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Abstract

We investigated theoretically the change of electronic properties of Si δ-doped GaAs layer as a function of temperature. We studied the influence of temperature on the donor concentration for a nonuniform distribution, which is taken as different from the known Gaussian distribution. In order to obtain the electronic structure we have calculated self-consistent Schrödinger - Poisson equations. We have seen that the change of the electronic properties as dependent on temperature is less pronounced at higher doping concentration.

Key Words: δ-doped GaAs, electronic structure, temperature-dependence.

1. Introduction

Delta (δ, planar)-doped semiconductor structures have recently attracted much attention because of its potential technological applications in electronic and photonic devices [1,2], as well as being a source of basic research [3-16]. A typical δ-doped semiconductor contains a sheet of impurity atoms located within a few atomic layers of crystal and thus the doping profile along the growth direction z can be described by the Dirac's δ-function [17], i.e. $N_d(z) = N_d^{2D}\delta(z)$, where N_d^{2D} is the 2D donor concentration. This profile neglects the random distribution of donors in the doped layer, which is valid in the high-density limit [18].

Silicon is widely used as the n-type dopant in GaAs growth using molecular beam epitaxy (MBE). When Si donors are localized into an atomic plane during epitaxial growth, a sheet of ionized donors produces a V-shaped potential well which confines the electron motion along the direction perpendicular to a δ-doped plane and leads to formation of a quasi-two-dimensional electron gas (2DEG). The eigenstates of such a carrier gas are subbands with energies which depends on the shape of the space-charge potential. This subband structure has been calculated by solving Schrödinger - Poisson equations self-consistently.

In this study, for electrostatic potential profiles Poisson equation and for quantized carriers Schrödinger equation was solved self-consistently as dependent on temperature. We have investigated the influence of temperature on the δ-doping concentration for nonuniform distribution. The effect of diffusion of donor impurities along the growth direction has been compared in our previous studies [12, 14] for both the uniform distribution and nonuniform distribution. We conclude that the electronic structure are quite sensitive to the type of the donor distribution when the donor thickness is large, and the confinement is more effective for uniform distribution.

2. Theory

Our calculations are based on a self-consistent solution of Schrödinger and Poisson equations, in the one particle effective-mass approximation. The δ-doped layer is assumed to be inserted into an infinite quantum well whose thickness is L_0. The quantized energy levels E_i and their corresponding envelope functions $\psi_i(z)$ satisfy the following Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + V_H(z) + V_{xc}(z)\right)\psi_i(z) = E_i\psi_i(z), \tag{1}$$

where m^* is the electron effective mass, z is the direction perpendicular to the δ-doped layer, $V_H(z)$ is the effective Hartree potential, and $V_{xc}(z)$ is the exchange-correlation potential. The exchange-correlation interaction on the subband structure is only very weak [6,19]. Hence we can confidently neglect this effect. The Hartree approximation for the confining potential $V_H(z)$ is obtained by solving the Poisson equation:

$$\frac{d^2V_H(z)}{dz^2} = -\frac{4\pi e^2}{\varepsilon}[N(z) - N_d(z)]. \tag{2}$$

The relation relates the electron density to the wavefunctions

$$N(z) = \sum_{i=1}^{n_d} n_i|\psi_i(z)|^2, \tag{3}$$

where ε is the GaAs dielectric constant, $N_d(z)$ is the total density of ionized dopants, i is subband index and n_d is the number of filled states. The temperature-dependent concentration of electrons in the ith subband depends on the Fermi energy according to

$$n_i = \frac{m^*k_BT}{\pi\hbar^2}\ln\{1 + \exp[(E_F - E_i)/k_BT]\}, \tag{4a}$$

and at zero temperature for $E_i \leq E_F$ it is given as

$$n_i = \frac{m^*}{\pi\hbar^2}(E_F - E_i), \tag{4b}$$

where k_B is Boltzmann constant and E_F represents the Fermi energy. The position of the Fermi energy is calculated using a given donor concentration. In this work, the nonuniform distribution is different from a Gaussian distribution as used by A Ben Jazia et al. [11] and other authors. The nonuniform distribution is taken as

$$N_d(z) = \frac{N_d^{2D}}{\Delta z\{1 - \exp[-|L_0/\Delta z|]\}}\exp[-|2z/\Delta z|], \tag{5}$$

where L_0 is the well width and barriers are assumed to be infinitely high, Δz is thickness of the donor distribution and N_d^{2D} is the 2D donor concentration.

A flow chart of the self-consistent calculation is given in our previous study [13]. The self-consistent calculation of Eqs. (1)-(5) gives the electronic structure for Si δ-doped GaAs layer.

3. Results and Discussion

For the nonuniform distribution, we have calculated the electronic structure of Si δ-doped GaAs layer as a function of the temperature. In Figure 1 the confining potential, the subband energies with their squared envelope wavefunctions are shown for T = 0 K and T = 300 K, with $L_0 = 300$ Å, $N_d^{2D} = 5 \times 10^{12}$ cm^{-2} and $\Delta z = 20$ Å. The solid curves represent the obtained results at T = 0 K and the dashed curves at T = 300 K. As can be seen from Eq. 4a, due to both the exponential term in the logarithm and the linear prefactor term, the charge density increases with increasing temperature. The envelope wavefunctions of the higher subbands are more extended in the z direction, thus the electrons in the lowest subband has a lower mobility than the electrons in the higher subbands since the electrons in the lowest subband are mostly confined around the impurity ions and the scattering mechanism is predominant. Also, we see that temperature has a certain effect on the shape of the effective potential because of thermal excitation of electrons from the lowest subband into the higher ones. At the same time we see that, at the room temperature the higher subbands contribute to the mobility. By considering this property, at high temperature δ-doping can be used to increase the electron mobility in semiconductor devices.

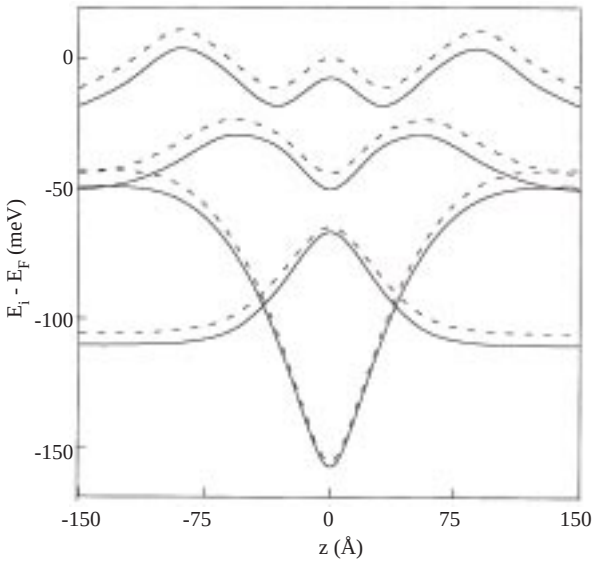

Figure 1. The effective potential profiles, the subband energies with their squared envelope wavefunctions at T = 0 K and T = 300 K, with $L_0 = 300$ Å,$N_d^{2D} = 5 \times 10^{12}$ cm^{-2} and $\Delta z = 20$ Å. The solid curves are results for T = 0 K and the dashed curves are results for T = 300 K. All values are referred to the Fermi energy level.

In Figure 2, the depth of the effective potential is shown as a function of temperature for different doping concentrations, with $L_0 = 300$ Å, and $\Delta z = 20$ Å. The depth of the effective potential depends strongly on increasing the doping concentration, but changes slightly with temperature.

The Fermi energy level is plotted versus temperature for the different doping concentrations in Figure 3. As shown in this figure, the Fermi level is very sensitive to the δ-doping concentration. As expected, while the Fermi energy increases with increasing the doping concentration, but it decreases with increasing the temperature. The Fermi energy curvature which decreases with temperature, is less pronounced at higher doping concentration.

For different doping concentrations, the change of the subband occupations as a function of the temperature are summarised in Table 1. Due to the high electron density in a δ-doped structure, more than one subband is populated. As shown in this table, the changes of the subband occupations are very sensitive to the δ-doping concentration and temperature. It is clear that, the distribution of the electrons over the levels depends on donor concentration and temperature.

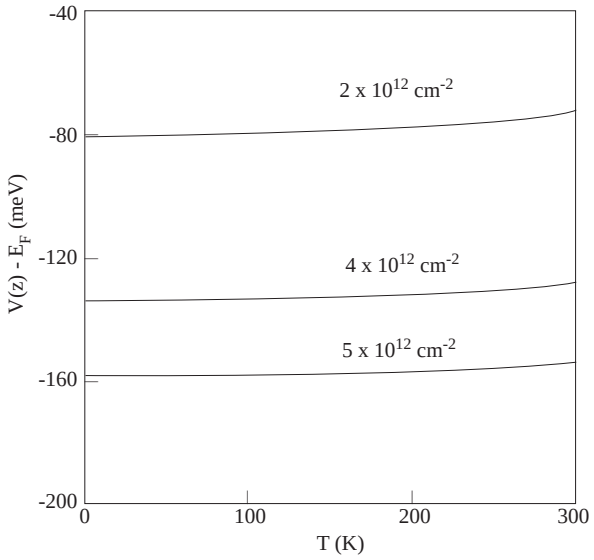

Figure 2. The depth of the effective potential versus temperature for different doping concentrations, with $L_0 = 300$ Å, and $\Delta z = 20$ Å. All values are relative to the Fermi level.

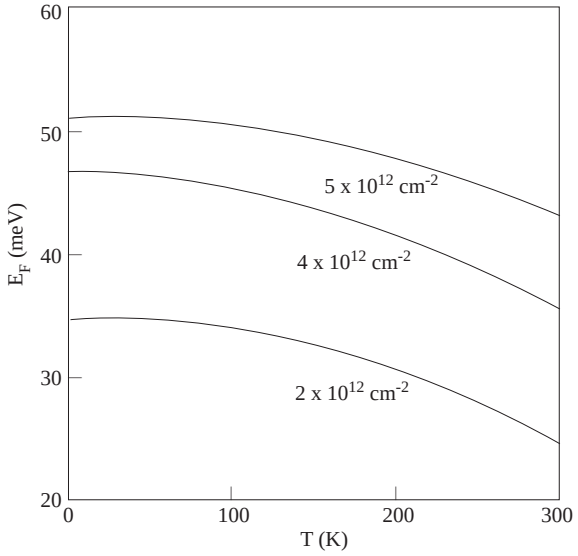

Figure 3. The Fermi energy level as a function of temperature for different doping concentrations, with $L_0 = 300$ Å, and $\Delta z = 20$ Å.

The ground E_1(a), first excited E_2 (b) and second excited E_3 (c) subband energies are shown as a function of temperature and doping concentration in Figure 4(a, b and c), respectively. As can be seen from these figures by increasing the δ-doping concentration, the subband energies are significantly changed. The subband energies change with increasing temperature since the subband occupation increases with temperature. This behavior is also seen in Table 1. In the subband energies near the Fermi energy, this changing is more evident.

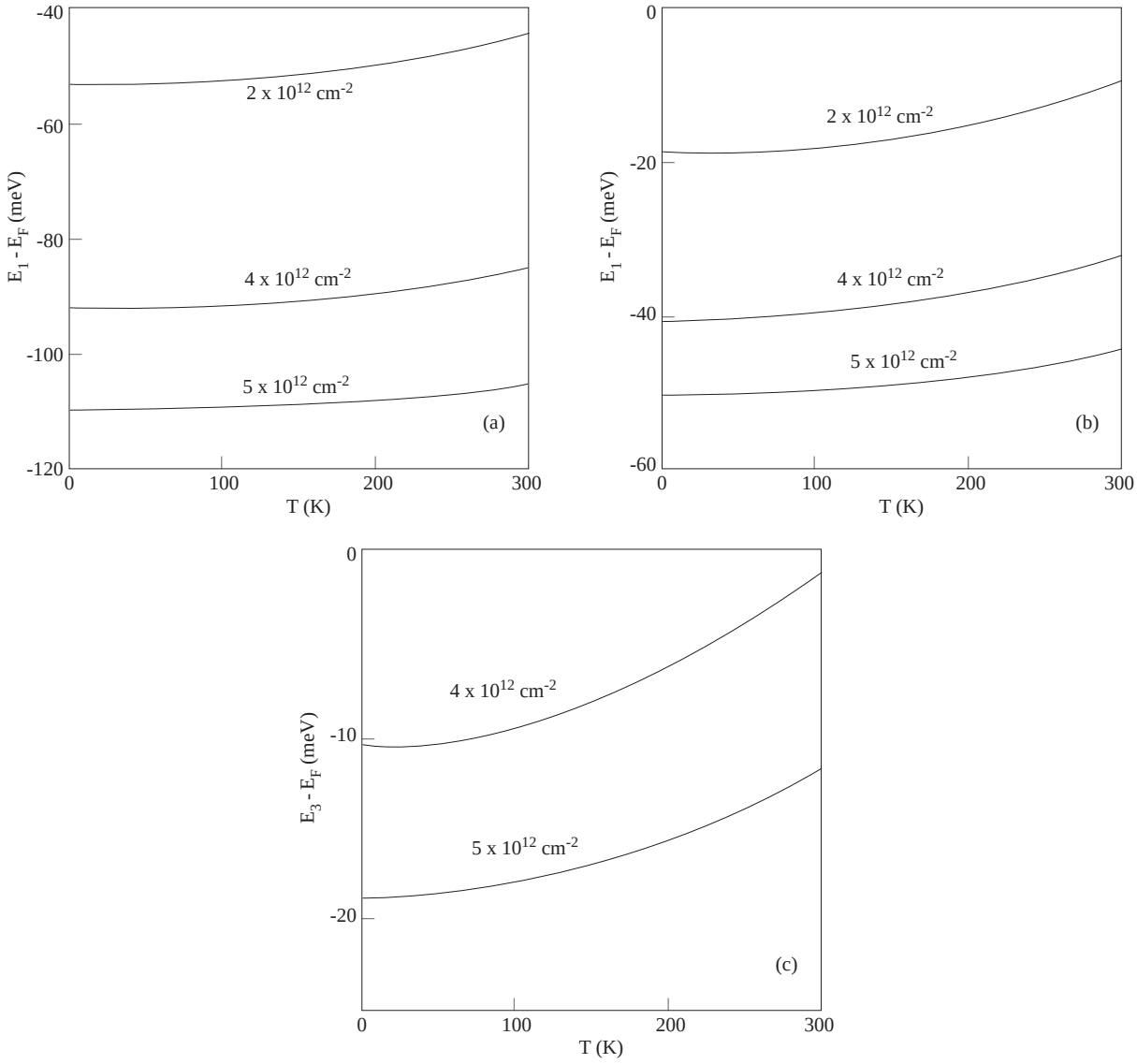

Figure 4. The calculated values of (a) the ground (b) the first excited and (c) the second excited subband energies as a function of temperature for different donor concentrations, with $L_0 = 300$ Å, and $\Delta z = 20$ Å. All subband energies are relative to the Fermi energy level.

As a general feature at a high-doping concentration ($N_d^{2D} = 5 \times 10^{12}$ cm^{-2}) the effective potential, the subband energies and Fermi energy level change slightly with temperature while at a low-doping concentration ($N_d^{2D} = 2 \times 10^{12}$ cm^{-2}) these changes were large. We have seen that the density of the carriers that appear due to the impurity atoms are more efficiently than the temperature on the subband structure.

4. Conclusion

We have investigated the changes of the electronic structure of Si δ-doped GaAs as dependent on the δ-doping concentration and the temperature for a nonuniform distribution. In this study, the nonuniform distribution is different from the Gaussian distribution used by other authors. To determine the electronic properties such as the effective potential, the subband energies, the subband occupations and Fermi energy level, the self-consistent methods of the Schrödinger and Poisson equations were used. It is shown that the subband structure changes significantly with increasing δ-doping concentration. An increasing doping

concentration in the δ-doped layer gives rise to the formation of a deeper potential profile and the electronic density profile becomes more localized around the δ-doped GaAs layer. These features can be used in controlling the confinement of carriers in δ-doped semiconductor devices. For many applications in devices and in many experimental situations, N_d^{2D} is definitely one of the most important physical quantity and it can be used as a tunable parameter for these systems.

Table 1. For T=0 K and T=300 K the obtained values of the subband occupations as dependent on different doping concentrations, with L_0 = 300 Å.

Temperature	N_d^{2D} (10^{12} cm^{-2})	Δz (Å)	$n_i(10^{12}$ cm$^{-2})$ i=1	i=2	i=3
T=0 K	2	20	1.484	0.515	–
T=300 K			1.364	0.635	–
T=0 K	4	20	2.574	1.131	0.294
T=300 K			2.496	1.077	0.426
T=0 K	5	20	3.081	1.404	0.515
T=300 K			2.964	1.355	0.680

Temperature has a certain effect on the electronic structure because of thermal excitation of electrons from the lowest subband into the higher ones. Also at the room temperature the higher subbands contribute to the mobility. Due to this property, at high temperatures δ-doping can be used to increase the electron mobility in semiconductor devices. From the self-consistent calculations, we have seen that the change of the electronic properties as dependent on temperature is less pronounced at higher doping concentration. At room temperature, the carriers which appear due to the impurity atoms lie more efficiently in the subband structure.

The δ-doping method gives ultimate control of the narrow doping profile. Novel, improved semiconductor devices have been developed by using δ-doping layer.

References

[1] E. F. Schubert, A. Fischer and K. Ploog, *IEEE Trans. Electron Devices,* **33**, (1986), 625.

[2] K. Ploog, M. Hauser and A. Fischer, *Appl. Phys. A,* **45**, (1988), 233.

[3] A. C. Maciel, M. Tatham, J. F. Ryan, J. M. Worlock, R. E. Nahory, J. P. Harbison and L. T. Florez, *Surf. Sci.*, **228**, (1990), 251.

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

[5] J. C. Egues, J. C. Barbosa, A. C. Notari, P. Basmaji and L. Ioriatti, *J. Appl. Phys.*, **70**, (1991), 3678.

[6] M. H. Degani, *Phys. Rev. B*, **44**, (1991), 5580.

[7] M. H. Degani, *J. Appl. Phys.*, **70**, (1991), 4362.

[8] M. L. Ke, J. S. Rimmer, B. Hamilton, J. H. Evan, M. Missious, K. E. Singer and P. Zalm, *Phys. Rev. B,* **45**, (1992), 14114.

[9] M. L. Ke, J. S. Rimmer, B. Hamilton, M. Missious, B. Khamsehpour, J. H. Evans, K. E. Singer and P. Zalm, *Surf. Sci.*, **267**, (1992), 65.

[10] S. M. Shibli, L. M. Scolfaro, J. R. Leite, C. A. C. Mendonça, F. Plentz and A. Meneses, *Appl. Phys. Lett.*, **60**, (1992), 2895.

[11] A. Ben Jazia, H. Mejri, H. Maaref and K. Souissi, *Semicond. Sci. Tech.*, **12**, (1997), 1388.

[12] E. Ozturk, Y. Ergun, H. Sari, I. Sokmen, *Superlattices and Microstructures*, **28**, (2000), 35.

[13] E. Ozturk, Y. Ergun, H. Sari, I. Sokmen, *Appl. Phys. A*, **73**, (2001), 749.

[14] E. Ozturk, Y. Ergun, H. Sari, I. Sokmen, *Journal of Applied Physics,* **91**, (2001), 2118.

[15] E. Ozturk, Y. Ergun, H. Sari, I. Sokmen, *Semicond. Sci. Tech.*, **16**, (2001), 421.

[16] E. Ozturk, Y. Ergun, H. Sari, I. Sokmen, *Appl. Phys. A,* 2002 (to be published).

[17] J. C. Henning and J.P. Ansems, *Semicond. Sci. Tech.*, **2**, (1987), 1.

[18] J. Kortus and J. Monecke, *Phys. Rev. B*, **49**, (1994), 17216.

[19] P. M. Koenraad et al., *Semicond. Sci. Tech.*, **5**, (1990), 861.