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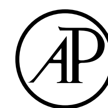

Electronic structure of modulation-doped heterostructures: electric field effects

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Self-consistent energy levels of electrons in modulation-doped GaAs/$Ga_{1-x}Al_xAs$ heterostructures are presented and their dependence on various device parameters are examined. The results of the calculation of the electric field effects on the shape of the confinement potential, the electron concentration and the shape of the wavefunction are presented.
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Key words: heterostructures, polarization, GaAs/$Ga_{1-x}Al_xAs$.

1. Introduction

The two-dimensional electron gas (2DEG) of a modulation-doped GaAs/$Ga_{1-x}Al_xAs$ heterostructure is now widely used in high-speed electronic devices such as high electron mobility transistors. The basic idea of modulation doping is to introduce impurities in barrier material so that the electron mobility will be improved as a result of spatial separation of electrons and their parent ionized impurities. The most important parameters that determine the 2DEG properties (mobility and electron concentration) are: the spacer-layer thickness, the donor doping concentration in n-GaAlAs, the Al mole fraction in $Ga_{1-x}Al_xAs$, and the background impurity concentration in the GaAs region. These parameters are optimized to obtain highest possible 2DEG mobilities and electron concentrations in the channel.

The great interest in the properties of 2DEG has led to a number of calculations of their energy levels and other electronic properties [1–4]. The methods employed for the calculation include self-consistent numerical solutions of the Schrödinger and Poisson equations [1–3], and variational calculations [4–8]. The earlier variational calculations involved various approximations such as the Hartree approximations [4], the neglect of tunnelling to the barrier region [5, 6] and the use of the finite or infinite triangular potential well [7]. The reader is referred to excellent reviews by Weisbuch [9], Hiyamizu [10], and Morkoc [11] for detailed discussions of electronic and transport properties of modulation-doped heterostructures. In this work, we present our self-consistent calculations of energy levels with and without the external electric field. The next section gives a description of the calculation. The results and conclusions are summarized in Section 3.

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2. Theory

To determine the energy levels and charge transfer in single heterojunctions we have to solve the coupled Poisson and Schrödinger equations self-consistently,

$$\frac{d^2V_H(z)}{dz^2} = \frac{4\pi e}{\kappa}\left[\sum_i n_i\chi_i^2(z) - N_D^+(z) + N_A^-\right], \tag{1}$$

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m(z)}\frac{\partial}{\partial z} + \frac{\hbar^2}{2m(z)}(k_x^2+k_y^2) + V_b(z) - eV_{sc}(z)\right]\chi_i(z) = E_i\chi_i(z), \tag{2}$$

where

$$V_{sc}(z) = V_H(z) + V_{xc}(z), \tag{3}$$

and $V_{xc}(z)$ is the exchange-correlation potential, $V_b(z)$ is the barrier potential, n_i is the areal concentration of electrons in the ith subband, N_D^+ and N_A^- are the donor and acceptor concentrations, κ is the static dielectric constant and $m(z)$ is the position-dependent effective mass.

At finite temperature T, the chemical potential μ is given by,

$$n_i = m_i\frac{k_BT}{\pi\hbar^2}\ln\left[1+\exp\left(\frac{\mu - E_i}{k_BT}\right)\right]. \tag{4}$$

At $T = 0$ K, this equation reduces to

$$n_i = \frac{m_i}{\pi\hbar^2}(\mu - E_i)\Theta(\mu - E_i), \tag{5}$$

where Θ is the step function. We need to supplement the above equations with the boundary conditions $\chi_i \to 0$ as $z \to \pm\infty$ and $\frac{1}{m(z)}\frac{\partial\chi_i}{\partial z}$ should be continuous everywhere. We further require the heterojunction to be in electrical equilibrium,

$$\sum_i n_i + \int_{-\infty}^{+\infty} dz(N_A^- - N_D^+) = 0. \tag{6}$$

At $T = 0$ K, the sharpness of the Fermi–Dirac distribution function introduces further simplifications and the acceptor and donor contributions to $V_{sc}(z)$ becomes

$$V_A(z) = \frac{2\pi e}{\kappa}N_A^- z(z - l_A) \tag{7}$$

$$V_D(z) = -\frac{2\pi e}{\kappa}(N_D - N_{b,A})(z + l_D + w)^2 + V_0, \tag{8}$$

where l_A and l_D are acceptor and donor depletion lengths, respectively, w is the spacer thickness and $N_{b,A}$ is the concentration of acceptors in the barrier region and V_0 is the integration constant needed for the continuation of the potential at w. In the depletion length approximation the charge balance equation can be written as

$$N_Dl_D = \sum_i n_i + N_{dep} + N_{b,A}(w + l_D), \tag{9}$$

where $N_{dep} = N_Al_A$. The transferred charge is $\sum_i n_i = N_s$.

We follow a self-consistent variational procedure to solve the coupled Poisson and Schrödinger equations [5]. We choose a modified Fang–Howard [8, 12] trial wavefunction which allows wavefunction penetration into the barrier region. We use an expression parametrized by Hedin and Lundquist [13] for the local exchange-correlation potential.

The electric field effects are included in the calculation by modifying the wavefunctions with exponentially

Table 1: Parameters used in self-consistent calculations.

Al content	$x = 0.3$
Acceptor concentration in GaAs	$N_{dep} = 0.5 \times 10^{11}$ cm^{-2}
Donor concentration in AlGaAs	$N_D = 2.0 \times 10^{18}$ cm^{-3}
Spacer layer thickness	$w = 60$ Å
Donor binding energy	$E_D = 60$ meV
Effective masses	$m(\text{GaAs}) = 0.070m_0$
	$m(\text{AlGaAs}) = 0.088m_0$
Dielectric constants	$\kappa(\text{GaAs}) = 13.1$
	$\kappa(\text{AlGaAs}) = 12.2$
Barrier height	$V_b = 225$ meV

decaying parts as discussed by Bastard [8]. We define a quantity P, which corresponds to the electron polarization in case where only the wavefunction distorts under an electric field, as

$$P = \langle ez \rangle_{F=0} - \langle ez \rangle_F, \tag{10}$$

where F denotes the strength of the applied electric field [14, 15].

The calculation of the expectation values is performed by using a modified Fang–Howard [8] trial wavefunction,

$$\chi_i(z) = \begin{cases} M \exp(\kappa_b z/2) & z \leq 0 \\ N(z + z_0) \exp(-bz/2), & z \geq 0, \end{cases} \tag{11}$$

in the case of no external electric field. The self-consistent potential profile with subband energies and E_F are determined through a simultaneous solution of eqns (1) and (2).

The external electric field is considered to modify the trial wavefunction into the form

$$F_i(z) = \chi_i(z) \exp(-\beta z), \tag{12}$$

and the term $\gamma F z$ is added to the Hamiltonian. The self-consistent calculation is repeated as in the zero-field case with the new wavefunction and Hamiltonian.

3. Results and conclusions

The parameters required for the self-consistent solution of the coupled Poisson and Schrödinger equations are listed in Table 1. These parameters are chosen to correspond to the experimental work of Hiyamizu *et al.* [16]. The donor binding energies are determined by considering the experimental results of Ishibashi *et al.* [17] and Ishikawa *et al.* [18]. We use a value of $E_D = 60$ meV corresponding to the case of AlAs mole fraction $x = 0.3$. We have tested the sensitivity of the energy levels to all the parameters in the calculation.

The calculated self-consistent potential V_{sc}, the ground subband and Fermi energy are shown in Fig. 1. It is known that the exchange and correlation are not as important in the present system as in the Si inversion or accumulation layers, but they affect the results quantitatively. Exchange and correlation pushes the subband energy E_0 and E_F down, and results in a higher N_s value. This also means that the inclusion of exchange and correlation increases the carrier concentration at which the Fermi level crosses into the second subband. From the penetration of the wavefunction we deduce that the average position of electrons is shifted in the negative z-direciton by about 17 Å from the case of infinite barrier height. This shift seems to be insensitive to the amount of charge transferred N_s, in the electric quantum limit we are considering.

Figure 2 shows the 2DEG concentration N_s as a function of spacer layer thickness w. The experimental

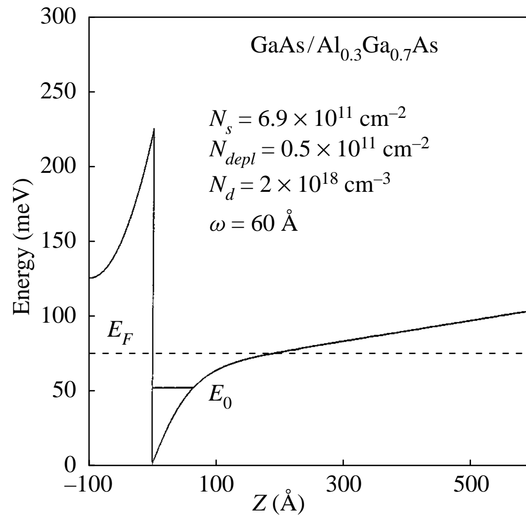

Fig. 1. The calculated self-consistent potential, the ground subband E_0, and Fermi energy E_F with parameters shown in the inset.

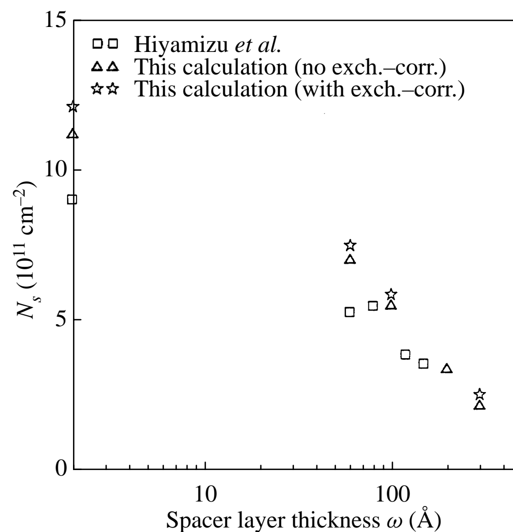

Fig. 2. The calculated 2DEG concentration N_s as a function of the spacer layer thickness w. The experimental results are from Hiyamizu *et al*. [16] obtained at 5 K without illumination.

results are taken from Hiyamizu *et al.* [16]. The agreement between our calculated values and experiment is rather good.

Figure 3 shows the 2DEG concentration N_s as a function of donor doping concentration N_D. Although the overall agreement with the experimental results of Hiyamizu *et al.* [16] is good, the discrepancies become larger for large donor concentrations. This depends rather sensitively on the spacer layer thickness w.

Figure 4 shows the dependence of self-consistently calculated N_s on the barrier height V_b. Increasing V_b means increasing energy separation between the donor level in GaAlAs and the ground subband level in GaAs thus more electrons are transferred to the GaAs region. This is also why the delta-doping increases N_s as a

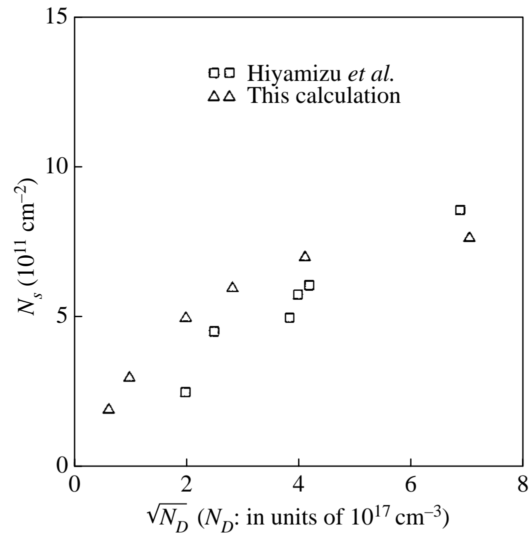

Fig. 3. The calculated 2DEG concentration N_s as a function of the donor concentration N_D. The experimental results are from Hiyamizu *et al*. [16] obtained at 77 K.

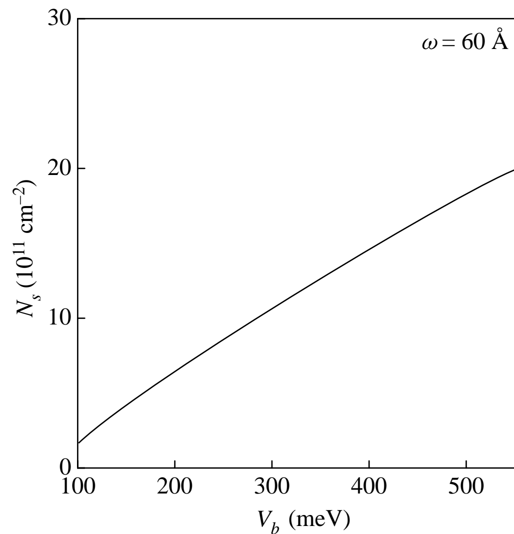

Fig. 4. The dependence of N_s on the barrier height V_b.

result of the confinement effect which pushes the δ-subband energy level up in GaAlAs, resulting in larger effective barrier height.

We calculated also the P values defined by eqn (10) by repeating the whole self-consistent calculation for each value of the applied electric field F. Figure 5 shows P values as a function of applied electric field F, for the calculated values of $N_D = 2 \times 10^{18}$ cm^{-3} and $N_D = 1.3 \times 10^{18}$ cm^{-3} corresponding approximately to the experimental case of Harris *et al*. [19]. The behaviour of ground subband electrons under the applied

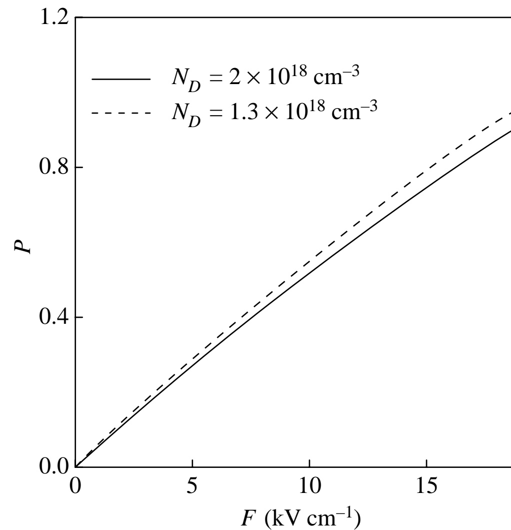

Fig. 5. The calculated P values as a function of applied electric field for donor concentrations $N_D = 1.3 \times 10^{18}$ cm^{-3} and $N_D = 2 \times 10^{18}$ cm^{-3}.

electric field is as expected. The lower value of N_D produces lower N_s which also means that the subband energy level is pushed up corresponding to decreased confinement. This is why we observe higher P values for lower N_D.

The nonparabolicity of the conduction band of GaAs is not taken into account in this work, except that we take an effective mass ($m = 0.07m_0$) slightly larger than the value at the conduction band minimum of bulk GaAs. This affects the kinetic energy which has only a small contribution to the subband energy. We have also neglected the image term in the Hamiltonian. The effect of this term is apparently extremely small and is discussed in detail by Stern and Das Sarma [3].

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