DOI 10.1007/s11182-017-0962-5

Russian Physics Journal, Vol. 59, No. 10, February, 2017 (Russian Original No. 10, October, 2016)

PHYSICS OF SEMICONDUCTORS AND DIELECTRICS

STABILITY OF QUASI-TWO-DIMENSIONAL ELECTRON-HOLE LIQUID IN SEMICONDUCTOR STRUCTURES OF THE TYPE-II

A. A. Vasilchenko,[1] G. F. Kopytov,[2] V. S. Krivobok,[3,4] D. A. Ermokhin[1] UDC 538.915

Analytical expressions are obtained for the energy of a quasi-two-dimensional electron-hole liquid (EHL) and the threshold value of the barrier height for electrons, above which formation of the direct EHL is impossible. It is shown that the state with a quasi-two-dimensional EHL can be energetically favorable in semiconductors with the anisotropy of masses and (or) a large number of equivalent valleys. A comparison of the calculation results with the experimental data for the Si/SiGe/Si *structure is made.*

Keywords: electron-hole liquid, binding energy, exciton.

INTRODUCTION

Studying properties of electron-hole systems is one of the rapidly developing areas of modern condensed matter physics. At present, most attention is paid to low-dimensional electron-hole systems, in which the role of the Coulomb interaction increases. Theoretical and experimental works in this area are focused primarily on the systems with a finite number of particles (excitons [1, 2], trions [3, 4], and electron-hole complexes with the number of particles less than 10 [5, 6]).

Less studied are the properties of quasi-two-dimensional EHL in semiconductor structures, particularly in the structures with heterojunctions of the type-II. First, the possibility of the formation of a quasi-two-dimensional EHL in silicon MOS-structures was shown in [7, 8]. Recently, EHL was found in $SiO_2/Si/SiO_2$ quantum wells [9, 10] and in $Si/Si_{1-x}Ge_x/Si$ heterostructures [11-15]. Si/SiGe/Si quantum wells are the structures of the type-II, in which the SiGe layer forms a barrier for electrons and a quantum well for holes. The barrier height at $x = 0.1$ is about 10 meV, and the well depth is of about 90 meV.

The aim of this work is to find the energy and equilibrium density of a quasi-two-dimensional EHL. To calculate the energy, the density functional theory is used and to account for the exchange-correlation energy, a standard local density approximation is applied. Earlier, the density functional theory has been successfully applied to study the properties of a three-dimensional EHL in semiconductors [16, 17].

FORMULATION OF THE PROBLEM

It is necessary to calculate the total energy of a quasi-two-dimensional electron-hole system

[1]Kuban State Technological University, Krasnodar, Russia, e-mail: a_vas2002@mail.ru; spacedreamer@yandex.ru; [2]Kuban State University, Krasnodar, Russia, e-mail: g137@mail.ru; [3]Lebedev Physical Institute of the Russian Academy of Sciences, Russia, e-mail: krivobok@sci.lebedev.ru; [4]National Research Nuclear University "MEPhI", Moscow, Russia. Translated from Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika, No. 10, pp. 151–155, October, 2016. Original article submitted July 4, 2016.

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

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

The exciton system of units is used: energy is measured in the units of $Ry_{ex} = e^2/2ka_{ex}$, and the length – in the units of $a_{ex} = k\hbar^2/\mu e^2$, where μ is the reduced mass and k is the dielectric constant.

Varying Eq. (1) over the densities n_e and n_h, we get two Schrödinger equations:

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

where $i = e, h$. Thus, the problem is reduced to solving the two one-dimensional nonlinear Schrödinger equations for the particles in the first and second wells, which are described by the potentials $V_{\text{eff},e}(z) = V_c(z)+V_{xc,e}(z)+U_e(z)$ and $V_{\text{eff},h}(z) = -V_c(z)+V_{xc,h}(z)+U_h(z)$, where $V_{xc}(z)$ is the exchange-correlation potential, and the electrostatic potential is derived from the Poisson equation:

$$V_c(z) = 8\pi\int_{-\infty}^{z}(z - z')[n_h(z') - n_e(z')]dz'. \quad (3)$$

The external potentials for electrons and holes are given by

$$U_i(z) = \begin{cases} 0, & |z| \le d/2, \\ U_i, & |z| > d/2, \end{cases} \quad (4)$$

where d is the well (barrier) width. In this choice of the external potentials, energy is measured from the band gap of the semiconductor creating a quantum well (barrier). Further, we consider a heterostructure of the type-II, for which $U_e < 0$ and $U_h > 0$.

If only the lower size quantization level is filled, the carrier densities are given by the expressions

$$n_e(z) = N_e\psi_{0,e}^2(z), \; n_h(z) = N_h\psi_{0,h}^2(z), \quad (5)$$

where N_e and N_h are the two-dimensional electron and hole densities, respectively. Below, the index "0" at variables is omitted.

The kinetic energy can be written as follows:

$$T_i[n_i] = \frac{\pi\mu}{g_i m_{d,i}}N_i^2 + N_i\left(E_i - \int V_{\text{eff},i}(z)\psi_i^2(z)dz\right), \quad (6)$$

where g_i is the number of equivalent valleys and $m_{d,i} = (m_{x,i}m_{y,i})^{1/2}$. In Eq. (6), the first term corresponds to the total kinetic energy of carriers along the electron-hole layer, and the second term – to the kinetic energy across the layer. For simplicity, further we assume that $g_h = 1$ and the hole masses are isotropic $m_h = m_{z,h} = m_{d,h}$, and introduce the notations: $m_z = m_{z,e}$, $m_d = m_{d,e}$.

For the exchange-correlation energy, we use the local density approximation

$$E_{xc}[n_e, n_h] = \int dz e_{xc}(n_e, n_h), \tag{7}$$

where $e(n_e, n_h)$ is the exchange-correlation energy of electrons and holes per unit volume.

Then, the exchange-correlation potentials have the form

$$V_{xc,e}(z) = \frac{de_{xc}}{dn_e}, \; V_{xc,h}(z) = \frac{de_{xc}}{dn_h}. \tag{8}$$

In general, the form of the expression for e_{xc} is unknown. In case of neutral electron-hole plasma $n_e(z) = n_h(z) = n(z)$, there is an approximation formula for the exchange-correlation energy $\varepsilon_{xc} = e_{xc}/n$ [18]

$$\varepsilon_{xc} = \frac{1}{2}\frac{a + br_s}{c + dr_s + r_s^2}, \tag{9}$$

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

THEORETICAL MODEL AND DISCUSSION

In general case, the system of nonlinear equations (2) - (9) must be solved numerically. In this section, a model is constructed that allows us to obtain analytical results for the energy of a quasi-two-dimensional EHL.

We take $\varepsilon_{xc} = -0.91K/r_s$, where $K = 1$ without taking into account the electron-hole correlations (exchange energy of electrons or holes). Further, we take $K = 1.3$ (this value follows from Eq. (9) in the vicinity of $r_s \approx 1$). Within the framework of this model, no Coulomb contribution to the energy is taken into account. Note that the Coulomb energy always increases the total energy.

Assume that the wave function of holes is determined only by the confinement potential $U_h(z)$, which is a rectangular well with the width d. We believe the well depth U_h for holes large enough to take the wave function of holes in the form $\psi_h(z) = (2/d)^{1/2}\cos(\pi z/d)$. Below, energy is measured from the energy level of holes.

For electrons, $U_e(z) = 0$ at $|z| \le d/2$. In this case, only the exchange-correlation potential remains in the Schrödinger equation. For electrons, we take the wave function with the parameter b in the form $\psi_e(z) = (1/(\pi^{1/2}b))^{1/2}\exp(-z^2/(2b^2))$. We expand $V_{xc,e}(z)$ in series and, taking into account only the quadratic term with respect to z, we obtain from the Schrödinger equation for electrons $b = 1.45\mu^{3/5}/(m_z^{3/5}K^{3/5}N_e^{1/5})$. The energy level for electrons is $E_e = -0.95K^{6/5}N_e^{2/5}(m_z/\mu)^{1/5}$. Taking into account the electron Fermi energy $E_F = 2\pi\mu N_e/g_e m_d$, we obtain for the threshold value of the barrier $\Delta = -U_e$, above which no spatially-direct EHL can be formed, the following expression:

$$\Delta_c = 0.95K^{6/5}N_e^{2/5}\left(\frac{m_z}{\mu}\right)^{1/5} - \frac{2\pi\mu}{g_e m_d}N_e. \tag{10}$$

After all of these assumptions, we obtain as a result the energy per one electron-hole pair:

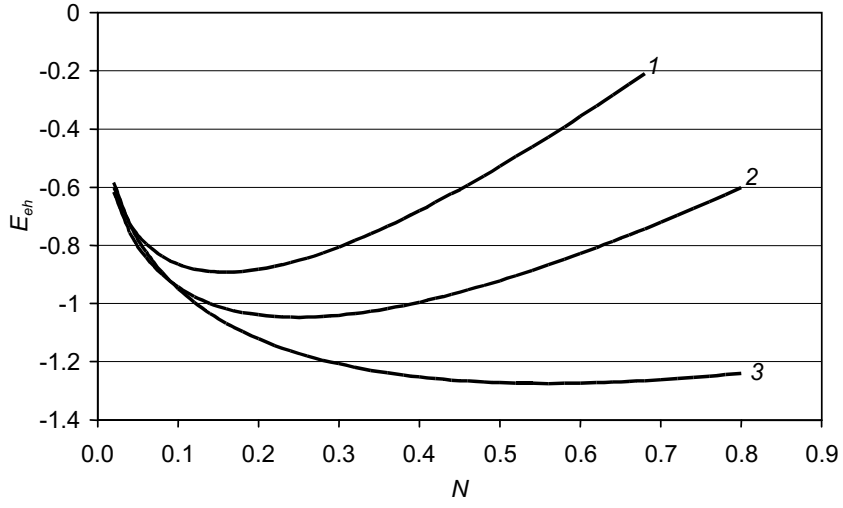

Fig. 1. Dependence of the energy per one electron-hole pair on the two-dimensional concentration of pairs, $d = 1$: $m_z = m_d = m_h$, $g_e = 1$(*1*) , $m_z == m_d = m_h$, $g_e = 2$ (*2*), and $m_d = m_h = 10m_z$, $g_e = 1$ (*3*).

$$E_{eh} = -0.69K^{6/5}\left(\frac{m_z}{\mu}\right)^{1/5} N_e^{2/5} - \frac{1.24K}{d^{1/3}} N_h^{1/3} + \pi\frac{\mu}{g_e m_d} N_e + \pi\frac{\mu}{m_h} N_h + U_e(1-\mathrm{erf}(d/2b)) . \qquad (11)$$

First term in Eq. (11) is the exchange and transverse kinetic energy of electrons, the second term is the exchange energy of holes, the third term is the longitudinal kinetic energy of electrons, the fourth term is the longitudinal kinetic energy of holes, and the last term is the energy of electrons in an external potential. For the neutral EHL, $N_e = N_h = N$.

Formation of EHL is possible, if it is stable with respect to the decay into free excitons, that is, when the binding energy of an electron-hole pair, equal to $-E_{eh}$, is higher than the exciton binding energy. In [19, 20], it is shown that in the structures of the type-II at $d > 1$, the exciton binding energy is close to the binding energy of a three-dimensional exciton. Let us consider the case of isotropic masses and $g_e = 1$. In this case, the sum of the longitudinal kinetic energies of electrons and holes is independent of masses. In Eq. (11), the last term always reduces the energy. Therefore, to exclude the effect of the barrier on the energy, we take $U_e = 0$. For equal electron and hole masses, the binding energy of an electron-hole pair is less than the binding energy of an exciton (curve *1* in Fig. 1) and EHL cannot form.

Note that a similar result was obtained for the three-dimensional EHL [16]. As can be seen from Eq. (11), for the quasi-two-dimensional EHL, the binding energy depends on the anisotropy of the electron masses. The effect of the anisotropy of electrons masses on the energy of an electron-hole pair is shown in Fig. 1 (curve *3*). With a further increase in the ratio m_d/m_z, the binding energy and equilibrium density increase. With increasing number of valleys, the binding energy also increases (curve *2* in Fig. 1). Thus, the state with the EHL can be energetically favorable in semiconductors with the anisotropy of masses and (or) a large number of equivalent valleys.

The proposed model is well suited to the Si/SiGe/Si heterojunctions. Recent experiments [11-15] have shown that in such a structure, a quasi-two-dimensional EHL can be formed. The authors of [14] studied the SiGe/Si quantum wells with the width of 5 nm with various content of Ge and showed that the threshold value of the barrier for electrons is of about 7 meV, the equilibrium density is of 10^{12} cm^{-2}, and the binding energy is of 19 meV for the Ge concentration of about 3%. In these experiments, the SiGe layer grown on the (100) silicon surface is strained, and we used the following parameters for the calculations [20]: $g_e = 4$, $m_z = 0.19m_0$, $m_d = 0.42m_0$, and $m_h = 0.19m_0$ (m_0 is the free electron mass). For these parameters, we obtain from Eq. (10) $\Delta_c \approx 8$ meV , which is in good agreement with the experimental results. Like silicon, we have taken the reduced mass $\mu = 0.126$, then, $a_{ex} \approx 5$ nm and $E_{ex} \approx 13$ meV .

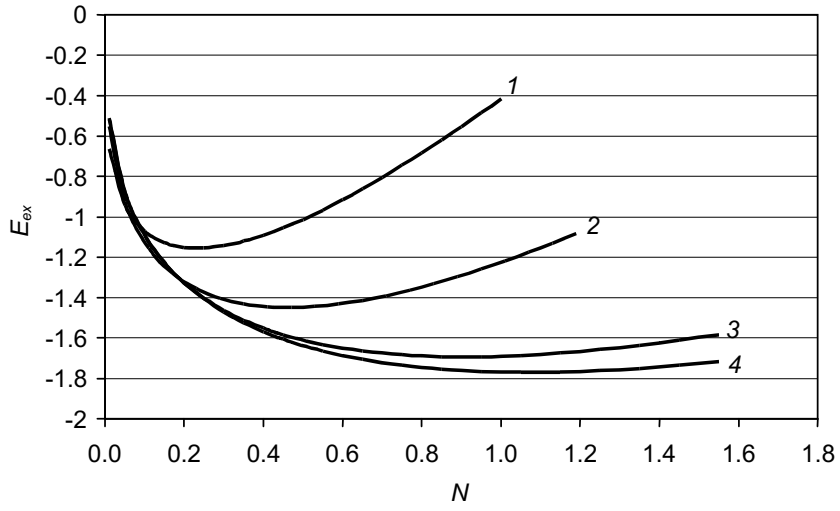

Fig. 2. Dependence of the energy per one electron-hole pair on the two-dimensional concentration of pairs, d = 1: the strained SiGe layer (*1*), the (100) surface, $m_z = 0.918m_0$, $m_d = 0{,}19m_0$, $m_h = 0.53m_0$, $g_e = 2$ (*2*), the (110) surface, $m_z = 0.315m_0$, $m_d = 0.324m_0$, $m_h = 0.53m_0$, $g_e = 4$ (*3*), and the (111) surface, $m_z = 0.258m_0$, $m_d = 0.358m_0$, $m_h = 0.53m_0$, $g_e = 6$ (*4*).

Figure 2 shows the dependence of the energy per one electron-hole pair on the two-dimensional concentration of pairs. In case of the strained SiGe layer (curve *1* in Fig. 2), the equilibrium carrier density $N = 0.23$ (about 10^{12} cm^{-2}) and the binding energy equal to 1.15 (about 15 meV) are obtained. Equilibrium density is in a very good agreement with the experimental data, while the binding energy is somewhat different from those.

At low concentrations of Ge, it should be expected that for the structure with an unstressed SiGe layer, the effective masses of charge carriers and the number of valleys would be the same as for silicon. Figure 2 shows the results of calculations for various silicon surfaces (curves *2–4*). For the (100) surface, the minimum energy is achieved at $N_e = 0.4$, which corresponds to the concentration of $1.6 \cdot 10^{12}$ cm^{-2}. For the (110) surface, the binding energy of the electron-hole pair and the equilibrium density significantly increase in comparison with the results for the (100) surface. This result is associated with an increase both in the number of valleys and the electron density-of-states mass m_d. For the (111) surface, the binding energy is close to that for the (110) surface, while the equilibrium density of pairs increases slightly. The latter result is mainly due to an increase in the number of valleys. For the (111) surface, the equilibrium density of electron-hole pairs is $N_{eq} = 4 \cdot 10^{12}$ cm^{-2}. The three-dimensional density of electron-hole pairs can be estimated as $n \approx N_{eq} / d \approx 8 \cdot 10^{18}$ cm^{-3}, which is more than 2 times greater than the equilibrium density of the three-dimensional liquid [16].

CONCLUSIONS

In this paper, we proposed an original method for the approximate analytical solution of the nonlinear Schrödinger equation. This method allowed to analytically express the energy of the quasi-two-dimensional EHL through such parameters as electron and hole masses, anisotropy of masses, and the number of equivalent valleys and to find the value of the barrier for electrons, above which the formation of the spatially direct quasi-two-dimensional EHL is impossible. The influence of the anisotropy of electron masses and the number of valleys on the energy of the electron-hole pair is studied. It is shown that in contrast to the three-dimensional EHL, in a quasi-two-dimensional case, the anisotropy of the electron masses increases the electron-hole binding energy.

A comparison with the experimental results is made for the Si/SiGe/Si structures with the strained SiGe layer. For the equilibrium density of electron-hole pairs and a critical barrier height, a satisfactory agreement between the model and experimental results is obtained.

It is shown that the properties of the quasi-two-dimensional EHL depend on the anisotropy of electron masses and the number of valleys in silicon. The highest binding energy and pair density are obtained for the (111) silicon surface. The proposed model can be easily generalized to structures, in which there is a barrier for holes and a quantum well for electrons. The analytical results obtained can be used to estimate the parameters of the quasi-two-dimensional EHL in other semiconductors.

The work was supported in part by the Russian Foundation for Basic Research and by the Ministry of Education and Science of the Krasnodar Region (Project No. 16-42-230280)

REFERENCES

1. Y. Sidor, B. Partoens, F. M. Peeters, *et al*., Phys. Rev. B, **73**, 155334 (2006).
2. L. V. Butov, A. C. Gossard, and D. S. Chemla, Nature, **418**, 751 (2002).
3. A. S. Bracker, E. A. Stinaff, D. Gammon, *et al*., Phys. Rev. B, **72**, 035332 (2005).
4. E. Anisimovas and F. M. Peeters, Phys. Rev. B., **68**, 115310 (2003).
5. A. A. Vasilchenko and D. M. Tolkachev, Mod. Phys. Lett. B, **30**, 1650013 (2016).
6. K. Kärkkäinen, M. Koskinen, M. Manninen, and S. M. Reimann, Solid State Commun., **130**, 187 (2004).
7. P. D. Altukhov, A. V. Ivanov, Yu. N. Lomasov, and A. A. Rogachev, Pisma Zh. Exp. Teor. Fiz., **38**, 5 (1983).
8. P. D. Altukhov, A. V. Ivanov, Yu. N. Lomasov, and A. A. Rogachev, Pisma Zh. Exp. Teor. Fiz., **39**, 432 (1984).
9. N. Pauc, V. Calvo, J. Eymery, *et al*., Phys. Rev. Lett., **92**, 236802 (2004).
10. N. Pauc, V. Calvo, J. Eymery, *et al*., Phys. Rev. B, **72**, 205325 (2005).
11. V. V. Zaitsev, V. S., Bagaev, T. M. Burbaev, *et al*., Physica E, **40**, 1172 (2008).
12. V. S., Bagaev, V. V. Zaitsev, V. S. Krivobok, *et al*., Zh. Exp. Teor. Fiz., **134**, 988 (2008).
13. V. S., Bagaev, V. S. Krivobok, Nikolaev S. N., *et al*., Phys. Rev. B, **82**, 115313 (2010).
14. V. S., Bagaev, V. S. Krivobok, S. N. Nikolaev, *et al*., Pisma Zh. Exp. Teor. Fiz., **94**, 63 (2011).
15. V. S., Bagaev, V. S. Krivobok, S. N. Nikolaev, *et al*., Zh. Exp. Teor. Fiz., **144**, 1045 (2013).
16. Electron-Hole Drops in Semiconductors [in Russian], ed. by C. D. Jeffries and L. V. Keldysh, Nauka, Moscow (1988).
17. N. N. Sibeldin, Problems of Condensed Matter Physics: Quantum Coherence Phenomena in Electron-Hole and Coupled Matter-Light Systems, ed. by A. L. Ivanov and S. G. Tikhodeev, Oxford Univ. Press, **139**, 227 (2008).
18. P. Vashishta and R. K. Kalia, Phys. Rev. B, **10**, 6492 (1982).
19. V. S., Bagaev, V. S. Krivobok, V. P. Martovitskii, and A. V. Novikov, Zh. Exp. Teor. Fiz., **136**, 1154 (2009).
20. C. Penn, F. Schäffler, G. Bauer, and S. Glutsch, Phys. Rev. B, **59**, 13314 (1999).