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CONDENSED MATTER

Multicomponent Electron–Hole Liquid in Si/SiGe Quantum Wells

A. A. Vasil'chenko*

Kuban State University, Krasnodar, 350040 Russia

**e-mail: a_vas2002@mail.ru*

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The density functional theory is used to calculate the energy of an electron–hole liquid in $Si/Si_{1-x}Ge_x/Si$ quantum wells. Three one-dimensional nonlinear Schrödinger equations for electrons and light and heavy holes are solved numerically. It is shown that, in shallow quantum wells (small x), both light and heavy holes exist in the electron–hole liquid. Upon an increase in the Ge content, a transition to a state with one type of holes occurs, with the equilibrium density of electron–hole pairs decreasing by more than a factor of 2.

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INTRODUCTION

Low-dimensional systems, in particular, two-dimensional layers in semiconductors, exhibit new properties as compared to three-dimensional samples of the same compounds, because spatial confinement leads to the enhancement of particle–particle interaction effects. One of such systems is a quasi-two-dimensional electron–hole liquid (EHL). The possibility of the formation of a quasi-two-dimensional EHL was shown for the first time in [1, 2]. Recently, the EHL was discovered in $SiO_2/Si/SiO_2$ quantum wells [3, 4] and in $Si/Si_{1-x}Ge_x/Si$ heterostructures [5–11].

Si/SiGe/Si quantum wells are type-II structures in which the SiGe layer forms a barrier for electrons and a quantum well for holes. Experimental results indicate that the properties of the EHL are modified upon the variation of the Ge content in the SiGe layer. In particular, an unusual structure in the EHL emission spectrum of SiGe/Si quantum wells with a low Ge content (a few percent) was found experimentally in [10, 11]. The shape of the condensed-phase line was explained by invoking the idea of a multicomponent EHL containing both heavy and light holes. It is noteworthy that the observed fine structure in the EHL emission spectra disappears as the Ge content in the quantum well increases.

The aim of this work is to calculate the energy of the quasi-two-dimensional EHL in SiGe/Si quantum wells in the presence of two types of holes. The calculations are carried out using the density functional theory.

MODEL

Let us consider a quasi-two-dimensional EHL with electrons and light and heavy holes. The total energy of such an electron–hole system can be written as

$$\begin{aligned} E_t[n_e, n_{hh}, n_{hl}] &= T_e[n_e] + T_{hh}[n_{hh}] + T_{hl}[n_{hl}] \\ &+ \frac{1}{2}\int V_c(z)(n_e(z) - n_h(z))dz + \int U_e(z)n_e(z)dz \\ &+ \int U_{hh}(z)n_{hh}(z)dz + \int U_{hl}(z)n_{hl}(z)dz \\ &+ E_{xc}[n_e, n_{hh}, n_{hl}]. \end{aligned} \quad (1)$$

Here, T_e, T_{hh}, and T_{hl} are the kinetic energies of electrons and heavy and light holes, respectively; $V_c(z)$ is the Coulomb potential; E_{xc} is the exchange–correlation energy; $U_e(z)$, $U_{hh}(z)$, and $U_{hl}(z)$ are the external potentials for electrons and heavy and light holes, respectively; n_e, n_{hh}, and n_{hl} are the densities of electrons and heavy and light holes, respectively; and $n_h = n_{hh} + n_{hl}$.

Excitonic units are used, so that the length and energy are measured in units of $a_{ex} = k\hbar^2/\mu e^2$ and $Ry_{ex} = e^2/2ka_{ex}$, respectively, where μ is the reduced mass and k is the dielectric constant. The values $\mu = 0.126$ and $k = 11.5$ corresponding to bulk silicon are taken, which yields $a_{ex} \approx 5$ nm and $Ry_{ex} \approx 13$ meV.

The Kohn–Sham equations for quasi-two-dimensional electrons and heavy and light holes can be written as [12, 13]

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

where $i = e$, hh, and hl.

Thus, the problem is reduced to the solution of three one-dimensional nonlinear Schrödinger equations with the potentials $V_{\text{eff},e}(z) = V_c(z) + V_{xc,e}(z) + U_e(z)$, $V_{\text{eff},hh}(z) = -V_c(z) + V_{xc,hh}(z) + U_{hh}(z)$, and $V_{\text{eff},hl}(z) = -V_c(z) + V_{xc,hl}(z) + U_{hl}(z)$, where $V_{xc}(z)$ is the exchange–correlation potential and $V_c(z)$ is the electrostatic potential obtained 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 the formula

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

where d is the width of the well (barrier).

The quantity Δ_i is introduced to take into account splitting between light and heavy holes. Let $\Delta_e = \Delta_{hh} = 0$; then, the energy is measured from the band gap of the semiconductor that forms the quantum well (barrier). Below, a type-II heterostructure, where $V_e < 0$, $V_{hh} > 0$, and $V_{hl} > 0$, is considered.

When only the lower quantum-confinement level is occupied, the carrier densities are given by expressions

$$n_e(z) = N_e\psi_{0,e}^2(z), \quad n_{hh}(z) = N_{hh}\psi_{0,hh}^2(z), \quad n_{hl}(z) = N_{hl}\psi_{0,hl}^2(z), \quad (5)$$

where N_e, N_{hh}, and N_{hl} are the two-dimensional densities of electrons and heavy and light holes, respectively. The subscript 0 will be omitted below.

The kinetic energy is written as

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

Here, the first and second terms correspond to the kinetic energy of charge-carrier motion parallel and perpendicular to the electron–hole layer, respectively.

The approximation $E_{xc}[n_e, n_{hh}, n_{hl}] = E_{xc}[n_e, n_h]$ is used for the exchange–correlation energy [14]. Then, in the local density approximation, the exchange–correlation potentials are written as

$$V_{xc,e}(z) = \frac{d(n_e\varepsilon_{xc})}{dn_e}, \quad V_{xc,hh}(z) = \frac{d(n_h\varepsilon_{xc})}{dn_{hh}}, \quad V_{xc,hl}(z) = \frac{d(n_h\varepsilon_{xc})}{dn_{hl}}. \quad (7)$$

The following expression is used for the exchange–correlation energy [15]:

$$\varepsilon_{xc} = \frac{1}{2}\frac{a + br_s}{c + dr_s + r_s^2}, \quad (8)$$

where $r_s = (3/(4\pi n_k))^{1/3}$ $(k = e, h)$, $a = -4.8316$, $b = -5.0879$, $c = 0.0152$, and $d = 3.0426$.

An electrically neutral EHL, where $N_e = N_{hh} + N_{hl} = N$, is considered here. The energy per electron–hole pair will be measured from the lowest heavy-hole energy level E_{hh} in an empty well: $E_{eh} = -E_{hh} + E_t/N$.

Taking into account that the Fermi energy of charge carriers with the density-of-states effective mass $m_{d,i} = (m_{x,i}m_{y,i})^{1/2}$ and the number of equivalent valleys of g_i equals $E_{\text{F},i} = 2\pi\mu N_i/g_i m_{d,i}$, we have

$$E_{hh} + \frac{2\pi\mu N_{hh}}{g_{hh}m_{d,hh}} = E_{hl} + \frac{2\pi\mu N_{hl}}{g_{hl}m_{d,hl}}. \quad (9)$$

From this equation, we find that, for the electrically neutral EHL and $g_i = 1$,

$$N_{hl} = N_e\frac{m_{d,hl}}{m_{d,hh} + m_{d,hl}} - \frac{m_{d,hh}m_{d,hl}}{m_{d,hh} + m_{d,hl}}\frac{E_{hl} - E_{hh}}{2\pi\mu}. \quad (10)$$

If Eq. (10) yields $N_{hl} < 0$, we have to take $N_{hh} = N_e$ and $N_{hl} = 0$.

RESULTS

The calculations were carried out for $Si/Si_xGe_{1-x}/Si$ structures using the parameters [16–18] $\Delta_{hl} = 16.6x$, $g_e = 4$, $g_{hh} = g_{hl} = 1$, $m_{z,e} = 0.198m_0$, $m_{d,e} = 0.44m_0$, $m_{z,hh} = 0.28m_0$, $m_{d,hh} = 0.2m_0$, $m_{z,hl} = 0.18m_0$, $m_{d,hl} = 0.25m_0$ (here, m_0 is the free-electron mass), $V_e = -7.7x$, and $V_{hh} = V_{hl} = 53.7x$.

The results of the numerical solution of the Schrödinger equations are shown in Fig. 1. It is seen that the wavefunctions of light holes and electrons overlap to a larger extent than those of heavy holes and electrons. Therefore, the presence of light holes in the EHL reduces the energy owing to a decrease in the Coulomb energy. The incomplete overlap of electron and hole wavefunctions results in the formation of an attractive Coulomb potential for electrons, which exceeds the barrier for electrons. One can see from Fig. 1 that the Coulomb and exchange–correlation potentials at the center of the quantum well are about $-0.6Ry_{\text{ex}}$ and $-0.7Ry_{\text{ex}}$, respectively. For holes within the quantum well, the repulsive Coulomb potential is compensated by the exchange–correlation potential. In our model, the effective potentials for light and heavy holes differ only within the quantum well by the value of Δ_{hl}.

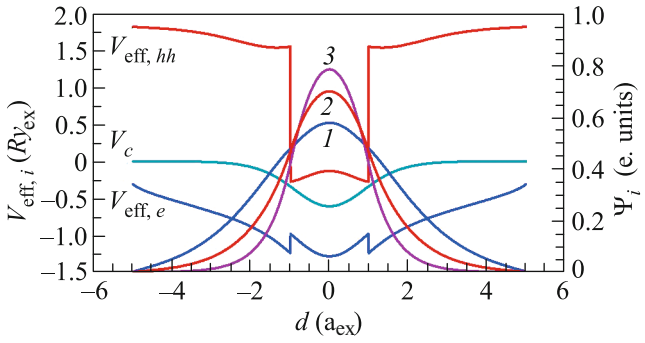

Fig. 1. (Color online) Profiles of the potentials and wavefunctions for (*1*) electrons, (*2*) light holes, and (*3*) heavy holes obtained with the parameters $N = 0.29$, $N_{hl} = 0.082$, $x = 0.034$, and $d = 2$.

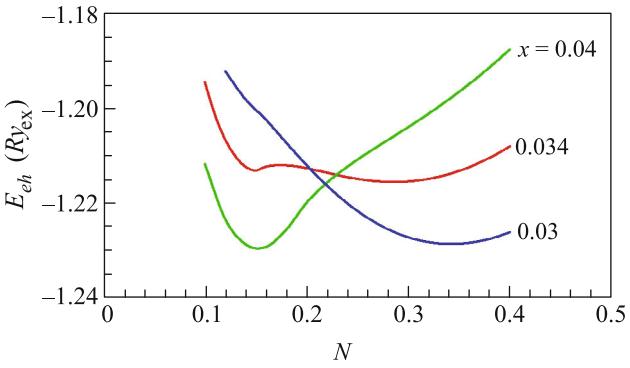

Fig. 2. (Color online) Energy per electron–hole pair versus the two-dimensional electron–hole pair density for $d = 2$.

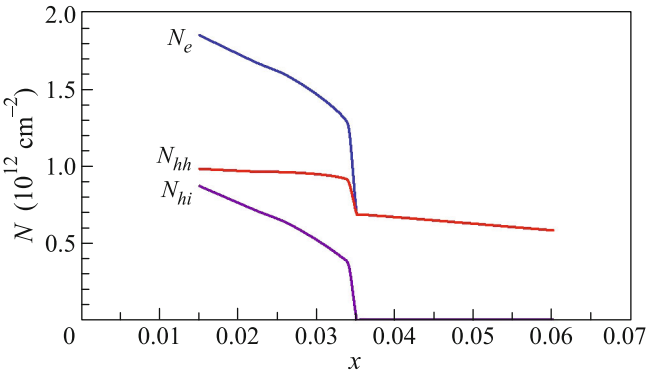

Fig. 3. (Color online) Electron and heavy and light-hole densities versus the Ge content in the SiGe layer for $d = 2$.

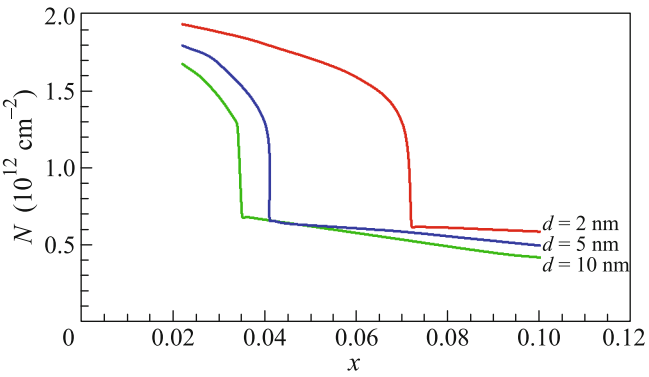

Fig. 4. (Color online) Equilibrium electron–hole pair density versus the Ge content in the SiGe layer.

Figure 2 shows the energy per electron–hole pair versus the two-dimensional pair density for a quantum well with a width of $d = 2$ (10 nm). For $x = 0.03$, the energy minimum is attained for $N = 0.34$, and the EHL is three-component with a light-hole density of $N_{hl} = 0.12$. With increasing Ge content, the energy curve acquires two minima. The EHL at the first minimum (at a smaller value of N) contains only heavy holes, and the EHL at the second minimum contains both light and heavy holes. For $x = 0.034$, the two energy minima are almost equal. With a further increase in x, there remains one energy minimum (two-component EHL) and the equilibrium electron–hole pair density decreases. Apart from an increase in the splitting of energy levels between light and heavy holes, the transition to the two-component state is also caused by an increase in the energy of light holes in the external potential. We note that, for $x = 0.03$, light holes are present almost in the entire range of electron–hole pair densities (Fig. 2). For $x = 0.034$ and 0.04, light holes with a low density begin to appear near the first energy minimum, and at $N = 0.3$, the density of light holes becomes $N_{hl} = 0.087$ and 0.071 for $x = 0.034$ and 0.04, respectively.

The transition from a three-component to a two-component EHL with increasing x occurs rather abruptly. This is clearly demonstrated in Fig. 3. It is noteworthy that, for small x, the densities of light and heavy holes are close to each other. Upon the transition from a three-component to a two-component EHL, the equilibrium density of electron–hole pairs is more than halved.

Calculations were carried out for structures with different widths of quantum wells. The results of these calculations are shown in Fig. 4. One can see that, as the width of quantum wells decreases, the transition to the two-component EHL occurs at a larger Ge content. This dependence on the well width is caused by the stronger effect of the external potential on the splitting between the energy levels of heavy and light holes in shallow narrow quantum wells.

Calculations taking into account the presence of both light and heavy holes in the EHL yield good agreement with the experimental data. Indeed, it was

shown in [10] that, for $d = 5$ nm and $x < 0.05$, there exists the three-component EHL, which agrees reasonably well with the calculation results. The experimental value of the equilibrium electron–hole pair density in the three-component EHL, which is $N = 1.6 \times 10^{12}$ cm^{-2} for $d = 5$ nm [10], agrees well with the calculated values (Fig. 4). According to [6], the quasi-two-dimensional EHL that appears in a structure with $d = 2$ nm and $x = 0.09$, is, apparently, two-component. The calculations for such a structure yield $N = 6 \times 10^{11}$ cm^{-2} (Fig. 4), which is in good agreement with the experiment [6].

CONCLUSIONS

The energy of the EHL in Si/SiGe/Si heterostructures with different widths of quantum wells (barriers) and Ge contents has been calculated. It has been shown that a three-component EHL is formed in shallow quantum wells (low Ge content). With increasing Ge content, the transition to a two-component EHL takes place, and the equilibrium density of electron–hole pairs decreases significantly. The results of the calculations agree with the experimental data.

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