Calculation of charge carrier concentration profile and magnetoresistance in modulation doped structures with a wide potential well

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Abstract. We investigated Fermi charge carriers’ concentration profile in modulation doped structures with a wide quantum well. We have formulated hydrodynamic equations both in the absence of magnetic field and in parallel magnetic field. We have obtained analytical solutions for the carrier concentration as a function of the tangential coordinate in the potential well. In a quantum area near the interface, we carried out quantum mechanical calculations taking into account the effect of electric and magnetic fields. The carrier concentration profile and magnetoresistance in parallel magnetic field are presented for modulation doped Si/SiGe/Si structures.

1. Introduction

We investigate the properties of the charge carrier systems with the Fermi statistics in modulation doped structures with a wide quantum well. All carriers in the two-dimensional conducting channel are formed due to the ionization of impurities in the doped layer, separated from the quantum well by the spacer. We study the carrier system with a sufficiently high density, such that effectively three-dimensional inhomogeneous electron state is formed. The carrier concentration profile is asymmetric due to significant interaction of the electrons with the electric field of the doped layer. In such structures the calculations of the Fermi electron state becomes difficult to calculate since screening effects are to be taken into account.

The problem of calculating such carrier concentration profile for self-consistent confinement potential has a long history. It was solved numerically many times (in particular, in ref. [1]). Approximate analytical solutions were only performed with some simplifying assumptions (in particular, in ref. [2]). The screening was assumed to be much smaller than the well width, which is satisfied only for very high doping level. However, carrier systems with the screening length comparable to the well width are of interest because of greater mobility and significant effects of magnetoresistance [3].

Calculations of Fermi carriers’ states in modulation doped structures in strong magnetic fields require consideration of the self-consistent effect of the screening and the magnetic field, so, the problem becomes even more complicated.

This paper is devoted to derivation of the charge carrier concentration profile model in modulation doped structures both in the absence of magnetic field and in parallel magnetic field. The point of our work is to consider the screening effect without further simplifying assumptions. We have
formulated a hydrodynamic model and obtained an analytical solution for the charge carrier concentration as a function of the transverse coordinate in the quantum well. In a quantum area (near the interface) we solved the Schrödinger equations.

2. Calculation of carriers’ concentration profile in a potential well without magnetic field

In this paper, we study the carrier system with a sufficiently high density a wide quantum well. In such system, the de Broglie wavelength of electrons is smaller than the potential well width. So the characteristic length of change of the wave function (the length of the de Broglie wavelength $\lambda$) is smaller than the characteristic length of potential variation (quantum well width $L$). In this case an effectively three-dimensional inhomogeneous electron state is formed. This electron system is quasi-classical (except for regions near the interface) and the hydrodynamic approximation can be used.

Within the hydrodynamic approach, we calculated a three-dimensional charge carrier concentration $n(z)$, which changes only in transversal coordinate $z$, on the basis of the thermodynamic condition of total energy conservation:

$$\mu + E_{\text{int}} = \text{const}$$ (1)

Here $\mu = \mu(n(z)) = \left(\frac{3\pi^2}{2}\right)^{2/3} \frac{h^2}{m_k^{2/3}} n(z)^{2/3}$ is the chemical potential of the charge carrier system, $E_{\text{int}} = E_{\text{int}}(n(z)) = e \cdot \Phi(z)$ is the electrostatic interaction energy. The electrostatic potential $\Phi$ is determined by the Poisson equation

$$\frac{d^2 \Phi}{dz^2} = \frac{4\pi \cdot e}{\chi} n(z),$$

where $\chi$ is the permittivity of the medium.

We are considering structures with the impurity layer is located far enough from the quantum well, so that the distance between the ions and charge carriers is far greater than the distance between the ions in the doped layer. In this case we can assume that charge carriers interact with the whole ions’ layer. Then the Poisson equation implies

$$e \cdot \frac{d\Phi}{dz} = e \left( E_i - \frac{4\pi \cdot e}{\chi} \int_0^z n(\zeta) \cdot d\zeta \right)$$ (2)

Here, $z=0$ is a coordinate of the interface from the side of the doped layer and $E_i$ is the unscreened field of the ions’ layer.

Differentiating (1) and taking into account (2), we get the equation for $n(z)$:

$$-E_0 + K_0 \int_0^z n(\zeta) \cdot d\zeta = \left[ n(z) \right]^{1/3} \cdot \left( \frac{dn}{dz} \right).$$ (3)

Here $E_0 = \frac{2 \cdot e \cdot m \cdot E_i}{3(3\pi)^{2/3} \cdot h^2}$, $K_0 = \frac{8\pi \cdot e^2 \cdot m}{3(3\pi)^{2/3} \cdot h^2 \cdot \chi}$.

The equation (3) describes the equilibrium of attractive forces of electrons to the ions’ layer (the left-hand side of the equation) and the repelling forces of electrons by the Fermi pressure (the right-hand side of the equation) in each interval $dz$ in the potential well.

We solved (3) with the boundary condition $\frac{dn}{dz}\big|_{z=L} = 0$, which means that on the right boundary of the potential well the ions’ field is fully offset by the field of charge carriers. We have obtained the analytical solution of the equation (3) in terms of hypergeometric functions:

$$z(n) = L - K \cdot n_L^{-5/6} \cdot \left( n_L^{2/3} \right) \cdot F\left(\frac{2}{5}, \frac{1}{2}, \frac{7}{5}, \sqrt{(n/n_L)^{2/3} - 1}\right)$$ (4)
with $K = \frac{3}{8} \left( \frac{5 \cdot (3\pi)^{2/3} \cdot \hbar^2 \cdot Z}{8\pi \cdot e^2 \cdot m} \right)^{1/2}$ and $n_z = n|_{z=L}$. Then $n(z)$ is given by the inverse function to $z(n)$.

It is remarkable that our solution is valid for any ratio between the screening length and well width. Detailed solution of the integro-differential equation (3) is given in ref. [4].

Calculation by formula (4) gives a sharp peak for $n(z)$ in the area immediately adjacent to the barrier (Figure 1). In this area, the hydrodynamic model is no longer applicable. Due to a rapid increase of Fermi energy, Fermi wave vector $k_F$ increases faster than $z$, i.e. $dk_F/k_F \geq dz/2\pi z$. So, there are not enough particles with a definite wavelength $dz/2\pi$. The intersection of curves in the inset of Figure 1 shows the coordinate $z \geq z_B$ where hydrodynamic model starts to be valid.

![Figure 1](image_url)

Figure 1. Concentration profile of holes in Si/SiGe/Si structure with doping level $N_i=2.2 \cdot 10^{11} \text{ cm}^{-2}$, $L=30 \text{ nm}$, $U_B=92 \text{ meV}$. Solid red line is calculations using hydrodynamic model. Blue line is computed using Schrodinger equation in mean-field approximation.

In quantum area we have to solve the effective Schrodinger equation

$$-rac{\hbar^2}{2m} \frac{d^2 \Psi(z)}{dz^2} + V(z) \cdot \Psi(z) = E \cdot \Psi(z)$$

We have used the electron wave in the well as $\Psi_w(z) = A_0 \exp(k_B z)$, where $l = (\hbar^2 / 2m e E_J)^{1/3}$, $k_B$ is the wave vector in the barrier. The coefficients $A_0$ and $\delta$ were calculated from the continuity condition of wave function and its derivative at $z=0$.

The coefficient $C_0$ and the value of $n_L$ were chosen so that $\int_{L_p}^L n(z)dz = N_i$, where $N_i$ is a two-dimensional density of ions, $L_p$ is depth of penetration into the barrier, $L_p<0$.

We described the quasi-classical area using the hydrodynamic approach and quantum area using the Schrodinger equation. The results of our calculations according to the above model are presented in Figure 2. This profile differs substantially from the symmetrical concentration profile of two-dimensional charge carrier system in a quantum well with quantum confinement levels.
3. Calculation of carriers’ concentration profile in a potential well in parallel magnetic field

Now we study the charge carrier system in a magnetic field applied parallel to the two-dimensional layers (along the x-axis). We consider the Fermi system with $\lambda < L$. Moreover, we study charge carrier system that satisfies the condition $k_F \cdot \lambda_H > 1$, where $\lambda_H = (\hbar c/eH)^{1/2}$ is the magnetic length. In this case the electron wave function is formed at the scale smaller than the magnetic length. In this case the hydrodynamic approach is applicable. We neglect spin-related effects, because the Zeeman spin splitting in a parallel field is small (in p-Si/SiGe/Si quantum well) [5].

In an external magnetic field, in addition to electrical forces, Lorentz force $F = e\frac{v}{c}[v \times H]$ acts on the charge carriers. Since the magnetic field is directed along the x-axis and the transversal velocity is zero in the equilibrium state, then the Lorentz force has only z-component: $F_z = -e\frac{v}{c} H_x$. The charge carriers in a magnetic field have a local velocity $v_z(z) = h^{-1} \cdot \partial \varepsilon_k(z) / \partial k$, where $\varepsilon_k(z)$ is the total energy of the charge carriers. The velocity $v_z$ has different signs near the opposite interfaces (according to the slope of the charge carrier profile). There are local currents $J_y$ in the quantum well. (Currents lines are closed and the resulting drift current in the y-direction is zero.)

The Fermi carrier system possesses diamagnetic properties. The diamagnetic susceptibility $\chi_{dia}$ is given by $\chi_{dia}(z) = -\frac{1}{3} \cdot \frac{e^2}{c} \cdot \frac{3^{1/3} \cdot \pi^{-4/3}}{4 \cdot m c^2} \cdot n^{1/3}(z)$. An induced magnetic field $H_{ind}$ arises due to diamagnetic effect: $H_{ind}(z) = 4\pi \cdot \chi_{dia}(z) \cdot H$. The total magnetic field $\tilde{H}_{ind}(z) = H + H_{ind}(z)$ is the sum of external field and the induced field. From the Maxwell equation

$$\text{rot} \tilde{H}_{ind} = \frac{4\pi}{c} \tilde{J} + \frac{\partial \tilde{E}}{\partial t},$$

where $\tilde{J}$ is the total current, and time derivative is zero (because we consider the steady state), we get

$$\frac{\partial}{\partial z} H_{ind}(z) = \frac{4\pi}{c} J_y(z)$$

Substituting $J_y(z) = e \cdot n(z) \cdot v_z(z)$ we obtain $v_z(z) = -\frac{1}{12} \cdot \frac{e}{c} \cdot \frac{3^{1/3} \cdot \pi^{-4/3}}{m} \cdot H_x \cdot \frac{1}{3} \cdot n^{-3/3}(z) \cdot \frac{\partial n(z)}{\partial z}$.

Then the force balance equation takes the form
\[-E_0 + K_o \cdot \int_0^z n(z) \cdot d\zeta = \left( n(z) \right)^{1/3} + K_i \cdot \left( n(z) \right)^{5/3} \frac{d}{dz}(n(z)). \] (5)

Here \( K_i = \frac{e^2}{c^2} \frac{H_i^2}{54 \cdot 3^{1/3} \cdot \pi^{2/3} \cdot h^2}. \) This equation describes the equilibrium of attractive forces of electrons to the ions’ layer (the left-hand side of the equation) and Lorentz force and the repelling forces of electrons by the Fermi pressure (the right-hand side) in each interval \( dz \) in the potential well.

In a magnetic field, the Fermi gas pressure changes due to the diamagnetic effect. Although magnitude of the induced magnetic field \( H_{\text{ind}}(z) \) is quite small, the effect depends upon the derivative of total field \( H + H_{\text{ind}}, \) and thus the influence of diamagnetic effect becomes substantial. The changing total magnetic field is related to the local current \( J_y(z) \) through the Maxwell equation and therefore it is related to the pressure of carriers’ gas. This current flows orthogonal to the magnetic field and also orthogonal to the pressure gradient, and creates additional pressure.

We solved (5) with the boundary conditions \( \frac{dn}{dz}(z=L) = 0. \) While the integro-differential equation (5) is quite complicated we managed to solve it analytically

\[ z(n) = L - 3 \left( \frac{6}{5} K_o \right)^{-1/2} \left( n_L^{-1/6} \cdot \int_1^y \frac{dy}{\left( y^3 - 1 \right)^{1/2}} + K_i \cdot n_L^{-3/2} \cdot \int_1^y \frac{dy}{\left( y^3 - 1 \right)^{1/2}} + \frac{5}{n_L} \cdot \frac{K_i}{n_L} \cdot \left( y - 1 \right) \right) \]

where the \( n_L \) is the charge carrier density on the right interface.

Then \( n(z) \) is given by the corresponding inverse function to \( z(n) \). It is remarkable that our solution is valid for any ratio between the screening length and well width.

In this way we have obtained formula that describes the descending branch of the charge carrier concentration profile in the quantum well in parallel magnetic field (see Figure 3).

**Figure 3.** Holes’ concentration profile in Si/SiGe/Si structure with doping level \( N_i=2.2 \cdot 10^{11} \text{ cm}^{-2}, L=30 \text{ nm}, \) the parallel magnetic fields \( H=1, 5, 8, 12 \text{ Tesla}. \)

In quantum area (near the interface) we have to solve the effective Schrödinger equation numerically taking into account the effect of electric and magnetic fields. Figure 3 shows our calculations of the profile of carriers’ concentrations in the modulation doped Si/SiGe/Si structures. The concentrations’
peak degrades with a magnetic field. The carrier density decreases in the region of the maximum. The rotation of the charge carriers under the magnetic field leads to “mixing” of carriers and redistribution of the carriers density in the quantum well.

Let us briefly discuss the magnetoresistance in a parallel magnetic field in modulation doped structures. In structures with a low charge carrier concentrations the giant magnetoresistance is associated with an orbital effect in a strong parallel magnetic field [6]. In the above structures with a sufficiently high doping level the carriers are located mainly near the interface in a region with a width of less than two Bohr radii \( r_c \approx 10^{-5} \sim 10^{-6} \text{ cm} \), thus the effect of orbital motion is weak for them. (Such a large value \( r_c \) is connected with high average density of particles in the peak concentrations.) Positive magnetoresistance is caused by a decrease in the number of particles, which give a defining contribution to the drift current, and also a decrease in its average velocity (carriers’ mobility). Figure 4 shows the calculation of the resistivity \( \rho_{xx} \) in the electric field \( E_{appl} \) applied along the x-axis (parallel to the magnetic field) for the Si/SiGe/Si structure with doping level \( N_i=2.2\cdot10^{11} \text{ cm}^{-2} \). It also shows the observed magnetoresistance from the ref. [3].

![Figure 4. Magnetoresistance in a parallel magnetic field (\( E_{appl} II H \)). The black line is the experiment [3]. The red circles are our calculations.](image)

4. Conclusions
We have formulated hydrodynamic model and obtained analytical solutions for Fermi electrons’ concentration of as a function of tangential coordinate in the potential well and applied parallel magnetic field. These solutions are valid for any ratio between the screening length and well width. In a quantum area near the interface we carried out quantum mechanical calculations. The charge carrier concentration profile is significantly asymmetric, but becomes flatter in the strong magnetic field. Magnetoresistance is due to the carriers’ redistribution along the quantum well width with magnetic field.

References
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