Influence of temperature on the electronic properties of Si $\delta$-doped GaAs structures

E. Ozturk$^{1,a}$, Y. Ergun$^{1}$, H. Sari$^{1}$, and I. Sokmen$^{2}$

$^1$ Cumhuriyet University, Department of Physics, 58140 Sivas, Turkey
$^2$ Dokuzeylul University, Department of Physics, Izmir, Turkey

Received: 1 October 2001 / Received in final form: 20 March 2002 / Accepted: 4 October 2002
Published online: 29 November 2002 – © EDP Sciences

Abstract. We have investigated theoretically the electronic structure of Si $\delta$-doped GaAs layers at $T = 0$ K and at room temperature. For a nonuniform distribution, we have studied their sensitivity to the donor concentration and the donor thickness. In this study, nonuniform distribution is different from Gaussian distribution used by other authors. From the self-consistent calculation, we have seen that at room temperature carriers which appear due to the impurity atoms are more efficient than temperature on the subband structure.

PACS. 73.90.+f Other topics in electronic structure and electrical properties of surfaces, interfaces, thin films, and low-dimensional structures

1 Introduction

During recent years, epitaxial-growth techniques have been currently used to prepare $\delta$-doped semiconductor structures, in which a sheet of impurity atoms is localized within a few monolayers of the material. Experimentally, $\delta$-doping profiles are achieved by growth interruption during epitaxial-growth by molecular beam epitaxy (MBE). If the doping thickness becomes smaller than other relevant length-scales, the doping profile can be mathematically described by a Dirac’s $\delta$-function. This profile neglects the random distribution of donors in the $\delta$-doping layer, which is valid in the high density limit [1].

The ionized impurities in the $\delta$-doped GaAs layer form a V-shaped potential well, and the electron energies are quantized into two-dimensional (2D) subband for motion perpendicular to the growth surface. The subband structure has been calculated by solving Schrödinger and Poisson equations self-consistently. The $\delta$-doped GaAs has attracted interest from both physics and applications [2,3]. The most widely used dopant atoms in GaAs are silicon and beryllium, which act as $n$-type and $p$-type dopant, respectively. The $\delta$-doping technique has been used widely to introduce carrier-confinement effects [4–10]. Due to this property of localizing impurities in space, $\delta$-doping is used in devices to give rise to quantum confinement of carriers [11,12]. This doping method gives ultimate control of the narrow doping profile and will play a significant role in future quantum electronic and photonic devices research.

In the present paper, by using a new alternative method explained in [13] we have calculated theoretically the electronic structure of Si $\delta$-doped GaAs by solving Schrödinger and Poisson equations self-consistently at $T = 0$ K and at room temperature. We have investigated the influence of the $\delta$-doping concentration, the $\delta$-layer thickness and temperature on the subband structure for nonuniform distribution. In this work, nonuniform distribution is different from Gaussian distribution used by Ben Jazia et al. [9] and other authors. The effect of diffusion of donor impurities along the growth direction has been compared in [10] for both a uniform distribution and a nonuniform distribution.

2 Theory

The electronic structure of a Si $\delta$-doped GaAs layer has been investigated by using a self-consistent calculation in the effective-mass approximation. We have calculated the confining potential, the charge density, the subband energies, the subband occupations and the Fermi energy level self-consistently by solving Schrödinger and Poisson equations.

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

$$\frac{d^2V(z)}{dz^2} = -\frac{4\pi e^2}{\varepsilon}[N(z) - N_0(z)] \tag{2}$$
where \(m^*\) is the electron effective mass, \(z\) is the direction perpendicular to the \(\delta\)-doped layer, \(V(z)\) is the guessed V-shaped potential profile with different slopes (Fig. 1), and \(V_{\text{ex}}(z)\) is the exchange-correlation potential, \(\varepsilon\) is the GaAs dielectric constant and \(N_0(z)\) is the total density of ionized dopants. The exchange-correlation interaction on the subband structure is only very weak [14]. Hence we can confidently neglect this effect hereafter.

The wave functions in these different regions are expressed as

\[
\psi_i(z) = \begin{cases} 
A \exp[Kz] & \text{I. region} \\
A_1 \chi_1(z) + B_1 \chi_2(z) & \text{II. region} \\
A_2 \chi_2(z) + B_2 \chi_2(z) & \text{III. region} \\
A_3 \chi_3(z) + B_3 \chi_3(z) & \text{IV. region} \\
A_4 \chi_4(z) + B_4 \chi_4(z) & \text{V. region} \\
A_5 \chi_5(z) + B_5 \chi_5(z) & \text{VI. region} \\
A_6 \chi_6(z) + B_6 \chi_6(z) & \text{VII. region} \\
B \exp[-Kz] & \text{VIII. region} 
\end{cases}
\]

(3)

where \(A_i[\chi(z)]\) and \(B_i[\chi(z)]\) are Airy and Bairy functions, respectively and

\[
K = \sqrt{\frac{2m^*(V_0 - E_i)}{\hbar^2}}
\]

\[
\chi_1(z) = \left(\frac{m^*(L_0 - L_1)^2}{2\hbar^2V_1^2}\right)^{1/3} \times \left(V_0 - \frac{2V_1}{L_0 - L_1} \left(z + \frac{L_0}{2}\right) - E_i\right)
\]

(4)

\[
\chi_2(z) = \left(\frac{m^*(L_1 - L_2)^2}{2\hbar^2V_2^2}\right)^{1/3} \times \left(V_0 - V_1 - \frac{2V_2}{L_1 - L_2} \left(z + \frac{L_1}{2}\right) - E_i\right)
\]

(5a)

By using the boundary conditions and the normalization condition for the wave functions, the energy levels and the wave functions can be obtained. The details about this method can be seen in our previous study [13]. The density of electrons is related to the wavefunctions by the relation

\[
N(z) = \sum_{i=1}^{n_d} n_i |\psi_i(z)|^2
\]

(4)

where \(n_i\) is the temperature-dependent number of electrons per unit area in the \(i\)th subband given by

\[
n_i = \frac{m^* k_B T}{\pi \hbar^2} \ln \left(1 + \exp \left(\frac{(E_F - E_i)}{k_B T}\right)\right)
\]

(5a)

and at zero Kelvin

\[
n_i = \frac{m^*}{\pi \hbar^2} (E_F - E_i)
\]

(5b)

where \(n_d\) is the number of filled states, \(i\) is subband index, \(k_B\) is Boltzmann constant and \(E_F\) is Fermi energy.

It is known that if there is atomic diffusion from an initial \(\delta\)-distribution, the final distribution should be a Gaussian distribution. But in our calculation we use an exponential donor distribution which is given in equation (7). We can easily get the analytical solutions by using the exponential distribution, and also we know from our previous study that the difference between the results of the exponential distribution and the Gaussian are not significant [15]. Due to this fact, we used an exponential distribution in our calculations as \(N_0(z) = A \exp[-|2z|/\Delta z]\). We should point out that the donor distribution in the \(x-y\) plane is uniform.

From the condition that the total number of electrons must equal the total number of donors:

\[
\sum_i n_i = N_0^{2D}
\]
By using the condition which is given in equation (6) we obtain the nonuniform distribution in the range from $-\frac{L_0}{2}$ up to $\frac{L_0}{2}$ as below,

$$N_d(z) = \frac{N_a^{2D}}{\Delta z \{1 - \exp[-|L_0/\Delta z|]\}} \exp[-|2z/\Delta z|]$$  \hspace{1cm} (7)

where $L_0$ is the top width of the V-shaped confining potential which is taken as a constant in our calculation (see Fig. 1), $\Delta z$ is the thickness of the donor distribution and $N_a^{2D}$ is the 2D donor concentration.

Initially we approximate the potential by a series of linear potentials with fixed $L_1, L_2, V_1, V_2, V_3$ (Fig. 1). The approximate potential is taken as a initial condition in self-consistent calculation, and after first iteration the obtained potential is a continuous curve.

The self-consistent calculation of equations (1–7) gives the subband structure.

### 3 Results and discussion

We have calculated the electronic structure of a Si δ-doped GaAs layer for a nonuniform distribution at $T = 0$ K and $T = 300$ K. In Figures 2a and 2b the confining potential and the electronic density profiles are shown for three different doping concentrations ($N_a^{2D} = 1.5, 3, 5 \times 10^{12}$ cm$^{-2}$), respectively. The solid curves represent the obtained profiles at $T = 0$ K and the dashed curves at $T = 300$ K. By increasing the doping concentration both the depth of the confining potentials and the density profiles are importantly changed as can be seen in these figures. At high doping concentrations, an increasing charge density in the δ-layer gives rise to the formation of a deeper potential energy profile and the electronic density profile is more localized around the δ-doped GaAs layer. These features could be used in controlling the confinement of carriers in devices using this type of doping.

As can be seen from equation (5a), the charge density increases slightly with increasing temperature owing to both the exponential term in the logarithm and the linear prefactor term. 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. The depth of the effective potential energy increases with charge density, thus at higher doping concentrations and temperatures, its effects are more significant on the subband structure. When the temperature is raised to 300 K, the change curvature of the effective potential and the density profile is less pronounced at higher doping concentrations as can be seen from Figures 2a and 2b.

The subband energies and the Fermi energy level as a function of doping concentration are shown in Figure 3. The solid curves represent the energy levels at $T = 0$ K and the dashed curves at $T = 300$ K. The thick solid curves indicate the Fermi energy for $T = 0$ K and the thick dashed curves for $T = 300$ K. As shown in this figure, the change of the subband energies and Fermi level is very sensitive to the δ-doping concentration. The subband energies increase with increasing temperature because temperature changes the subband occupation as can be seen from Table 1. As expected, while the Fermi energy level increases with increasing the doping concentrations, it decreases with increasing temperature. As can be seen from Figures 2a, 2b and 3 at a low-doping concentration ($N_a^{2D} = 1.5 \times 10^{12}$ cm$^{-2}$) the confining potential, the charge density, the subband energies and the Fermi energy level strongly change with temperature while at high-doping concentration ($N_a^{2D} = 5 \times 10^{12}$ cm$^{-2}$) these changes are small. We have seen that at room temperature, the carriers which appear due to the impurity
The calculated values of the subband energies and Fermi energy level as a function of donor concentration. The solid curves represent the energy levels for $T = 0$ K and the dashed curves for $T = 300$ K. The thick solid curves indicate the Fermi energy at $T = 0$ K and the thick dashed curves at $T = 300$ K with $L_0 = 500$ Å, and $\Delta z = 20$ Å.

atoms are more efficient than temperature on the subband structure.

In Figures 4a and 4b we show the confining potential and the density profile for three different doping thicknesses ($\Delta z = 20, 50, 100$ Å), respectively. The solid curves indicate the obtained profiles at $T = 0$ K and the dashed curves at $T = 300$ K. As seen in these figures, the confining potential and the density profile are quite sensitive to the thickness of the donor distribution. Since at the narrow doping thickness the donor impurities distribution is at a small range than that of the wider donor thickness, the effective potential is deep, the band bending is larger and the density profile is more localized. Due to this feature of localizing impurities in space, $\delta$-doping is used in semiconductor devices to rise the carrier confinement. The temperature dependence of the confining potential curvature and of the density profile is more evident at wider donor thickness.

The subband energies and the Fermi energy level versus the $\delta$-doping thickness are shown in Figure 5. The solid curves display the obtained energy levels at $T = 0$ K and the dashed curves at $T = 300$ K. The thick solid curves show the Fermi energy for $T = 0$ K and the thick dashed curves for $T = 300$ K. Both the subband energy levels and Fermi energy decrease with increasing donor thickness as can be seen from this figure. The variation of the subband energies and Fermi level as dependent on temperature is smaller for narrow donor thickness.

For different doping concentrations and different doping thicknesses, the change of the subbands occupation as dependent on the temperature are summarized in Table 1. Due to the high electron density in a $\delta$-doped structure, more than one subband is populated. As shown in this table, the change of the subbands occupation is very sensitive on the $\delta$-doping concentration, on the $\delta$-layer thickness and on temperature. It is clear that the electron distribution over the levels is dependent on donor concentration, on the thickness of the donor distribution and on temperature. Thus, both the donor concentration and the donor thickness can be used as fitting parameters in these systems.

4 Conclusions

We have investigated the changes of the subband structure of Si $\delta$-doped GaAs as dependent on $\delta$-doping concentration, on $\delta$-layer thickness and on temperature by
Table 1. For $T = 0$ K and $T = 300$ K the obtained values of the subband occupations as dependent on different doping concentrations and different donor thicknesses.

<table>
<thead>
<tr>
<th>Temperature</th>
<th>$N_d^{2D}$ ($10^{12}$ cm$^{-2}$)</th>
<th>$\Delta z$ (Å)</th>
<th>$n_i$ ($10^{12}$ cm$^{-2}$)</th>
<th>$i = 1$</th>
<th>$i = 2$</th>
<th>$i = 3$</th>
<th>$i = 4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T = 0$ K</td>
<td>1.5</td>
<td>20</td>
<td>0.987</td>
<td>0.345</td>
<td>0.166</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$T = 300$ K</td>
<td>3</td>
<td>20</td>
<td>1.907</td>
<td>0.761</td>
<td>0.330</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$T = 0$ K</td>
<td>5</td>
<td>20</td>
<td>2.845</td>
<td>1.265</td>
<td>0.565</td>
<td>0.322</td>
<td>-</td>
</tr>
<tr>
<td>$T = 300$ K</td>
<td>5</td>
<td>50</td>
<td>2.578</td>
<td>1.356</td>
<td>0.688</td>
<td>0.376</td>
<td>-</td>
</tr>
<tr>
<td>$T = 0$ K</td>
<td>5</td>
<td>100</td>
<td>2.161</td>
<td>1.381</td>
<td>0.872</td>
<td>0.584</td>
<td>-</td>
</tr>
<tr>
<td>$T = 300$ K</td>
<td>5</td>
<td>100</td>
<td>2.131</td>
<td>1.314</td>
<td>0.883</td>
<td>0.670</td>
<td>-</td>
</tr>
</tbody>
</table>

using a new alternative method and a nonuniform distribution. We use a nonuniform distribution which is different from Gaussian distribution used by other authors. We have calculated the electronic properties such as the effective potential, the density profile, subband energies, subband occupations and Fermi energy level by solving Schrödinger and Poisson equations self-consistently. We have shown that the subband structure depends strongly on doping concentration and donor thickness. By increasing the $\delta$-doping concentration and the $\delta$-doping thickness, the electronic structure is significantly changed. Thus, both the donor concentration and the donor thickness can be used as tunable parameters for these systems. We have seen that the dependence of the electronic properties on temperature is less pronounced at high doping concentration and narrow donor thickness.

The $\delta$-doping technique is very interesting because it represents the ultimate technological limit for impurity profiles; the technique has resulted in a series of novel electronic and photonic devices.

References