Electron Spectrum of δ-doped Quantum Wells by Thomas – Fermi Method at Finite Temperatures

V.Grimalsky, L.M.Gaggero-S., S.Koshevaya, A.Garcia-B.

Abstract – Electron spectrum of δ-doped quantum well in *n*-GaAs is investigated by means of Thomas – Fermi (TF) method at finite temperatures. This method shows fast convergence and good accuracy. At 2D doping $10^{13}\ldots2\times10^{13}$ cm^{-2}, the simplest TF method (T = 0) can be used up till the temperatures $T \leq 200$ K.

I. Introduction

The doping of semiconductors down to atomic resolution (δ-doping) has recently become possible as a natural development of the increasing precision of modern molecular beam epitaxy (MBE) growth techniques. The work on *n*-type δ-doped structures was primarily on GaAs semiconductors, and revealed considerable information on the subband structure and the mobilities of these systems through electrical and optical measurements [1–4]. On the other hand, the investigation in Si is more scare, due mainly to the difficulties found to incorporate dopants in a well controlled way during the MBE growth of Si [5].

The electron spectrum of δ-doped quantum wells can be calculated from solving the Schrödinger equation jointly with the Poisson one [6]. Nevertheless, this direct approach is complicated, and its convergence is slow. To investigate δ-doped quantum wells, it is possible with a simpler approach based on the statistical Thomas-Fermi (TF) method. Moreover, a main problem with using the direct approach is to find an appropriate initial approximation that can be obtained namely with TF.

II. Basic Equations

Consider a single δ-doped electron quantum well within *n* type semiconductor. Generally, the equation for the single electron potential energy $V = -e\varphi$ is the Poisson one (in absolute units):

$$\frac{d^2V}{dz^2} = \frac{4\pi e^2}{\varepsilon}\{-n[V] + n_{2d}\delta(z) + N_d(z)\} \qquad (1)$$

Here *n* is the electron concentration, which is the functional of V, φ is electric potential, n_{2d} is the 2D doping concentration, N_d is the 3D concentration of ionized donors; ε is the permittivity of semiconductor. The donors in 2D well are fully ionized whereas the volume impurities are ionized partially. $E_d \approx 0.01$ eV is the donor energetic level, N_{d0} is the donor doping concentration.

In TF method, the expression for *n[V]* can be obtained from the following formula:

$$N \equiv \int d^3\vec{r}\, n[V] = \iint d^3\vec{p}\, d^3\vec{r} f(\vec{p},\vec{r}) \qquad (2)$$

The Fermi distribution function is:

$$f(\vec{p},\vec{r}) = \frac{1}{4\pi^3\hbar^3}\frac{1}{1+\exp\left(\frac{E(\vec{p})+V(\vec{r})-\mu}{T}\right)}$$

The expression is given for electrons in the lowest parabolic Γ-valley (*n*-GaAs, GaN). Here $E(\mathbf{p}) = p^2/2m^*$ is the electron kinetic energy, μ is the Fermi energy, T is the temperature in energetic units; m^* is the effective mass. Therefore the formula for *n* is:

$$n[V] = N_C\Phi_{1/2}\left(\frac{\mu - V}{T}\right);$$

$$where \quad N_C = \frac{1}{2^{1/2}}\left(\frac{m^*T}{\pi\hbar^2}\right)^{3/2}, \qquad (3)$$

$$\Phi_{1/2}(v) = \frac{2}{\pi^{1/2}}\int_0^\infty \frac{u^{1/2}du}{1+\exp(u-v)}$$

Here N_C is the density of states in the conduction band, $\Phi_{1/2}(v)$ is the Fermi integral. In the case of *n*-Si, where the lowest valleys are lateral and the effective mass is anisotropic, and the integration over the quasi-momentum is more complex. The number of equivalent valleys should be taken into account too.

Below we use the atomic units: for distances $a_0^* = \varepsilon\hbar^2/(m^*e^2)$ and for energy $Ry^* = e^2/(2\varepsilon a_0^*)$. In undimensional variables, the basic equation of TF method for symmetrical δ-doped electron quantum well is:

$$\frac{d^2V}{dz^2} = 8\pi\{-n[V] + N_{d0}\times(2\exp(\frac{\mu - E_d - V}{T}) + 1)^{-1}\}; \qquad (4)$$

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

V. Grimalsky, L.M.. Gaggero-S., and S. Koshevaya are with CIICAp and Faculty of Sciences, the Autonomous University of State Morelos (UAEM), 62209, Cuernavaca, Mor., Mexico, E-mail: v_grim@yahoo.com; lgaggero@uaem.mx.
A. Garcia-B. is with Department of Mechatronics, the Polytechnic University of Pachuca (UPP), 43830, Pachuca, Hgo., Mexico; and with Advanced Materials and Devices Analysis Group, Institute for Microelectronics, TU Wien, 1040, Vienna, Austria, E-mail: barrientos@iue.tuwien.ac.at.

978-1-4244-7201-7/10/$26.00 © 2010 IEEE

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

The donor levels are assumed shallow and single charged [7].

The position of Fermi level μ has been obtained from the condition of neutrality:

$$n[V=0] = N_{d0} \times (2\exp(\frac{\mu - E_d}{T}) + 1)^{-1} \qquad (5)$$

Eq. (4) has been solved by the Newton method. The Fermi integral and its derivative have been approximated from [7]. The fast convergence has been demonstrated.

After calculation of $V(z)$, the energy levels E_j and wave functions $\Psi_j(z)$ of the discrete spectrum of the well have been computed from the Schrödinger equation:

$$\frac{d^2\Psi_j}{dz^2} - [V(z) - E_j]\Psi_j = 0; \int_{-\infty}^{+\infty} |\Psi_j|^2 \, dz = 1 \qquad (6)$$

The eigenproblem (6) has been solved by the shooting method.

To check the accuracy of TF method, it is possible to calculate also the electron concentration, due to localized states of the well [6]:

$$n(z) = \frac{T}{2\pi} \sum_j |\Psi_j(z)|^2 \times \log\left(1 + \exp\frac{\mu - E_j}{T}\right) \qquad (7)$$

In the limiting case $T = 0$ the Fermi distribution is step-like, the equation for TF method is:

$$\frac{d^2V}{dz^2} = -8\pi n[V], \quad n[V] = \frac{1}{3\pi^2}(-V)^{3/2}$$
$$\frac{dV}{dz}(z = +0) = 4\pi n_{2d}, \quad V(z \to \pm\infty) = 0 \qquad (8)$$

The donors are not ionized here $N_d(z) = 0$ and $\mu = 0$.

III. Results of Simulations

The simulations have been performed for *n*-GaAs. For *n*-GaAs the values are: $a_0^* = 9.14$ nm ≈ 10 nm, $Ry^* = 6.25$ meV. Typical results of simulations are given in Figs.1-4. One can estimate an applicability of the simplest version of TF method at $T = 0$ into the cases with $T > 0$.

It is seen that at 2D concentrations $n_{2d} = 10^{13}\ldots 2\times10^{13}$ cm^{-2} the results of TF method for the electron potential energy in the well $V(z)$ and the lowest energy levels (E_{s1}, E_{a1}) at $T = 0$ can be applied up till the temperatures $T \le 150\ldots200$ K (Figs.1,2, parts c,d). At smaller values of 2D doping $n_{2d} \le 5\times10^{12}$ cm^{-2}, TF method can be applied up till the temperatures $T \le 50\ldots70$ K (Figs.1,2, parts a,b). For higher energy levels, the coincidence takes place at lower temperatures T ≤ 70 K ($n_{2d} \sim 10^{13}$ cm^{-2}).

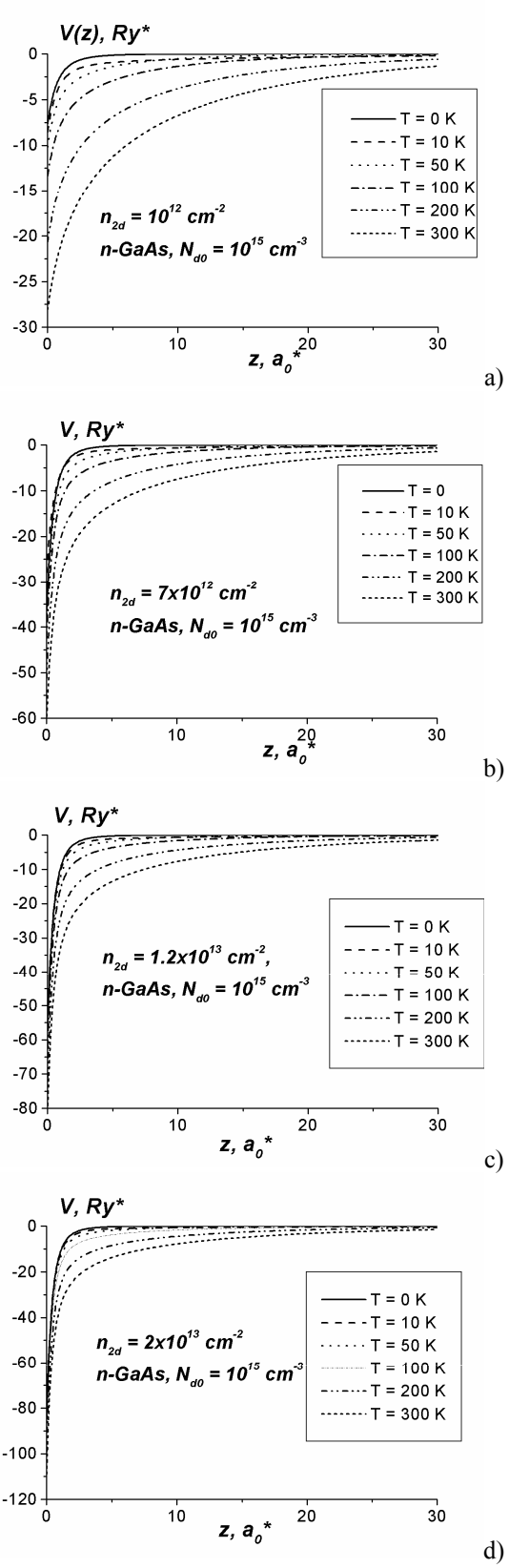
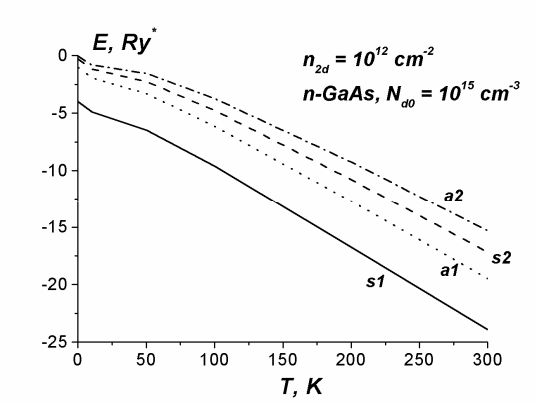
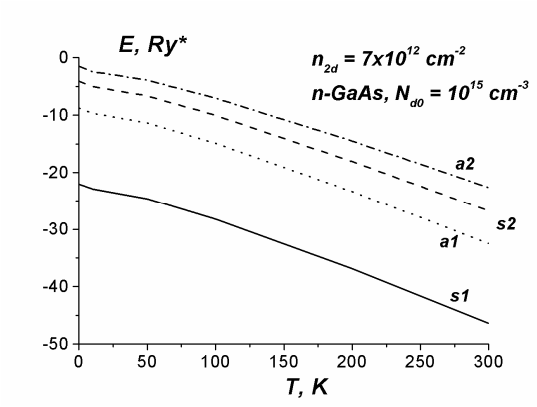


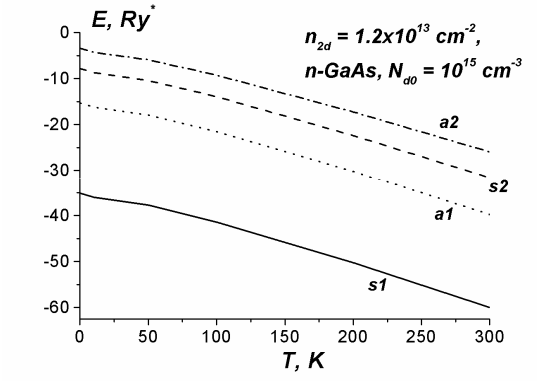
Fig.1. Profiles of electron potential energy $V(z)$ at different values of δ-doping n_{2d}. For *n*-GaAs $a_0^* = 9.14$ nm, $Ry^* = 6.25$ meV.



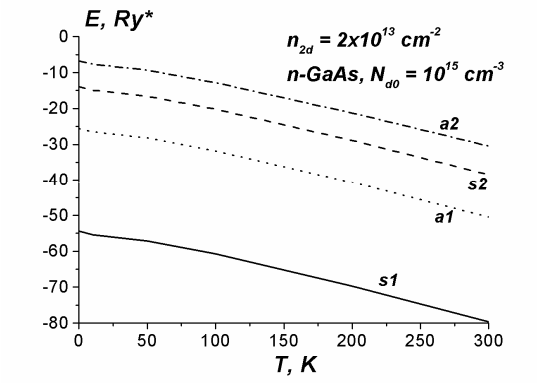
a)



b)



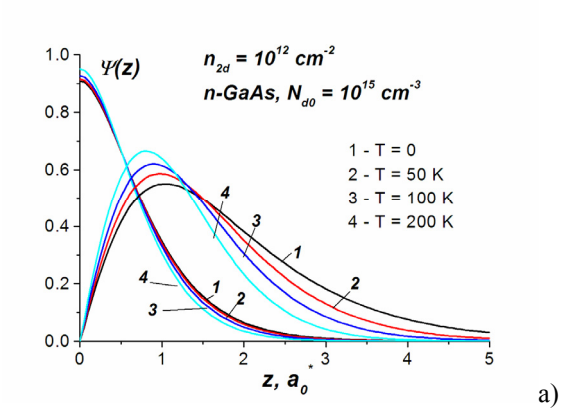
c)



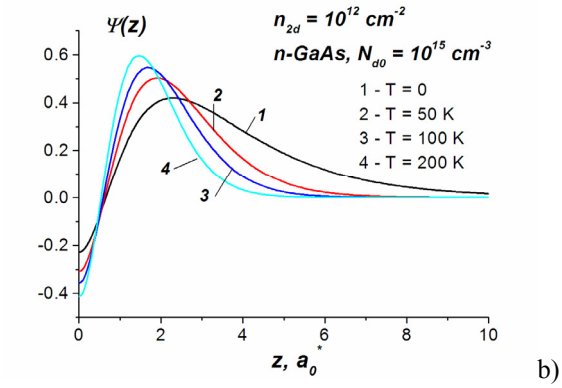
d)

Fig.2. Dependencies of the energy levels of the well of the lowest symmetric (s1,2) and antisymmetric (a1,2) states of the well.

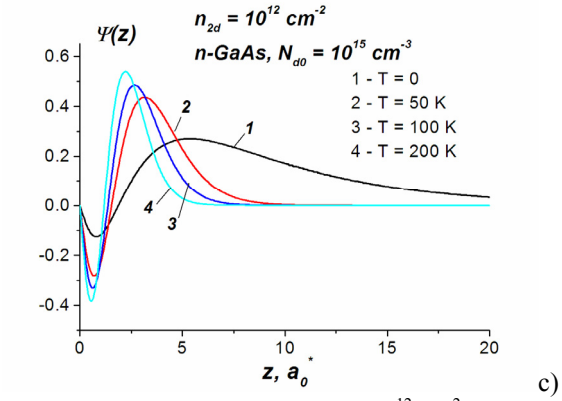
The calculated electron wave functions in the well are given in Figs.3,4. It is seen that TF method at T = 0 gives the correct results for the lowest symmetric and antisymmetric states up till the temperatures T ≤ 200 K, whereas for the second antisymmetric state there are some differences at 2D doping $n_{2d} \sim 10^{12}$ cm^{-2}. At higher 2D doping $n_{2d} \sim 10^{13}$ cm^{-2}, the wave functions for the higher state are just the same at $T = 0$ and $T = 200$ K (Fig. 4, c).



a)



b)



c)

Fig.3. Electron wavefunctions at $n_{2d} = 10^{12}$ cm^{-2}. Part a) is $\Psi_{s1}(z)$, $\Psi_{a1}(z)$; part b) is $\Psi_{s2}(z)$; part c) is $\Psi_{a2}(z)$.

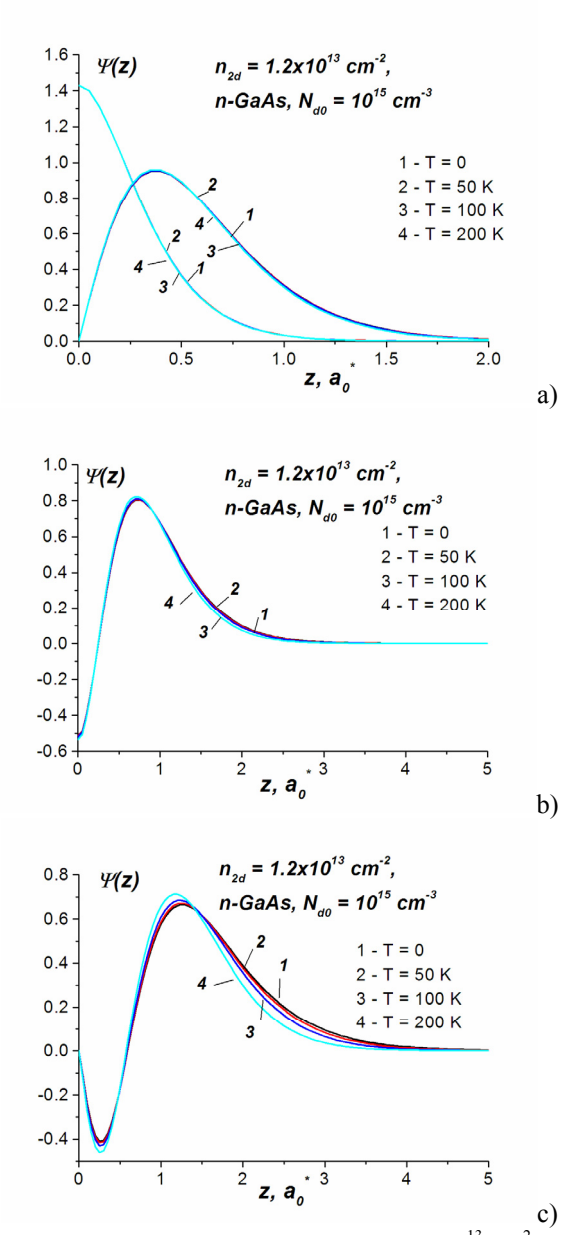


Fig.4. Electron wavefunctions at $n_{2d} = 1.2\times10^{13}$ cm^{-2}. Part a) is $\Psi_{s1}(z)$, $\Psi_{a1}(z)$; part b) is $\Psi_{s2}(z)$; part c) is $\Psi_{a2}(z)$.

In Fig. 5 the electron concentration $n(z)$ calculated both from TF method at $T = 200$ K (curve 1) and from the wave functions, Eq. 7, (curve 2) is given. A coincidence is demonstrated for the values $n \geq 10^{16}$ cm^{-3}. Moreover, TF method at $T = 0$ yields the same results for $n \geq 10^{18}$ cm^{-3}. Nevertheless, for $n < 10^{16}$ cm^{-3} there are differences between the curves 1 and 2. This fact seems natural, because TF method can be applied at high values of $n \geq 10^{17}$ cm^{-3}.

In TF method, it is possible to take into account the many-particle effects, like exchange-correlations. In the simplest approach, the additional electron potential energy $V_{xc} \approx -(2/\pi)(3\pi^2 n)^{1/3}$ should be used in Eqs. (3) and (8) [3]. Many particle effects can change the values of $n(z)$ at $n > 10^{18}$ cm^{-3} on 3…5%, as our simulations have demonstrated. But it is impossible to apply V_{xc} at $n < 10^{17}$ cm^{-3}, because in this case the basic TF method leads to essential errors, as seen from Fig. 5.

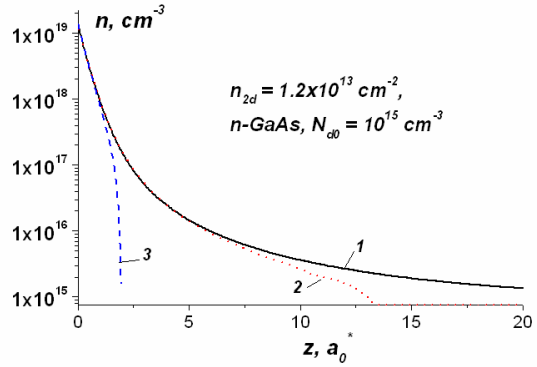


Fig. 5. The dependencies of electron concentration $n(z)$ calculated from TF method at $T = 200$ K (curve 1), from the wave functions (curve 2), and from TF method at $T = 0$ (curve 3).

IV. Conclusions

An application of Thomas – Fermi method at finite temperatures to δ-doped n-GaAs shows effectiveness and a good accuracy for calculation of the electron potential energy, wave functions and energy levels. It is possible to apply the simplest version of TF ($T = 0$) up till the temperatures $T \leq 200$ K at 2D doping levels $n_{2d} \sim 10^{13}$ cm^{-2}.

Acknowledgement

This paper was supported by SEP-CONACyT (Mexico).

References

[1] E.F. Schubert, A. Fischer, and K. Ploog, "The delta-doped field-effect transistor (δFET)", *IEEE Trans. Electron Devices*, vol. ED-33, pp. 625-632, 1986.

[2] K. Nakagawa, A.A. van Gorkum, and Y. Shiraki, "Atomic layer doped field-effect transistor fabricated using Si molecular beam epitaxy", *Appl. Phys. Lett.*, 1989, vol. 57, pp. 1869-1872.

[3] L.M. Gaggero-Sager, "Exchange and correlation via functional of Thomas-Fermi in delta-doped quantum wells", *Modelling Simul. Mater. Sci. Eng.*, 2001, vol. 9, pp. 1-5.

[4] E. Ozturk and I. Sokmen, "Intersubband transitions for single, double and triple Si δ-doped GaAs layers", *J. Phys. D,* 2003, vol. 36, pp. 2457-2464.

[5] W. Kiunke, E. Hammerl, I. Eisele e.a., "Electrical transport between delta layers in silicon", *J. Appl. Phys.*, 1992, vol. 72, pp. 3602-3610.

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

[7] Ying Fu and M. Willander, *Physical Models of Semiconductor Quantum Devices,* Dordrecht: Kluwer, 1999.