COMBINED METHOD FOR SIMULATING ELECTRON SPECTRUM OF δ-DOPED QUANTUM WELLS IN n-SI WITH MANY-BODY CORRECTIONS

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Abstract—The combined method to investigate the electron spectrum of single n-type δ-doped quantum wells in silicon is proposed. It is based on computing the electron potential energy by means of the Thomas-Fermi method at finite temperatures; then the obtained electron potential energy is applied to the iteration procedure with solving the Schrödinger equations for the electron spectrum and the Poisson one for the potential energy. The many-body corrections to the electron spectrum in the quantum well also have been investigated. The combined method demonstrates a rapid convergence. It is shown that that the simple Thomas-Fermi method gives a good approximation for the electron potential energy and for the total electron concentration within the well.

1. INTRODUCTION

The doping of semiconductors down to atomic resolution, or δ-doping, has recently become possible due to the modern molecular beam epitaxy growth techniques [1–37]. The δ-doping technique has been used to provide the carrier quantum confinement effects. Because the ionized impurity scattering is the principal factor that determines the carrier mobility, the advantage of the field effect transistor with the δ-doped channel over uniformly-doped materials is the smaller overlapping between impurities and carriers [2–4, 34, 35]. The infrared transitions between electron sublevels within δ-doped quantum wells are perspective for using in optoelectronics, especially, for infrared and terahertz modulators, switches, detectors, devices of nonlinear

optics, quantum computing, and lasers [3, 4, 9, 10, 18, 23–37]. For these purposes simple and exact methods to calculate the electron spectrum in quantum structures and the electron wave functions are of great interest.

The electron spectrum of δ-doped quantum wells can be calculated from solving the Schrödinger equation jointly with the Poisson one (SP) [28–35, 38–47]. It is possible to investigate δ-doped quantum wells also with a simpler approach based on the statistical Thomas-Fermi (TF) method [48–52]. The TF method is simpler, but the SP one is more exact and justified. When realizing SP method, the initial approximation is important for the convergence. Such an approximation can be taken from the simple TF theory. At higher values of electron concentrations $n > 10^{18} \, \text{cm}^{-3}$ the corrections to the potential electron energy due to many-body effects, like exchange-correlation, can be essential [38, 50] and should be included into the SP method. Note that last time there are some papers devoted to the calculations of δ-doped quantum wells by complicated *ab initio* methods, like density functional theory [53, 54].

In this paper the combined TF-SP method to calculate the electron spectrum in δ-doped n-Si is presented at finite temperatures. The electron potential energy within the well, the electron sublevels, the wave functions, and the total electron concentration have been calculated. This combined method shows a rapid convergence. It is demonstrated that the electron potential energies and electron concentrations calculated from TF method are practically the same as ones computed from SP ones. An influence of many-body effects, like exchange, has been investigated too. A specification of the iteration procedure for the case of high δ-doping has been proposed.

2. BASIC EQUATIONS

Consider a single δ-doped electron quantum well within n-Si. The plane of doping is aligned along the crystallographic axes. Below the atomic units are used for distances $a_0^* = \varepsilon \hbar^2 / (m_c e^2) \approx 0.52 \, \text{nm}$ and for energies $Ry^* = e^2 / (2\varepsilon a_0^*) \approx 0.12 \, \text{eV}$, where the effective mass of density of states in the conduction band is $m_c = \nu^{2/3} (m_\perp^2 m_{||})^{1/3} \approx 1.08 m_e \approx 10^{-27} \, \text{g}$, $\nu = 6$ is the number of the lowest non-equivalent electron valleys in Si [1, 35, 55]. In the case of n-Si the lowest valleys are lateral and the effective mass is anisotropic with the components $m_{||}$, $m_\perp$.

The Thomas-Fermi (TF) method at finite temperatures is applied to calculate the electron potential energy $V(z)$. With undimensional variables the basic equations of TF method for a symmetrical δ-doped

electron quantum well is [56]:

$$\frac{d^2V}{dz^2} = 8\pi \left\{ -n[V] + N_{d0} \times \left(2\exp\left(\frac{\mu - E_d - V}{T}\right) + 1 \right)^{-1} \right\};$$

$$\frac{dV}{dz}(z = +0) = 4\pi n_{2d}, \quad V(z \to \pm\infty) = 0 \tag{1}$$

where $\quad n[V] = \frac{1}{4}\left(\frac{T}{\pi}\right)^{3/2} \Phi_{1/2}\left(\frac{\mu - V}{T}\right);$

$$\Phi_{1/2}(v) \equiv \frac{2}{\pi^{1/2}} \int\limits_0^\infty \frac{u^{1/2}du}{1 + \exp(u - v)} \tag{2}$$

Here n_{2d} and N_{d0} are 2D and 3D donor concentrations, respectively; T is the temperature in energetic units. The donor levels are assumed shallow and single charged. Eq. (1) is the nonlinear Poisson one for the electron potential energy V in the electrostatics, where the concentrations of electrons $n[V]$ and ionized donors are calculated from the statistical theory [35, 55]. Note that Eqs. (1), (2) possess the same form both for n-Si and n-GaAs quantum wells.

The position of the Fermi level μ has been obtained from the condition of the total electric neutrality [1, 55]:

$$n[V = 0] = N_{d0} \times \left(2\exp\left(\frac{\mu - E_d}{T}\right) + 1 \right)^{-1} \tag{3}$$

Namely, the concentrations of electrons and the ionized donors outside the well are the same.

The nonlinear Eq. (1) has been solved by the Newton method. Namely, the following iteration scheme has been used:

$$V^{s+1} = V^s + \chi; \quad \frac{d^2\chi}{dz^2} - Q \cdot \chi = -\left(\frac{d^2V^s}{dz^2} - 8\pi\left\{ -n[V^s] \right.\right.$$

$$\left.\left. + N_{d0}\left(2\exp\left(\frac{\mu - E_d - V^s}{T}\right) + 1\right)^{-1}\right\}\right),$$

where $\quad Q \equiv 2\left(\frac{T}{\pi}\right)^{1/2} \Phi'_{1/2}(-\frac{V^s - \mu}{T})$ \hfill (4)

$$+ \frac{1}{T}\frac{16\pi N_{d0} \cdot \exp\left(-\frac{E_d + V^s - \mu}{T}\right)}{\left[2\exp\left(-\frac{E_d + V^s - \mu}{T}\right) + 1\right]^2}.$$

Because the scale $a_0^* \approx 0.52\,\text{nm}$ is quite small and comparable with the size of the lattice cell, the distributed 2D doping has been applied

in simulations. Namely, it is assumed that the donor concentration in the center of the structure is $n_{2d}(z) = n_{2d}/(\pi^{1/2}z_0)\exp(-(z/z_0)^2)$, these donors are fully ionized. Here z_0 is the transverse scale of 2D doping. When $z_0 = 0.5 - 1.5\,\text{nm}$, the results of simulations depend weakly on this parameter. In the simulations presented below it is $z_0 = 2a_0^* \approx 1\,\text{nm}$. When using the distributed 2D doping, the smooth dependence of $V(z)$ takes place in the central point $z = 0$.

The Fermi integral $\Phi_{1/2}$ and its derivative $\Phi'_{1/2}$ have been approximated from [35]. The rapid convergence of the TF method has been demonstrated, because the stabilization term $Q > 0$ in Eq. (4) provides stability. The numerical realization is simple, because it is necessary to solve a single equation for the electron potential energy V only. This iteration method is similar to the classical Gummel's approach for simulations of semiconductor devices [57].

After calculating the value of electron potential energy $V(z)$, the energy levels E_j, the wave functions $\Psi_j(z)$ of the discrete spectrum of the well, and also the electron concentration n have been computed from the Schrödinger equations [58]:

$$\frac{m_c}{m_{||}}\frac{d^2\Psi_j^{(1)}}{dz^2} - \{V(z) + V_{xc}\,[n] - E_j^{(1)}\}\Psi_j^{(1)} = 0;$$

$$\frac{m_c}{m_\perp}\frac{d^2\Psi_j^{(2)}}{dz^2} - \{V(z) + V_{xc}\,[n] - E_j^{(2)}\}\Psi_j^{(2)} = 0; \qquad (5)$$

$$\int_{-\infty}^{+\infty} |\Psi_j|^2 dz = 1$$

$$n(z) = \frac{T}{\pi}\sum_j\left\{\frac{m_\perp}{m_c}|\Psi_j^{(1)}(z)|^2 \times \log\left(1 + \exp\frac{\mu - E_j^{(1)}}{T}\right)\right.$$

$$\left. + 2\frac{(m_{||}m_\perp)^{1/2}}{m_c}\left|\Psi_j^{(2)}(z)\right|^2 \times \log\left(1 + \exp\frac{\mu - E_j^{(2)}}{T}\right)\right\} + n_{cont} \quad (6)$$

Here V_{xc} is the exchange-correlation correction to the electron potential energy due to many-body effects. It is the functional of the electron concentration [50]. In the expression for the electron concentration the term due to the continuous electron spectrum n_{cont} has been taken into account. It is unessential near the center of the well, where the influence of the localized electron wave functions is dominating, but is important at the periphery. In our simulations the value of n_{cont} is

taken as equal to the density of the charged donors in the volume of the semiconductor: $n_{cont.} = n[V = 0]$, see Eq. (3).

For different orientations of the valleys there are two Schrödinger equations for the wave functions $\Psi^{(1)}$, $\Psi^{(2)}$, as seen from Eq. (5), which are solved by means of the shooting method. In Eq. (6) it is taken into account that there are 2 valleys with the effective mass $m_{\parallel}$ is z-direction and 4 valleys with the mass $m_{\perp}$.

Thus, the idea of the combined method is as follows. Initially the potential electron energy $V(z)$ has been calculated by means of TF method from the single Eq. (4). The starting approximation for $V(z)$ is not essential at this stage. Then the SP method has been applied, where Eqs. (4)–(6) have been used jointly and the initial approximation for $V(z)$ has been taken there as the final value in TF method. At the final stage the corrections due to many-body effects have been taken into account.

3. RESULTS OF SIMULATIONS

The results of simulations are presented for the room temperature $300\,\mathrm{K}$, the donor concentration is $N_d = 10^{15}\,\mathrm{cm^{-3}}$. The values of 2D doping concentrations are taken within the interval $10^{12} - 10^{14}\,\mathrm{cm^{-2}}$. The donor level position is $E_d = -0.045\,\mathrm{eV}$, which is typical for the shallow donor impurities in Si [1, 55].

The forming of the quantum well in n-Si needs essentially higher doping values than in n-GaAs [51], because the effective mass of the density of states in silicon is much higher. In n-Si the exchange-correlation term in the undimensional electron potential energy is [38, 50]:

$$V_{xc} \approx -2 \left(1 + 0.025n^{-1/3} \log(1 + 35n^{1/3})\right) n^{1/3}. \qquad (7)$$

The dominating term in semiconductors is due to the exchange: $V_x \approx -2n^{1/3}$. The effects due to electron correlation are smaller for the electron concentrations $n \leq 10^{21}\,\mathrm{cm^{-3}}$ used here [50]. It is known [38, 59] that the many-body effects are unessential at smaller electron concentrations $n < 10^{18}\,\mathrm{cm^{-3}}$. Nevertheless, within the quantum wells in silicon the electron concentrations reach the values $n = 10^{19} - 10^{21}\,\mathrm{cm^{-3}}$, and the many-body effects can be important there and should be taken into account. So, in the difference of the preliminary results presented in [59], where the many-body effects were not taken into account, the main attention is paid to the cases of high δ-doping.

The dependencies of the electron potential energy $V(z)$ on the transverse coordinate z are given in Fig. 1, which are computed from
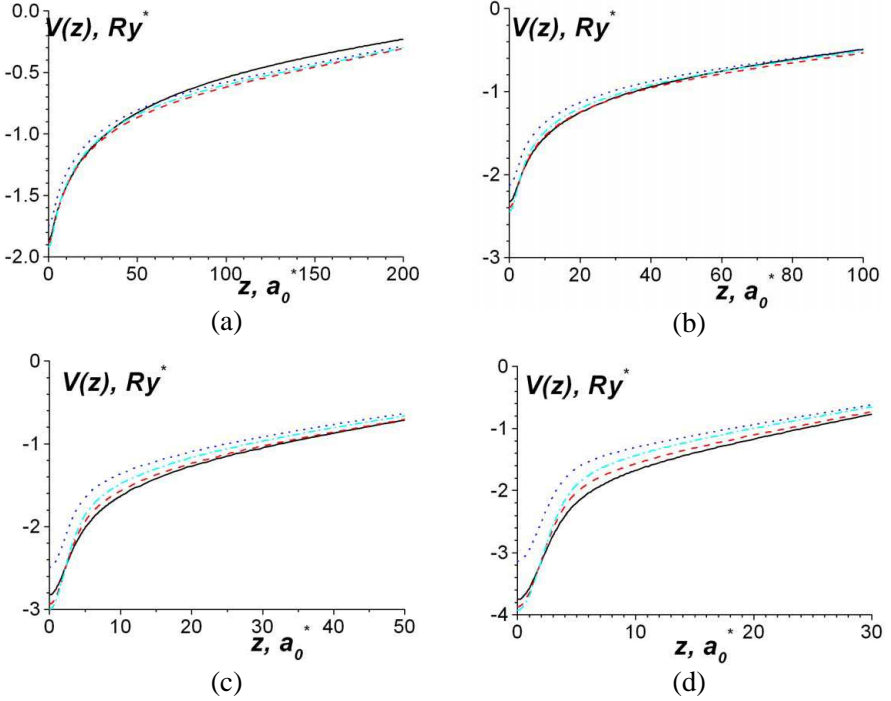
Figure 1. The dependencies of the electron potential energy $V(z)$ for different values of 2D doping. (a) is for $n_{2d} = 3 \times 10^{12}\,\mathrm{cm}^{-2}$, (b) is for $n_{2d} = 1 \times 10^{13}\,\mathrm{cm}^{-2}$, (c) is for $n_{2d} = 3 \times 10^{13}\,\mathrm{cm}^{-2}$, (d) is for $n_{2d} = 1 \times 10^{14}\,\mathrm{cm}^{-2}$; for all cases the donor concentration is $N_d = 1 \times 10^{15}\,\mathrm{cm}^{-3}$, $T = 300\,\mathrm{K}$. The solid lines are $V(z)$ computed from TF method; the dash lines are computed from SP one; the dot lines are from SP method with many-body corrections. The dash-dot lines are the sum of the electrostatic potential energy and the exchange correction $V + V_x$.

TF method, solid lines, then from SP one, dash lines, and, finally, from SP method with many-body corrections, dot lines. Also the sum of the electrostatic potential energy and the exchange correction $V + V_x$ is given, the dash-dot lines. The corresponding dependencies of the total electron concentrations $n(z)$ are given in Fig. 2. One can see that near the center of the well there are no differences between the values of $V(z)$ calculated from TF method and SP one without many-body corrections. The convergence of SP method is also rapid there. There are some differences in the calculated values of $V(z)$ at the periphery under smaller values of 2D doping $n_{2d} = 10^{12} - 3 \times 10^{12}\,\mathrm{cm}^{-2}$, see Fig. 1(a). This fact can be explained by a more essential influence of
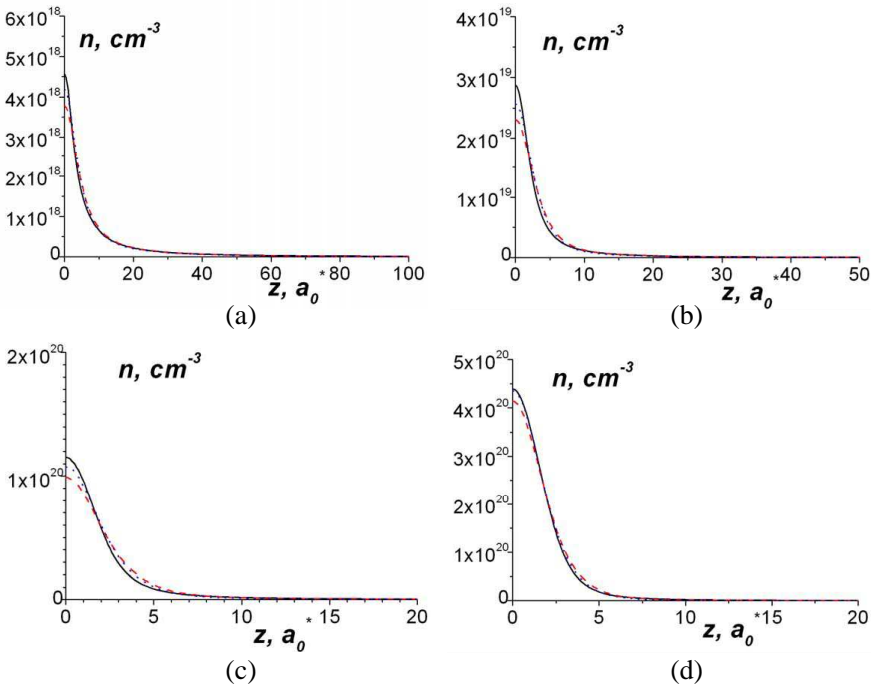
Figure 2. The dependencies of the total electron concentration $n(z)$ for different values of 2D doping. (a) is for $n_{2d} = 3 \times 10^{12}\,\text{cm}^{-2}$, (b) is for $n_{2d} = 1 \times 10^{13}\,\text{cm}^{-2}$, (c) is for $n_{2d} = 3 \times 10^{13}\,\text{cm}^{-2}$, (d) is for $n_{2d} = 1 \times 10^{14}\,\text{cm}^{-2}$; $N_d = 1 \times 10^{15}\,\text{cm}^{-3}$, $T = 300\,\text{K}$. The solid lines are from TF method; the dash lines are from SP one; the dot lines are from SP method with exchange.

the continuous electron spectrum there. Therefore, it seems natural to use TF method to calculate the electron energy at the periphery of the well $z \geq 100 a_0^*$ in the case of small values of 2D doping $n_{2d} = 10^{12} - 3 \times 10^{12}\,\text{cm}^{-2}$. Note that the electron gas is non-degenerated there, because the electron concentrations are $n \leq 10^{16}\,\text{cm}^{-3}$.

An influence of the exchange correction term V_x is unessential at smaller values of $n_{2d} \leq 10^{13}\,\text{cm}^{-2}$, and the convergence is still rapid. At higher values of $n_{2d} > 10^{13}\,\text{cm}^{-2}$ the convergence of the iterations is poor when the exchange term V_x is taken into account. To improve the iteration process, it is possible to choose the increased value of the parameter Q in Eq. (4). This value has been obtained numerically from the condition of the most rapid convergence, and the convergence takes place for all realistic values of 2D doping $n_{2d} \leq 2 \times 10^{14}\,\text{cm}^{-2}$. The iteration procedure has been finished when the maximum relative

error has reached the value $\leq 10^{-6}$.

One can see from Fig. 2 that under 2D donor concentrations $n_{2d} \sim 10^{12} - 10^{14} \, \text{cm}^{-2}$ the values of n computed both from TF method and from SP one without the exchange corrections practically coincide. Therefore, the simple TF method is effective for computing the electron spectrum of the δ-doped quantum wells. A small difference is in the center of the well, where TF method yields overestimated results. The exchange corrections result in changing the maximum values of the electron concentration in the center of the well under higher values
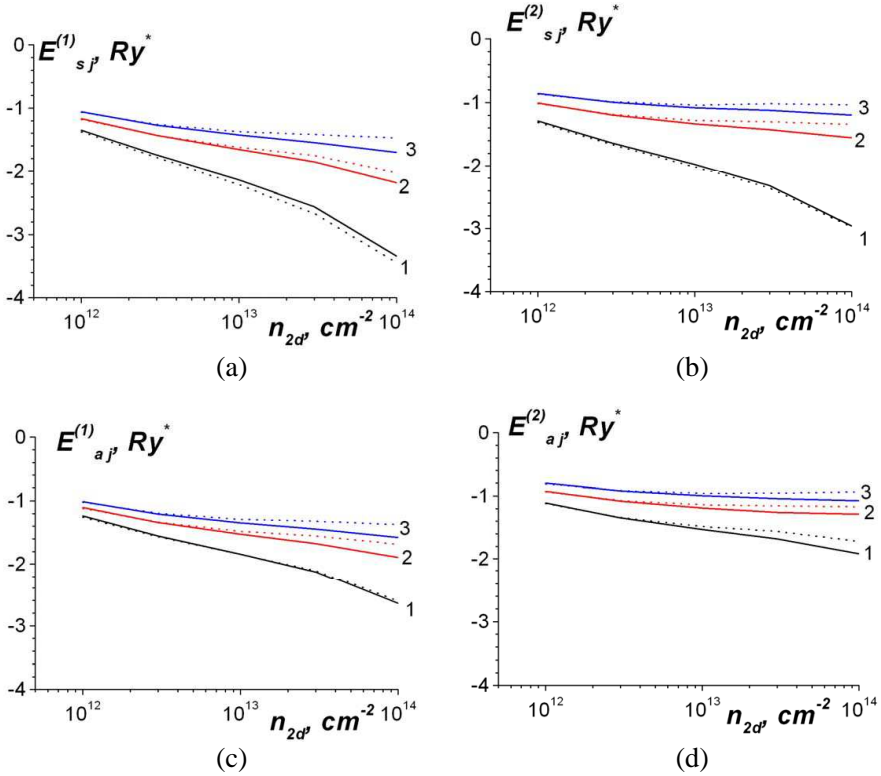

Figure 3. The dependencies of the lowest electron energies $E_j^{(1)}$, $E_j^{(2)}$ ($j = 1, 2, 3$) on the values of 2D doping for different valleys and different symmetries of wave functions for $n_{2d} = 10^{13} \, \text{cm}^{-2}$. (a) is for symmetric wave functions $\Psi^{(1)}(z)$, (b) is for symmetric wave functions $\Psi^{(2)}(z)$, (c) is for antisymmetric wave functions $\Psi^{(1)}(z)$, (d) is for antisymmetric wave functions $\Psi^{(2)}(z)$. The solid lines are from TF method; the dot lines are from SP method with exchange.

of 2D doping $n_{2d} > 10^{13}\,\mathrm{cm}^{-2}$. Nevertheless, because the difference between the electron potential energy calculated from TF method and the total electron energy $V + V_x$ calculated from SP method with many-body corrections is small, the TF method results in a small error even at high values of 2D doping.

The dependencies of energy sublevels on the 2D doping concentrations are given in Fig. 3. The solid lines are the results of TF theory, the dot lines are calculated form SP method with the exchange correction V_x. One can see that under the moderate doping values $n_{2d} \leq 10^{13}\,\mathrm{cm}^{-2}$ the values of the electron energy are practically the same for the lowest three sublevels. Under higher doping values the shift of energy sublevels due to many-body effects can be essential, but for the practical needs the difference of the energy sublevels is important. Such a difference between the first and second sublevels is the same both in TF and SP theories, when the values of 2D doping
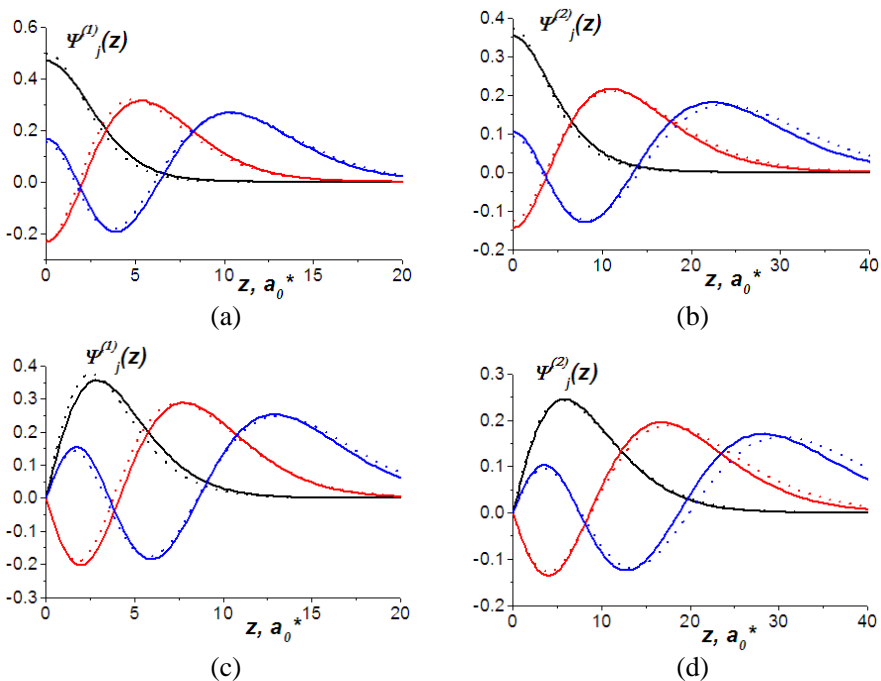

Figure 4. Wave functions for $n_{2d} = 10^{13}\,\mathrm{cm}^{-2}$. (a) is symmetric wave functions $\Psi^{(1)}(z)$, (b) is symmetric wave functions $\Psi^{(2)}(z)$, (c) is antisymmetric wave functions $\Psi^{(1)}(z)$, (d) is antisymmetric wave functions $\Psi^{(2)}(z)$. The solid lines are from TF method; the dot lines are from SP method with exchange.

are $n_{2d} \leq 10^{13}\,\mathrm{cm}^{-2}$.

The profiles of the wave functions are given in Fig. 4. The solid lines are the results of TF theory, the dot lines are calculated form SP method with the exchange correction V_x. It is seen that the localization of the wave functions for different valleys differs essentially. Under doping values $n_{2d} \leq 10^{13}\,\mathrm{cm}^{-2}$ there is no difference between the profiles of the electron wave functions computed within TF and SP methods.

A comparison with the complex *ab initio* methods based on the density functional theory [53, 54] shows that the SP method yields a good approximation for 2–3 lowest electron sub-levels. The results of both TF method and SP one are in a good agreement with the experimental data [36, 37, 58]. The higher energy sub-levels are computed with some errors, because an influence of the splitting of the electron valleys is important there [53]. This influence also can be included in the numerical method presented here.

The proposed combined method can be applied also for another quantum structures like selectively doped ones, when it is necessary to solve jointly the Poisson equation and the Schrödinder one.

4. CONCLUSIONS

A combined method to compute the electron spectrum of quantum wells in δ-doped n-Si has been developed, which is based on calculating the electron potential energy from the simple Thomas-Fermi method and then the using of the direct solving the Schrödinger equations and the Poisson one. An influence of many-body effects like exchange has been considered. The electron potential energy and the total electron concentration obtained from the Thomas-Fermi method practically coincide with ones calculated from the direct approach. The lowest energy levels also can be calculated from the Thomas-Fermi method. Both the Thomas-Fermi method and Schrödinger-Poisson one demonstrate a rapid convergence. The many-body corrections to the electron potential energy, like exchange, are essential under 2D doping values $n_{2d} > 10^{13}\,\mathrm{cm}^{-2}$. An improved algorithm for the simulation of the electron spectrum at higher doping levels has been proposed, which is based on the choice of optimum value of the stabilization term in the Poisson equation.

ACKNOWLEDGMENT

REFERENCES

1. Yu, P. Y. and M. Cardona, *Fundamentals of Semiconductors. Physics and Materials Properties*, Springer, New York, 2010.

2. Schubert, E. F., A. Fische, and K. Ploog, "The delta-doped field-effect transistor (δFET)," *IEEE Trans. Electron. Devices,* Vol. 33, No. 5, 625–630, 1986.

3. Ploog, K., "Delta- (δ-) doping in MBE-grown GaAs: Concept and device application," *J. Cryst. Growth,* Vol. 81, No. 4, 304–313, 1987.

4. Schubert, E. F., "Delta doping of III–V compound semiconductors: Fundamentals and device applications," *J. Vac. Sci. Technol.*, Vol. A8, No. 3, 2980–2996, 1990.

5. Nakagawa, K., A. A. van Gorkum, and Y. Shiraki, "Atomic layer doped field effect transistor fabricated using Si molecular beam epitaxy," *Appl. Phys. Lett.,* Vol. 54, No. 19, 1869–1871, 1989.

6. Word, C. E. C., G. Metze, J. Berry, and L. F. Eastman, "Complex free-carrier profile synthesis by 'atomic plane' doping of MBE GaAs," *J. Appl. Phys.,* Vol. 51, No. 1, 383–387, 1980.

7. Nakazato, K., R. J. Blaikie, and H. Ahmed, "Single-electron memory," *J. Appl. Phys.,* Vol. 75, No. 10, 5123–5136, 1994.

8. Zrenner, A., F. Koch, and K. Ploog, "Subband physics for a 'realistic' δ-doping layer," *Surf. Sci.*, Vol. 196, Nos. 1–3, 671–676, 1988.

9. Ullrich, B., C. Zhang, and K. V. Klitzing, "Quantum confined subband transitions of a GaAs sawtooth doping superlattice," *Appl. Phys. Lett.*, Vol. 54, No. 12, 1133–1135, 1989.

10. Ke, M. L., J. S. Rimmer, B. Hamilton, J. H. Evans, M. Missous, K. E. Singer, and P. Zalm, "Radiative transitions associated with hole confinement at Si δ-doped planes in GaAs," *Phys. Rev.,* Vol. B45, No. 24, 14114–14121, 1992.

11. Chang, C. Y., W. Lin, W. C. Hsu, T. S. Wu, S. Z. Chang, and C. Wang, "The δ-doped $In_{0.25}Ga_{0.75}As$/GaAs pseudomorphic high electron mobility transistor structures prepared by low-pressure metal organic chemical vapor deposition," *Jpn. J. Appl. Phys.,* Vol. 30, No. 6, 1158–1163, 1991.

12. Ni, W.-X., G. V. Hansson, J.-E. Sundgren, L. Hultman, L. R. Wallenberg, J.-Y. Yao, L. C. Markert, and J. E. Greene, "δ-function-shaped Sb-doping profiles in Si(001) obtained using a low-energy accelerated-ion source during molecular-beam epitaxy," *Phys. Rev.,* Vol. B46, No. 12, 7551–7558, 1992.

13. Kuo, T. Y., J. E. Cunningham, E. F. Schubert, W.T. Tsang, T. H. Chiu, F. Run, and C. G. Constad, "Selectively δ doped

quantum well transistor grown by gas source molecular beam epitaxy," *J. Appl. Phys.*, Vol. 64, No. 6, 3324–3327, 1988.

14. Gossmann, H.-J., C. S. Rafferty, A. M. Vredenberg, H. S. Luftman, F. C. Unterwald, D. J. Eaglesham, D. C. Jacobson, T. Boone, and J. M. Poate, "Time dependence of dopant diffusion in δ-doped Si films and properties of Si point defects," *Appl. Phys. Lett.,* Vol. 64, No. 3, 312–314, 1994.

15. Schubert, E. F., J. E. Cunningham, and W. T. Tsang, "Electron-mobility enhancement and electron-concentration enhancement in δ-doped n-GaAs at $T = 300\,\mathrm{K}$," *Solid State Commun.*, Vol. 63, No. 7, 591–594, 1987.

16. Liu, D. G., J. C. Fan, C. P. Lee, K. H. Chang, and D. C. Liou, "Transmission electron microscopy study of heavily delta-doped GaAs grown by molecular beam epitaxy," *J. Appl. Phys.*, Vol. 73, No. 2, 608–614, 1993.

17. Headrick, R. L., B. E. Weir, A. F. J. Levi, D. J. Eaglesham, and L. C. Feldman, "Si(100) (2×1) boron reconstruction: Self-limiting monolayer doping," *Appl. Phys. Lett.*, Vol. 57, No. 26, 2779–2781, 1990.

18. Zhu, J.-H., D.-W. Gong, B. Zhang, F. Lu, C. Sheng, H.-H. Sun, and X. Wang, "Admittance spectroscopy studies of boron δ-doped Si quantum wells," *Phys. Rev.*, Vol. B52, No. 12, 8959–8963, 1995.

19. Wang, Y., R. J. Hamers, and E. Kaxiras, "Atomic structure and bonding of boron-induced reconstructions on Si(001)," *Phys. Rev. Lett.*, Vol. 74, No. 3, 403–406, 1995.

20. Zheng, X., T. K. Carns, K. L. Wang, and B. Wu, "Electron mobility enhancement from coupled wells in delta-doped GaAs," *Appl. Phys. Lett.*, Vol. 62, No. 5, 504–506, 1993.

21. Gurtovoi, V. L., V. V. Valyaev, S. Y. Shapoval, and A. N. Pustovit, "Electron transport properties of double delta-doped GaAs structures grown by low-pressure metalorganic chemical vapor deposition," *Appl. Phys. Lett.*, Vol. 72, No. 10, 1202–1204, 1998.

22. Kiunke, W., E. Hammerl, I. Eisele, D. Schulze, and G. Gobsch, "Electrical transport between delta layers in silicon," *J. Appl. Phys.*, Vol. 72, No. 8, 3602–3605, 1992.

23. Sasagawa, R., H. Sugawara, Y. Ohno, H. Nakajima, S. Tsujino, H. Akiyama, and H. Sakaki, "Enhancement of intersubband transition energies in GaAs quantum wells by Si delta doping of high concentration," *Appl. Phys. Lett.*, Vol. 72, No. 6, 719–721, 1998.

24. Shena, T.-C., J.-Y. Ji, M. A. Zudov, R.-R. Du, J. S. Kline, and

J. R. Tucker, "Ultradense phosphorous delta layers grown into silicon from PH$_3$ molecular precursors," *Appl. Phys. Lett.,* Vol. 80, No. 9, 1580–1582, 2002.

25. Oberbeck, L., N. J. Curson, M. Y. Simmons, R. Brenner, A. R. Hamilton, S. R. Schofield, and R. G. Clark, "Encapsulation of phosphorus dopants in silicon for the fabrication of a quantum computer," *Appl. Phys. Lett.*, Vol. 81, No. 17, 3197–3199, 2002.

26. Oberbeck, L., N. J. Curson, T. Hallam, M. Y. Simmons, G. Bilger, and R. G. Clark, "Measurement of phosphorus segregation in silicon at the atomic scale using scanning tunneling microscopy," *Appl. Phys. Lett.*, Vol. 85, No. 8, 1359–1361, 2004.

27. Kul'bachinskii, V. A., V. G. Kytin, R. A. Lunin, V. G. Mokerov, A. P. Senichkin, A. S. Bugaev, A. L. Karuzskii, A. V. Perestoronin, R. T. F. van Schaijk, and A. de Visser, "Transport and optical properties of tin delta-doped GaAs structures," *Semiconductors,* Vol. 33, No. 7, 771–778, 1999.

28. Ahn, D., "Intersubband transitions in a δ-doped semiconductor with an applied electric field: Exact solutions," *Phys. Rev.*, Vol. B48, No. 11, 7981–7985, 1993.

29. Ozturk, E., "Optical intersubband transitions in double Si δ-doped GaAs under an applied magnetic field," *Superlattices and Microstructures,* Vol. 46, No. 5, 752–755, 2009.

30. Ozturk, E. and I. Sokmen, "The electric field effects on intersubband optical absorption of Si δ-doped GaAs layer," *Solid-State Commun.*, Vol. 126, No. 11, 605–609, 2003.

31. Ozturk, E. and I. Sokmen, "Intersubband transitions for single, double and triple Si δ-doped GaAs layers," *2003 J. Phys. D*, Vol. 36, No. 20, 2457–2464, 2003.

32. Kim, K. T., S. S. Lee, and S. L. Chiang, "Inter miniband optical absorption in a modulation doped Al$_x$Ga$_{1-x}$As/GaAs superlattice," *J. Appl. Phys.,* Vol. 69, No. 9, 6617–6624, 1991.

33. Ozturk, E. and I. Sokmen, "Effect of magnetic fields on the linear and nonlinear intersubband optical absorption coefficients and refractive index changes in square and graded quantum wells," *Superlattices and Microstructures,* Vol. 48, No. 3, 312–320, 2010.

34. Schubert, E. F., "Delta-doping of semiconductors: Electronic, optical, and structural properties of materials and devices," *Semiconductors and Semimetals,* Vol. 40, Chapter 1, 1–151, Elsevier, Amsterdam, 1994.

35. Fu, Y. and M. Willander, *Physical Models of Semiconductor Quantum Devices*, Kluwer, Dordrecht, NL, 1999.

36. Zeindl, H. P., T. Wegehaupt, I. Eisele, H. Oppolzer, H. Reisinger,

G. Tempel, and F. Koch, "Growth and characterization of a delta-function doping layer in Si," *Appl. Phys. Lett.*, Vol. 50, No. 17, 1164–1166, 1987.

37. Li, H.-M., K.-F. Berggren, W.-X. Ni, B. E. Sernelius, M. Willander, and G. V. Hansson, "Tunneling current spectroscopy of electron subbands in n-type δ-doped silicon structures grown by molecular beam epitaxy," *J. Appl. Phys.*, Vol. 67, No. 4, 1962–1968, 1990.

38. Ramdas Ram-Mohan, L., *Finite Element and Boundary Element Applications in Quantum Mechanics,* Oxford University Press, New York, Oxford, 2002.

39. Hurkx, G. A. M. and A. van Haeringen, "Self-consistent calculations on GaAs-Al$_x$Ga$_{1-x}$As heterojunctions," *J. Phys. C: Solid State Phys.*, Vol. 18, No. 29, 5617–5628, 1985.

40. Simserides, C. D. and G. P. Triberis, "A systematic study of electronic states in n-Al$_x$Ga$_{1-x}$As/GaAs/n-Al$_x$Ga$_{1-x}$As selectively doped double-heterojunction structures," *J. Phys.: Condens. Matter*, Vol. 5, No. 35, 6437–6446, 1993.

41. Xu, W. and J. Mahanty, "The influence of Si delta doping on the electronic structure of AlGaAs-GaAs-AlGaAs single quantum wells," *J. Phys.: Condens. Matter*, Vol. 6, No. 25, 4745–4762, 1994.

42. Simserides, C. D. and G. P. Triberis, "Looking for the maximum low-temperature conductivity in selectively doped Al$_x$Ga$_{1-x}$As-GaAs-Al$_x$Ga$_{1-x}$As double heterojunctions," *J. Phys.: Condens. Matter*, Vol. 8, No. 30, L421–L430, 1996.

43. Xu, W., "Self-consistent electronic subband structure in terahertz-driven two-dimensional electron gases," *Europhys. Lett.*, Vol. 40, No. 4, 411–416, 1997.

44. Green, T. J. and W. Xu, "Population inversion in an optically pumped single quantum well," *J. Appl. Phys.*, Vol. 88, No. 6, 3166–3169, 2000.

45. Xu, W., P. A. Folkes, and G. Gumbs, "Self-consistent electronic subband structure of undoped InAs/GaSb-based type II and broken-gap quantum well systems," *J. Appl. Phys.*, Vol. 102, No. 3, 033703-9, 2007.

46. Ozturk, E., "Effect of magnetic field on a p-type δ-doped GaAs layer," *Chinese Phys. Lett.,* Vol. 27, No. 7, 077302-5, 2010.

47. Shpatakovskaya, G. V., "Semiclassical model of the structure of matter," *Phys. Usp.*, Vol. 55, No. 5, 429–464, 2012.

48. Ioriatti, L., "Thomas-Fermi theory of δ-doped semiconductor structures: Exact analytical results in the high-density limit,"

Phys. Rev., Vol. B41, No. 12, 8340–8344, 1990.

49. Rodriguez-Vargas, I. and L. M. Gaggero-Sager, "Subband structure comparison between *n*- and *p*-type double delta-doped GaAs quantum wells," *Revista Mexicana de Fisica*, Vol. 50, No. 6, 614–619, 2004.

50. Gaggero-Sager, L. M., "Exchange and correlation via functional of Thomas-Fermi in delta-doped quantum wells," *Modelling Simul. Mater. Sci. Eng.,* Vol. 9, No. 1, 1–6, 2001.

51. Oubram, O., O. Navarro, L. M. Gaggero-Sager, J. C. Martínez-Orozco, and I. Rodríguez-Vargas, "The hydrostatic pressure effects on intersubband optical absorption of *n*-type δ-doped quantum well in GaAs," *Solid State Sciences,* Vol. 14, No. 4, 440–444, 2012.

52. Gülveren, B., "Quantum dot with N interacting electrons confined in a power-law external potential," *Solid State Sciences,* Vol. 14, No. 1, 94–99, 2012.

53. Drumm, D. W., A. Budi, M. C. Per, S. P. Russo, and L. C. L. Hollenberg, "*Ab initio* calculation of valley splitting in monolayer δ-doped phosphorus in silicon," *Nanoscale Research Letters*, Vol. 8, No. 1, 111–121, 2013.

54. Carter, D. J., N. A. Marks, O. Warschkow, and D. R. McKenzie, "Phosphorus δ-doped silicon: Mixed-atom pseudopotentials and dopant disorder effects," *Nanotechnology*, Vol. 22, No. 6, 065701-10, 2011.

55. Brennan, K. F., *The Physics of Semiconductors*, Cambridge Univ. Press, Cambridge, 1999.

56. Grimalsky, V., L. M. Gaggero-Sager, and S. Koshevaya, "Electron spectrum of delta-doped quantum wells by the Thomas-Fermi method at finite temperatures," *Physica B*, Vol. 406, No. 2, 2218–2222, 2011.

57. Gummel, H. K., "A self-consistent iterative scheme for one-dimensional steady state transistor calculations," *IEEE Trans. Electron. Dev.,* Vol. 11, No. 10, 455–465, 1964.

58. Rodriguez-Vargas, I., M. L. Gaggero-Sager, V. V. Grimalsky, M. E. Mora-Ramos, and R. Perez-Alvarez, "Electron spectrum of single *n*-type delta-doped quantum wells in Si," *PIERS Proceedings*, 248–251, Beijing, China, Mar. 26–30, 2007.

59. Grimalsky, V., L. M. Gaggero-Sager, S. Koshevaya, and M. C. Castrejon, "Combined method for simulating electron spectrum of δ-doped quantum wells in *n*-Si," *Proc. 28th Internat. Conference on Microelectronics (MIEL 2012)*, 305–308, Nis, Serbia, May 13–16, 2012.