DOI 10.1007/s11182-019-01645-8

Russian Physics Journal, Vol. 61, No. 11, March, 2019 (Russian Original No. 11, November, 2018)

QUASI-TWO-DIMENSIONAL ELECTRON-HOLE LIQUID IN AN ELECTRIC FIELD

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UDC 538.915

The density functional theory is used to determine the ground state of quasi-two-dimensional electron-hole liquid in an external electric field. The Schrödinger equations for electrons and holes are solved numerically. The equilibrium density of electron-hole liquid in $SiO_2/Si/SiO_2$ *quantum wells is found as a function of the quantum well width and electric field strength.*

Keywords: electron-hole liquid, equilibrium density, electric field.

INTRODUCTION

Condensation of excitons into electron-hole liquid (EHL) has been actively studied since the late 1960s. The properties of three-dimensional EHL in various semiconductors have been rather well studied [1, 2]. The properties of EHL in low-dimensional semiconductor structures are less studied. For the first time, the possibility of the formation of quasi-two-dimensional EHL in silicon MOS structures was shown in [3, 4]. These studies demonstrate the possibility of the formation of quasi-two-dimensional EHL consisting of two layers (the first layer with a surface density of N_1 and the second layer with a surface density of N_2, where $N_t = N_1 - N_2$ is the surface charge density). The properties of quasi-two-dimensional EHL are actively studied both theoretically [5–9] and experimentally [10–15].

In this paper, we use the density functional theory to calculate the energy of quasi-two-dimensional EHL in an external electric field. The method for solving the problem is similar to the method proposed in [8] for EHL in a zero electric field. In this work, calculations were performed for quantum wells (QWs) of various widths and satisfactory agreement was obtained between the calculated values of the equilibrium density and the experimental results [10] for the (100) silicon surface.

THEORETICAL MODEL

Let us consider EHL in $SiO_2/Si/SiO_2$ QWs in an external electric field directed perpendicular to the electron-hole layer. An electric field can be created by a gate located behind the SiO_2 layer. We introduce as a parameter the two-dimensional density of the gate charge N_t. Then, for an electro-neutral system, we write: $N_e = N_t + N_h$, where N_e and N_h are the two-dimensional densities of electrons and holes. In case of $N_t > 0$, we obtain a system of electron-hole pairs with the density $N_{eh} = N_h$ associated with an electron layer with the density N_t. In the opposite case $N_t < 0$, we obtain a system of electron-hole pairs with the density $N_{eh} = N_e$ associated with a hole layer with the density N_t.

Further, the exciton system of units is used, in which energy is measured in units of $\mathrm{Ry}_{\mathrm{ex}} = e^2/2ka_{\mathrm{ex}}$ and length is measured in units of $a_{\mathrm{ex}} = k\hbar^2 / \mu e^2$, where μ is the reduced mass and k is the dielectric constant. For silicon, μ =

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0.126 and k = 11.4, then, $a_{ex} \approx 5$ nm and $E_{ex} \approx 13$ meV . To calculate the energy of EHL, we use the model proposed in [8]. In the framework of the density functional theory, the total energy of quasi-two-dimensional EHL is written as

$$E_t[n_e, n_h] = T_e[n_e] + T_h[n_h] + \frac{1}{2}\int V_c(z)(n_e(z) - n_h(z))dz$$
$$+\int U_e(z)n_e(z)dz + \int U_h(z)n_h(z)dz + E_{xc}[n_e, n_h], \quad (1)$$

where T_e, T_h are the kinetic energies of charge carriers, $V_c(z)$ is the Coulomb potential, E_{xc} is the exchange-correlation energy, $U_e(z)$, $U_h(z)$ are the external potentials for electrons and holes, and n_e and n_h are the densities of electrons and holes.

To find the charge carrier densities, it is necessary to solve two Schrödinger equations for electrons and holes:

$$\left(-\frac{\mu}{m_{z,e}}\frac{d^2}{dz^2} + V_{\text{eff},e}(z)\right)\psi_{n,e}(z) = E_{n,e}\psi_{n,e}(z), \quad (2)$$

$$\left(-\frac{\mu}{m_{z,h}}\frac{d^2}{dz^2} + V_{\text{eff},h}(z)\right)\psi_{n,h}(z) = E_{n,h}\psi_{n,h}(z), \quad (3)$$

where $V_{\text{eff},e}(z) = V_c(z) + V_{xc,e}(z) + U_e(z)$, $V_{\text{eff},h}(z) = -V_c(z) + V_{xc,h}(z) + U_h(z)$, and $m_{z,e}$, $m_{z,h}$ are the charge carrier masses across the QW.

The exchange-correlation potentials have the following form:

$$V_{xc,e}(z) = \frac{d(n_e\varepsilon_{xc})}{dn_e},\ V_{xc,h}(z) = \frac{d(n_h\varepsilon_{xc})}{dn_h}. \quad (4)$$

For the exchange-correlation energy ε_{xc}, we use the formula proposed in [16]:

$$\varepsilon_{xc} = \frac{1}{2}\frac{a + br_s}{c + dr_s + r_s^2}, \quad (5)$$

where $r_s = (3/(4\pi n))^{1/3}$, a = –4.8316, b = –5.0879, c = 0.0152, and d = 3.0426.

External potentials for electrons and holes are defined by the expression

$$U_i(z) = \begin{cases} 0, & |z| \le d/2, \\ U_i, & |z| > d/2, \end{cases} \quad (6)$$

where d is the quantum well width and $i = e, h$.

The electrostatic potential is derived from the Poisson's equation

$$V_c(z) = 8\pi N_t z + 8\pi \int_{-\infty}^{z} (z - z')[n_h(z') - n_e(z')]dz'. \quad (7)$$

Equations (1)–(6) have the same form as in [8]. Equation (7) is distinguished by the first term, which takes into account an external electric field with the strength $8\pi N_t$.

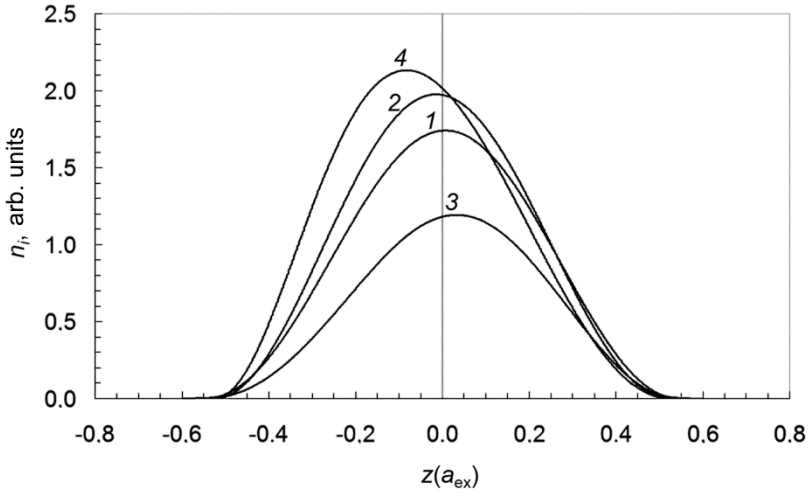

Fig. 1. Density profiles of electrons (*1*, *3*) and holes (*2*, *4*) for $N_t = -0.1$ (*1*, *2*) and –0.5 (*3*, *4*). $d = 1$, (111) Si.

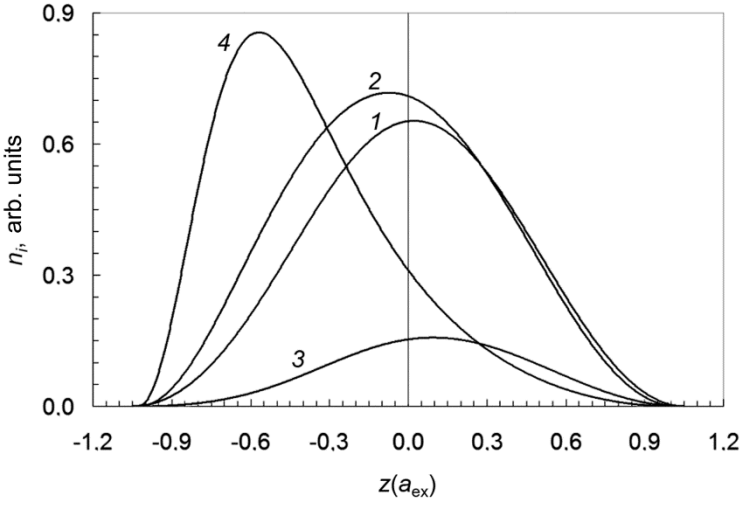

Fig. 2. Density profiles of electrons (*1*, *3*) and holes (*2*, *4*) for $N_t = -0.1$ (*1*, *2*) and –0.5 (*3*, *4*). $d = 2$, (111) Si.

RESULTS

The calculations were performed for the $SiO_2/Si/SiO_2$ QWs. For calculations, we used the following parameters [8]: the number of electron valleys $g_e = 2$ and the masses of the electron state density $m_{d,e} = 0.19m_0$, $m_{z,e} = 0.918m_0$, and $m_h = 0.53m_0$ for (100) Si, $g_e = 6$, $m_{z,e} = 0.258m_0$, $m_{d,e} = 0.358m_0$, and $m_h = 0.53m_0$ (m_0 is the free electron mass) for (111) Si, $U_e = 246$, $U_h = 384$.

Nonlinear Schrödinger equations (2) and (3) for electrons and holes were solved numerically. Figures 1 and 2 show the electron and hole density profiles for the ground state of the EHL for different values of the external electric field. For negative values of N_t, the external electric field is screened by holes and the hole density profile shifts toward negative values of z. As can be seen from Fig. 1, such a shift is rather weak for QWs with the width $d = 1$. For example, at $N_t = -0.5$, the density maximum is reached at $z = -0.08$ for holes and $z = 0.03$ for electrons.

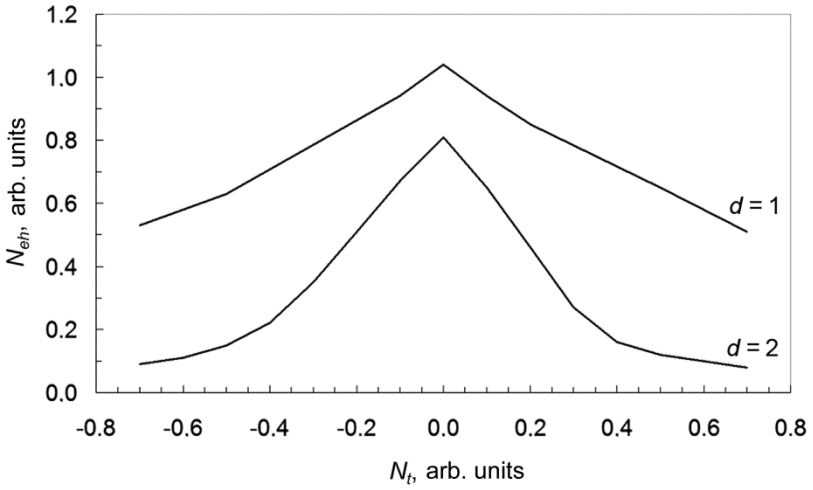

Fig. 3. Dependences of the equilibrium density of electron-hole pairs on the gate charge density for (111) Si.

For the QW width $d = 2$ (Fig. 2), the influence of an external electric field is much stronger than for a QW with the width $d = 1$. It can be seen that the overlap of the electron and hole densities decreases with increasing electric field strength. This separation of EHL leads to an increase in the Coulomb energy and a decrease in the equilibrium density of electron-hole pairs.

The decrease of the equilibrium density of EHL in an external electric field is clearly demonstrated in Fig. 3. It can be seen that the dependence $N_{eh}(N_t)$ has an almost symmetric form despite the difference in the effective masses of electrons and holes. This symmetry is explained by the fact that the main contribution to the change of energy in an electric field is made by the Coulomb and exchange-correlation energies. At $d = 2$ and $N_t = -0.4$ (or $N_t = 0.4$), the equilibrium density of the electron-hole pairs is $N_{eh} \approx 0.1$. This density corresponds to the parameter $r_s = 1/(\pi N_{eh})^{1/2} \approx 1.8$ and at such densities, an electron-hole plasma is formed. When $d = 1$, in the considered range of N_t (Fig. 3), the parameter r_s is always less than 1 and the ground state is EHL. Thus, in a wide QW, the EHL is destroyed at a smaller value of the electric field strength compared with a narrow QW.

Similar calculations were also performed for (100) Si. For this silicon surface, the equilibrium density of EHL in a zero electric field is much less than for (111) Si. Figure 4 shows the dependences of the equilibrium density of electron-hole pairs on the gate charge density for (100) Si. The form of the dependence $N_{eh}(N_t)$ is the same as for (111) Si. It can be seen that in case of $d = 2$, the equilibrium density decreases more with increasing electric field strength compared with the case of $d = 1$. At $d = 2$, the transition to an electron-hole plasma for (100) Si occurs in smaller electric fields than for (111) Si. It should be noted that the theoretical model uses the condition of local neutrality of EHL [8]. The EHL separation in an electric field will reduce the exchange-correlation energy and the transition to an electron-hole plasma should occur in even smaller electric fields.

CONCLUSIONS

In the present work, the density functional theory is used to calculate the energy of quasi-two-dimensional EHL and to find the equilibrium density of electron-hole pairs in the presence of an external electric field. The nonlinear Schrödinger equations for electrons and holes were solved numerically. The calculations were performed for EHL in $SiO_2/Si/SiO_2$ QWs for (100) and (111) silicon surfaces. The densities of electrons and holes are calculated as a function of the electric field strength and QW width. It has been shown that strong separation of electrons and holes occurs in wide QWs. The dependences of the equilibrium density of electron-hole pairs on the electric field strength and QW width for (111) Si and (100) Si are found. The calculated equilibrium density of electron-hole pairs decreases with

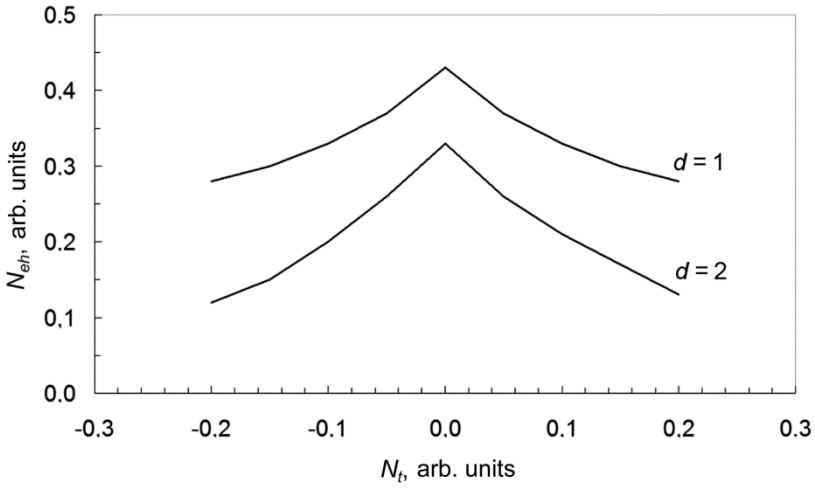

Fig. 4. Dependences of the equilibrium density of electron-hole pairs on the gate charge density for (100) Si.

increasing electric field strength. A particularly strong decrease of density occurs in wide QWs, in which an electric field can destroy the EHL. For (100) Si, the transition to an electron-hole plasma in wide QWs occurs in smaller electric fields than for (111) Si.

This work was supported by the Russian Foundation for Basic Research and the Administration of the Krasnodar Region (project No. 16-42-230280).

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