)	E_{lh0} (EFA)
2	13	8			8	3
3	16	11			9	4
4	19	15			11	6
5	22	18			12	7
6	25	22			13	9
7	28	25	7	2	15	10
8	31	28	7	2	16	12
9	34	31	8	3	18	13
10	37	34	8	3	19	15
20	63	65	13	9	33	30
30	88	93	20	16	47	45
40	113	121	26	24	62	60
50	136	148	33	31	76	75
60	159	174	40	39	90	89
70	181	199	47	48	105	103
80	203	225	54	56	119	118
90	224	249	62	64	134	132

carrier concentrations p_{2D}. We present results of TB and EFA calculations. The new input parameters in this case are $m^*_{hh}=0.62m_0$, $m^*_{lh}=0.081m_0$ and $m_{ed}=m^*_{hh}[1+(m^*_{lh}/m^*_{hh})^{3/2}]^{2/3}$. The energy zero is at the top of the GaAs valence band.

We have not found hh1 bound states for concentrations $p_{2D}=5$ and 6×10^{12} cm^{-2}. For all concentrations there is a large divergence between TB and EFA results for the energy E_{hh1}, while the coincidence for E_{lh0} is quite good. The relative differences between E_{hh0} (TB) and E_{hh0} (EFA) for the whole range of concentrations is about 27%.

Wagner *et al.*[7] have grown $Al_{1-x}Ga_xAs/GaAs/Al_{1-x}Ga_xAs$ quantum wells in which they place a Be doping spike with an intended dopant density of 8×10^{12} cm^{-2} at the center of the GaAs layer. If the energy difference between the two subbands is just given by the peak energy difference, they have found a subband separation of 36 meV. Our calculation refers to a simpler system, but we have obtained an energy difference of 26 meV (EFA) and 24 meV (TB) between the first and second hh levels, which gives a plausible approximation.

Richards *et al.*[8] have 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. For an acceptor concentration of 8×10^{12} cm^{-2}, they have obtained the difference $\Delta E_{h0l0}=E_{hh0}-E_{lh0}\approx19$ meV. Our result for this difference is 16 meV (EFA) and 15 meV (TB).

Damen *et al.*[9] have studied Be δ-doped GaAs. They have observed that in this system there are two levels for $p_{2D}=6\times10^{12}$ cm^{-2}. The Fermi level lies near to the last level. A difference of ≈21 meV between the Fermi level and the ground level has been measured in Ref. 9. Only within the TB calculation have we found a hh1 bound state for this concentration, which gives a difference of 25 meV between the Fermi level and the ground level.

In general, we can say that the results from the TB calculations are closer to the EFA results for Si δ-doped GaAs quantum well than for Be δ-doped GaAs quantum well.

We have compared self-consistent EFA calculations with semiempirical TB calculations for Si δ-doped and Be δ-doped quantum wells in GaAs. It is still too early to make a conclusion about this comparison. We need more calculations for several systems.

We have considered the self-consistent potential of δ-doped quantum wells obtained in Thomas-Fermi approximation as an external potential in a semiempirical tight-binding model. The numerical results obtained for Si δ-doped GaAs and Be δ-doped GaAs are satisfactory. We think that a further development of this scheme is possible.

This work was partially supported by National Fund for Scientific Investigations, Bulgaria through Grant No. X-646. S.V. is especially indebted to the CONACyT (Mexico) for support.

*Author to whom correspondence should be addressed. Electronic address: lgaggero@cantera.reduaz.mx

[1] L. Ioriatti, Phys. Rev. B **41**, 8340 (1990).

[2] G. Tempel, F. Muller, N. Scharz, F. Koch, G. Weiman, H. P. Zeindl, and I. Eisele, Surf. Sci. **228**, 247 (1990).

[3] C. A. C. Mendoca, F. Plentz, J. B. B. Oliveira, E. A. Meneses, L. M. R. Scolfaro, D. Beliaev, S. M. Shibli, and J. R. Leite, Phys. Rev. B **48**, 12 316 (1993).

[4] A. C. Maciel, M. Tatham, J. F. Ryan, J. M. Worlock, R. E. Nahory, J. P. Harbison, and L. T. Florez, Surf. Sci. **228**, 251 (1990).
[5] L. M. Gaggero-Sager, M. E. Mora-Ramos, and A. Contreras-Solorio, Phys. Rev. B **51**, 6286 (1998).
[6] G. M. Sipahi, R. Enderlein, L. M. R. Scolfaro, and J. R. Leite, Phys. Rev. B **53**, 9930 (1996).
[7] J. Wagner, A. Ruiz, and K. Ploog, Phys. Rev. B **43**, 12 134 (1991).
[8] D. Richards, J. Wagner, H. Schneider, G. Hendorfer, M. Maier, A. Fischer, and K. Ploog, Phys. Rev. B **47**, 9629 (1993).
[9] T. C. Damen, M. Fritze, A. Kastalsky, J. E. Cunningham, R. N. Pathak, H. Wang, and J. Shah, Appl. Phys. Lett. **67**, 515 (1995).
[10] L. M. Gaggero-Sager and R. Pérez-Alvarez, J. Appl. Phys. **74**, 4566 (1995); K. Nakagawa, A. A. van Gorkum, and Y. Shiraki, Appl. Phys. Lett. **57**, 1869 (1989); L. M. Gaggero-Sager and M. E. Mora-Ramos, Mater. Sci. Eng., B **47**, 279 (1997).
[11] T. B. Boykin, Phys. Rev. B **54**, 8107 (1996); M. U. Erdogan, V. Sankaran, K. W. Kim, M. A. Stroscio, and G. J. Iafrate, J. Appl. Phys. **79**, 8675 (1996).
[12] M. C. Muñoz, V. R. Velasco, and F. García-Moliner, Phys. Rev. B **39**, 1786 (1989); D. A. Contreras-Solorio, V. R. Velasco, and F. García-Moliner, *ibid.* **47**, 4651 (1993); S. Vlaev, V. R. Velasco, and F. García-Moliner, *ibid.* **51**, 7321 (1995).
[13] M. Graf and P. Vogl, Phys. Rev. B **51**, 4940 (1995).
[14] E. Mendez and F. Agulló-Rueda, J. Lumin. **44**, 223 (1989); E. Mendez, F. Agulló-Rueda, and J. M. Hong, Phys. Rev. Lett. **60**, 2426 (1988); S. J. Kim, Y. T. Oh, S. K. Kim, T. W. Kang, and T. W. Kim, J. Appl. Phys. **77**, 2486 (1996).
[15] S. Vlaev, V. R. Velasco, and F. García-Moliner, Phys. Rev. B **49**, 11 222 (1994).
[16] D. J. Chadi, Phys. Rev. B **16**, 790 (1977); P. Vogl, H. P. H. Hjalmarson, and J. D. Dow, J. Phys. Chem. Solids **44**, 365 (1983); C. Priester, G. Allan, and M. Lannoo, Phys. Rev. B **37**, 8519 (1988).
[17] M. P. López Sancho, J. M. López Sancho, and J. Rubio, J. Phys. F **14**, 1205 (1984); **15**, 851 (1985).
[18] T. B. Boykin, G. Klimeck, R. Ch. Bowen, and R. Lake, Phys. Rev. B **56**, 4102 (1997).