Electron energy levels in a δ-doped layer in GaAs

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Calculated results for energy levels of electrons in a Si δ-doped layer in GaAs are presented at $T=0$ K and ambient temperature. Their sensitivity to the donor distribution is examined. The many-body exchange-correlation effects are taken into account in the local-density-functional approximation.

I. INTRODUCTION

The capability of confining carriers in a very narrow region is of great interest for many device applications. With the advances in molecular-beam epitaxy (MBE), it is possible to control the growth in such a way that the dopants can be localized during growth interruption, resulting in a doped region confined to a single atomic layer.[1] This so-called δ, or planar, doping of semiconductor structures has attracted considerable interest. The carriers released from the dopants are confined by the potential well induced by the space charges. The δ-doping technique represents the ultimate control of a dopant profile and certainly will play an important role in future quantum-electronic- and -photonic-device research. Profiles with full widths at half maximum (FWHM) of 30 and 20 Å determined by capacitance voltage have been reported for Si and Be-doped structures, respectively.[2,3]

Several experimental techniques such as infrared-absorption,[4] Raman,[5–7] and magnetotransport measurements,[8–11] have been used to study the electron energy levels formed in the doping induced potential well. Luminescence spectroscopy of a single δ-doped layer,[12,13] however, is complicated because the potential confining the electrons is repulsive for the photocreated holes and, due to this fact, a considerable reduction of the overlap between hole and electron wave functions occurs and therefore the radiative recombination probability is expected to be low. In order to ensure confinement of the photocreated holes, experimentalists have studied a single Si δ-doped layer in GaAs placed close to the GaAs surface or placed close to a heterointerface of GaAs and $Al_xGa_{1-x}As$. Since in these structures the photocreated holes can be confined, radiative recombination from the quasi-two-dimensional electron gas is observed.

For the theoretical point of view, a single δ-doped layer has been studied in the Hartree[8] and in the Thomas-Fermi approximations.[14] It has been proved that the semiclassical Thomas-Fermi approximation gives results that are equivalent to those obtained from the much more elaborate self-consistent approximation. However, in this study an ideal δ-doped layer was considered. The diffusion of donors along the growth direction and the presence of a *p*-type doped semiconductor background were neglected. Zrenner, Koch, and Ploog[8] have calculated the electron energy levels in the Hartree approximation at $T=0$ K and have considered the spread of the donor impurities in the calculations assuming that the donor impurities are distributed homogeneously in a finite sheet along the growth direction. This effect modified considerably the effective potential and consequently the electron energy levels. Recently Zrenner[15] has studied the influence of the *DX* center on the capacitance-voltage characteristics of a single δ-doped layer in GaAs close to a Schottky barrier at $T=300$ K, and concluded that *DX* centers are very important for a proper understanding of the experimental results.

In the present paper we present results of a self-consistent calculation of a single δ-doped layer in GaAs at $T=0$ K and ambient temperature. It is well known that the Hartree approximation overestimates the electron-electron interaction; we go beyond the Hartree approximation and use the local-density approximation[16] (LDA) in order to include many-body exchange-correlation effects. It is shown that in this system exchange and correlation effects are less important than the effect of finite, nonzero temperature on the electron energy levels. The effect of diffusion of the donor impurities along the growth direction is considered in two different models: (i) uniform distribution and (ii) nonuniform distribution. In the first case the dopants are distributed uniformly in a sheet of thickness Δz, and in the second case a Gaussian distribution is used to describe the donor doping along the growth direction. Our calculations reveal that the electronic subbands are quite sensitive to the donor distribution principally when Δz is large.

In Sec. II a description of the calculation approach, which is the self-consistent-field approximation within the Hohenberg-Kohn-Sham local-density approximation,[16] is given. The numerical results for the electron energy levels are presented in Sec. III. In Sec. IV we present our conclusions.

II. FORMALISM

We use the effective-mass approximation in order to describe the electrons in the host semiconductor and replace the localized donor charges by a z-dependent charge density that has been averaged over the x-y plane.

The interactions between electrons in the conduction band can be separated into a Hartree term due to the electrostatic potential of the total electron density and an exchange-correlation term. Hohenberg, Kohn, and Sham[16] have shown that such exchange-correlation potential is given by taking the functional derivative of the exchange-correlation part of the ground-state energy with respect to the electron density. The exchange-correlation potential energy is, in general, an unknown functional of the electron density $n(z)$, and in the simplest approximation—the local-density approximation—the exchange-correlation potential is approximated by the exchange-correlation contribution to the chemical potential of a homogeneous electron gas having a uniform electron density n_0 which is equal to the local electron density $n(z)$ of the inhomogeneous system. It is interesting to note that this simple approximation works surprisingly well and has been used very successfully to obtain ground-state properties of many systems.[17]

The problem is reduced to a one-body Schrödinger equation when LDA is used, with electrons moving in an effective potential which is a sum of the Hartree potential and the exchange-correlation potential.

Due to the translational symmetry in the x-y plane in our system, the wave functions can be written as

$$\Psi_{n\mathbf{k}}(\mathbf{r})=\frac{\exp(i\mathbf{k}\cdot\boldsymbol{\rho})}{\sqrt{S}}\xi_n(z)\ , \tag{1}$$

and the eigenvalues are given by

$$E_{n\mathbf{k}}=\varepsilon_n+\frac{\hbar^2k^2}{2m^*}\ , \tag{2}$$

where $\mathbf{k}$ is the wave vector of the electron parallel to the x-y plane, m^* is the effective mass, $\mathbf{r}=(x,y)$, S is the sample area, and $\xi_n(x)$ and ε_n are obtained from the one-dimensional Schrödinger equation

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}+V_H(z)+V_{\rm xc}(z)\right]\xi_n(z)=\varepsilon_n\xi_n(z)\ . \tag{3}$$

The Hartree potential due to the electrostatic interaction of the electrons with themselves and with the impurity charges is obtained from the following equation:

$$\frac{d^2V_H(z)}{dz^2}=-\frac{4\pi e^2}{\epsilon}[n(z)-N_I(z)]\ , \tag{4}$$

with

$$n(z)=\sum_i N_i|\xi_i(z)|^2\ , \tag{5}$$

and

$$N_i=\frac{m^*k_BT}{\pi\hbar^2}\ln\left[1+\exp\left[\frac{E_F-\varepsilon_i}{k_BT}\right]\right]\ , \tag{6}$$

N_i being the number of electrons per unit area in the ith subband, ϵ the dielectric constant, E_F the Fermi energy, and $N_I(z)$ the total density of ionized dopants $N_{D^+}-N_{A^-}$. The exchange-correlation potential $V_{\rm xc}(z)$ has been parametrized by several authors,[18,19] and different forms for $V_{\rm xc}$ give similar quantitative results for the subband energy levels. The simple analytic parametrization suggested by Hedin and Lundqvist[20] will be used here:

$$V_{\rm xc}(z)=-\frac{e^2}{2\epsilon a_0^*}\frac{2}{\pi\alpha r_s}[1+0.7734x\ln(1+x^{-1})]\ , \tag{7}$$

where $\alpha=(4/9\pi)^{1/3}$, $r_s=[4\pi a_0^{*3}n(z)/3]^{-1/3}$, $x=r_s/21$, and a_0^* is the effective Bohr radius.

The explicit temperature dependence of $V_{\rm xc}$ is neglected,[21] and we assume only an implicit temperature dependence which arises because $n(z)$ depends on temperature through the occupations of the self-consistent energy levels of the system.

The self-consistent solution of Eqs. (3)–(7) gives us the charge-density profile, the subband energy levels, and the effective potential.

III. NUMERICAL RESULTS

Equations (3)–(7) have been solved self-consistently considering two different distributions of donor impurities: (i) uniform, and (ii) nonuniform. In the first approximation, it is assumed that the donor impurities are distributed homogeneously in a sheet of thickness Δz; and in the second approximation, it is considered that a Gaussian distribution describes the donor impurity doping. It is shown that the electron energy levels are very sensitive to the donor distribution and generally the confinement is more effective for a uniform distribution.

The acceptor concentration is assumed to be constant in the whole system and equal to 5×10^{15} cm^{-3} and, to describe properly the potential band bending, a very thick system was considered in the calculation.

We first give results for δ doping at absolute zero temperature for several values of the thickness of the layer where the donors are distributed. For the nonuniform distribution this thickness corresponds to the full width at half maximum. Calculated energy levels for $N_D=8\times10^{12}$ cm^{-2} are shown in Fig. 1. The dashed curves correspond to the uniform distribution and the solid curves are results for a Gaussian distribution, both of which are calculated with inclusion of exchange and correlation. The occupation of the subbands N_i is another important quantity which can be obtained experimentally from Shubnikov–de Haas oscillations observed during magnetotransport measurements. Figure 2 shows the occupation of the subbands as a function of Δz and we note that the potential well accommodates more electrons for the uniform distribution than for the Gaussian distribu-

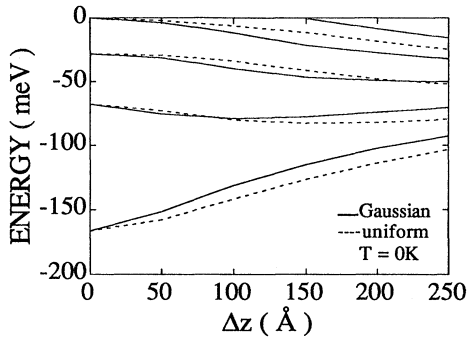

FIG. 1. Calculated values of the energy levels with inclusion of exchange and correlation of a δ-doped layer in GaAs at $T=0$ K. Solid curves are results for a Gaussian distribution with FWHM equal to Δz and dashed curves are results for a uniform distribution. All energies in this figure are relative to the Fermi energy and $N_D=8\times10^{12}$ cm^{-2}.

tion. The effective potential is presented in Fig. 3 for six different widths of the distribution Δz, 0, 50, 100, 150, 200, and 250 Å. As can be seen, the uniform distribution presents a stronger confinement than the nonuniform case, principally when Δz is large.

The electronic density for both cases, uniform and nonuniform distribution, are shown in Fig. 4 and it is clear that when the width Δz increases an accentuated difference between the uniform and nonuniform distribution occurs. Figure 4 shows that the electronic density for a uniform distribution is more localized than for a Gaussian distribution. Certainly this difference has some important implications in the transport properties of these structures.

The effects of exchange and correlation in the energy levels and in the effective potential can be seen from the differences between the solid and dashed curves in Fig. 5. In Fig. 5a $N_D=5\times10^{12}$ cm^{-2}, the donor distribution is

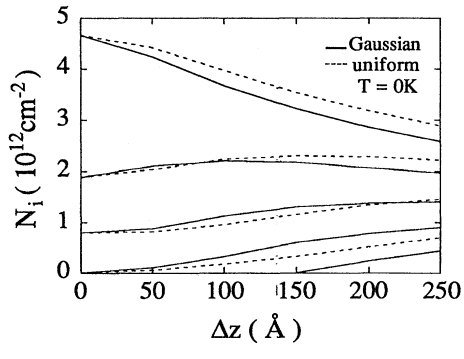

FIG. 2. Individual subband density N_i as a function of the thickness Δz. Solid curves are results for a Gaussian distribution and dashed curves are results for a uniform distribution. The donor concentration is $N_D=8\times10^{12}$ cm^{-2}.

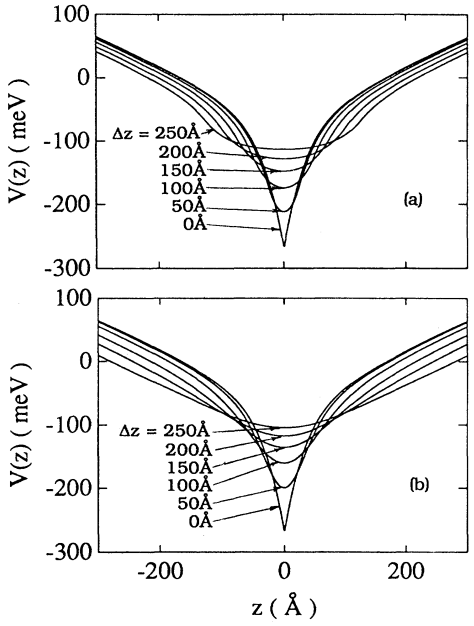

FIG. 3. Effective potential calculated at $T=0$ K and $N_D=8\times10^{12}$ cm^{-2} for various values of Δz assuming (a) uniform distribution, and (b) Gaussian distribution. The Fermi energy E_F is taken equal to zero.

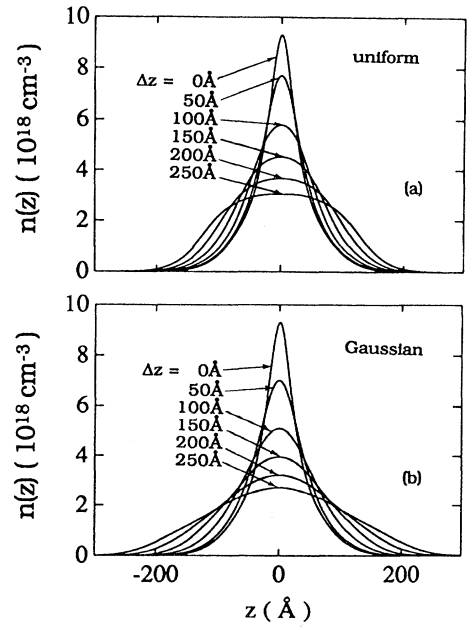

FIG. 4. Electronic density calculated at $T=0$ K and $N_D=8\times10^{12}$ cm^{-2} for various values of Δz assuming (a) uniform distribution, and (b) Gaussian distribution.

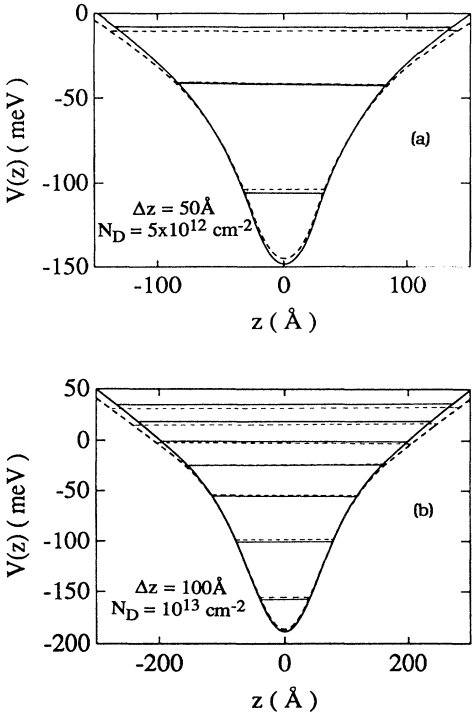

FIG. 5. Effective potential and energy levels for a δ-doped layer in GaAs with (solid curve) and without (dashed curve) exchange and correlation effects for (a) uniform distribution, $T=0$ K, $\Delta z=50$ Å, and $N_D=5\times10^{12}$ cm^{-2}, and (b) Gaussian distribution, $T=0$ K, $\Delta z=100$ Å, and $N_D=10^{13}$ cm^{-2}. All energies in these figures are relative to the Fermi energy E_F.

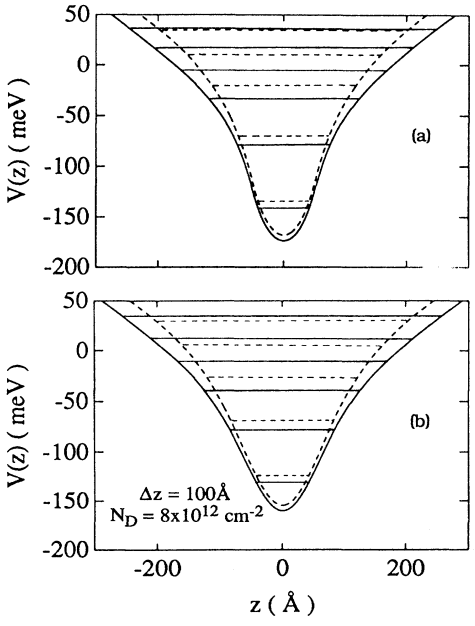

FIG. 6. Effective potential and energy levels for a δ-doped layer in GaAs for $T=0$ K (solid curve) and $T=300$ K (dashed curve) with $\Delta z=100$ Å and $N_D=8\times10^{12}$ cm^{-2}. (a) Uniform distribution, and (b) Gaussian distribution. All energies in these figures are relative to the Fermi energy E_F.

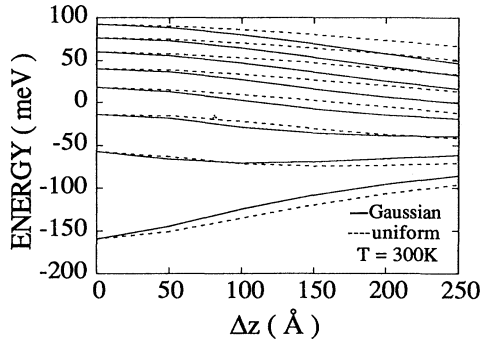

FIG. 7. Calculated values of the energy levels with inclusion of exchange and correlation of a δ-doped layer in GaAs at $T=300$ K. Solid curves are results for a Gaussian distribution with FWHM equal to Δz and dashed curves are results for a uniform distribution. All energies in this figure are relative to the Fermi energy and $N_D=8\times10^{12}$ cm^{-2}.

uniform, and $\Delta z=50$ Å, and in Fig. 5(b) a Gaussian distribution was used with $N_D=10^{13}$ cm^{-2} and $\Delta z=100$ Å. Inclusion of exchange and correlation lightly increases the carrier concentration in the well.

The change of the energy levels and the effective potential when the temperature is raised to 300 K for a δ-doped layer with $N_d=8\times10^{12}$ cm^{-2} and $\Delta z=100$ Å is shown in Figs. 6(a) and 6(b) for a uniform distribution and a Gaussian distribution, respectively. The temperature changes the occupation of the subbands, and lightly increases the carrier concentration in the well. The energy levels as a function of the width of the donor distribution are shown in Fig. 7 where the dashed curves represent the uniform distribution and solid curves the Gaussian distribution for $N_D=8\times10^{12}$ cm^{-2}. The occupation of the subbands as a function of Δz is presented in Fig. 8.

IV. CONCLUSIONS

We have studied the changes of the electron energy levels in a δ-doped layer in GaAs as a function of the

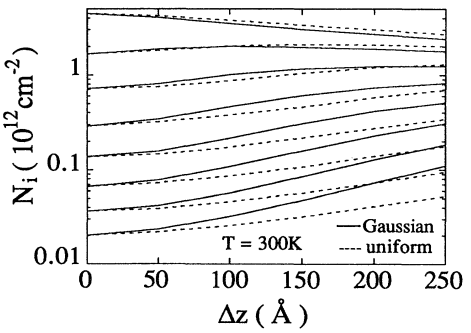

FIG. 8. Individual subband density N_i as a function of the thickness Δz. Solid curves are results for a Gaussian distribution and dashed curves are results for a uniform distribution. The donor concentration is $N_D=8\times10^{12}$ cm^{-2} and $T=300$ K.

donor distribution and concentration, and temperature. Two different models are used to describe the distribution of the donor impurities: (i) uniform, and (ii) nonuniform. In the uniform model the donors are homogeneously distributed in a sheet of thickness Δz, and for the second model a Gaussian with FWHM equal to Δz is used to describe the donor distribution. It is shown that the electronic subbands are quite sensitive to the donor distribution, and that the electronic confinement is more effective for uniform distributions. Many-body exchange-correlation effects are taken into account in the local-density approximation. It is shown that these effects are less important than the effects of finite nonzero temperature on the electron energy levels. The electron energy levels are very sensitive to all parameters involved in the calculation, such as the donor concentration and distribution, acceptor concentration, and temperature. The doping distribution depends strongly on how the sample is grown and in order to compare our results with the experimental results more information about the sample should be available.

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