

PHYSICS OF SEMICONDUCTORS AND DIELECTRICS

QUASI-TWO-DIMENSIONAL ELECTRON–HOLE LIQUID IN Si/SiO₂ QUANTUM WELLS

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To calculate the energy and equilibrium density of electron-hole pairs in SiO₂/Si/SiO₂ quantum wells (QWs), nonlinear Schrödinger equations for electrons and holes were numerically solved. Calculations were carried out for (100) and (111) silicon surfaces and various values of the QW width. It is shown that the binding energy of electron-hole pairs in a quasi-two-dimensional electron-hole liquid (EHL) is much higher than the binding energy in a three-dimensional EHL. The results of calculations are compared with the experimental results for a wide range of QW widths.

Keywords: electron-hole liquid, quantum well, equilibrium density, binding energy.

INTRODUCTION

Low-dimensional systems, in particular, two-dimensional layers in semiconductors, exhibit new properties in comparison with three-dimensional samples of the same compounds, which is explained by spatial limitations that enhance the effects of inter-particle interactions. One of such systems is a quasi-two-dimensional EHL, intensive studies of which have been conducted in recent years. Recently, EHL has been found in SiO₂/Si/SiO₂ QWs [1, 2], in Si/SiGe/Si heterostructures [3, 4], and in GaAs/AlAs superlattices [5]. The recombination radiation of nonequilibrium electron-hole pairs in SiO₂/Si/SiO₂ quantum wells was experimentally studied in [1, 2]. In these papers, the possibility of formation of a quasi-two-dimensional EHL has been demonstrated and its properties have been studied in detail as a function of the quantum well width.

The studies in this area are mainly aimed at creating new light-emitting devices. Of an obvious interest is also the verification of theoretical methods for systems with strong inter-particle interaction. One of these methods is the density functional theory. This theory has proved itself well in studying properties of a three-dimensional EHL (see the review [6]).

In this paper, the density functional theory is used to calculate the EHL energy and find the equilibrium density of electron-hole pairs in the SiO₂/Si/SiO₂ quantum wells.

STATEMENT OF THE PROBLEM

In the framework of the density functional theory, the total energy of a quasi-two-dimensional EHL can be written in the form

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

$$+ \int U_e(z)n_e(z)dz + \int U_h(z)n_h(z)dz + E_{xc}[n_e, n_h],$$

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

Below, the exciton system of units is used: energy is measured in the units $Ry_{ex} = e^2/2ka_{ex}$ and length is measured in the units $a_{ex} = k\hbar^2 / \mu e^2$, where μ is the reduced mass and k is the dielectric permittivity. For silicon, $\mu = 0.126$ and $k = 11.4$ and then, $a_{ex} \approx 5$ nm and $E_{ex} \approx 13$ meV.

Varying expression (1) with respect to the densities n_e and n_h , we obtain 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 $V_{\text{eff},e}(z) = V_c(z) + V_{xc,e}(z) + U_e(z)$, $V_{\text{eff},h}(z) = -V_c(z) + V_{xc,h}(z) + U_h(z)$, $m_{z,e}$ and $m_{z,h}$ are the masses of charge carriers across the QW.

The electrostatic potential is found from the Poisson equation

$$V_c(z) = 8\pi \int_{-\infty}^z (z - z') [n_h(z') - n_e(z')] dz' \quad (4)$$

and the external potentials for electrons and holes are given by the expression

$$U_i(z) = \begin{cases} 0, & |z| \leq d/2, \\ U_i, & |z| > d/2, \end{cases} \quad (5)$$

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

In what follows, we consider an EHL with the two-dimensional charge carrier concentrations $N_e = N_h = N$. The energy per one electron-hole pair is counted off from the lower energy levels of an electron $E_{0,e}$ and a hole $E_{0,h}$ in an empty well: $E_{eh} = -E_{0,e} - E_{0,h} + E_t/N$.

In case, when only the lower levels of the electron and hole energies are populated, the kinetic energy of charge carriers has the form

$$T_e[n_e] = \frac{\pi\mu}{g_e m_{d,e}} N_e^2 + N_e \left(E_{0,e} - \int V_{\text{eff},e}(z) \Psi_{0,e}^2(z) dz \right), \quad (6)$$

$$T_h[n_h] = \frac{\pi\mu}{m_{d,h}} N_h^2 + N_h \left(E_{0,h} - \int V_{\text{eff},h}(z) \Psi_{0,h}^2(z) dz \right), \quad (7)$$

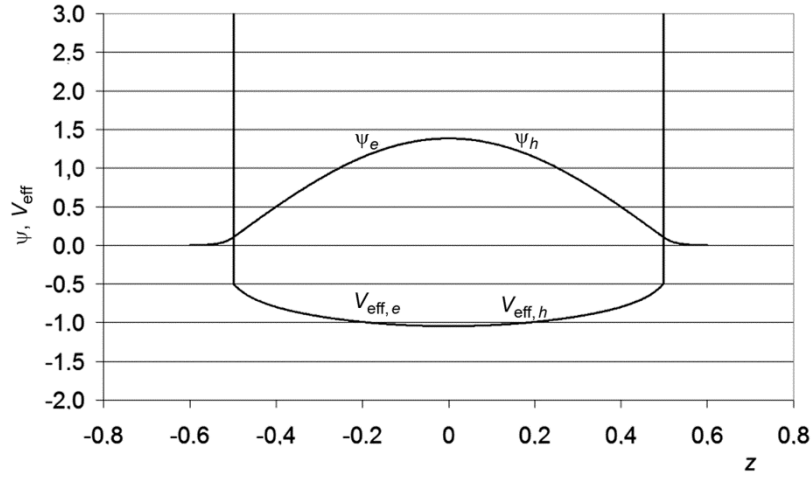


Fig. 1. Profiles of the effective potentials and wave functions in quantum wells with the width $d = 1$ and $N = 0.43$.

where g_i is the number of the equivalent valleys in the conduction band, $m_{d,e}$ and $m_{d,h}$ are the masses of state density of electrons and holes, respectively.

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

$$E_{xc}[n_e, n_h] = \int dz e_{xc}(n_e, n_h), \quad (8)$$

where $e(n_e, n_h)$ is the exchange-correlation energy of electrons and holes per unit volume. Then, the exchange-correlation potentials can be written as

$$V_{xc,e}(z) = \frac{de_{xc}}{dn_e}, \quad V_{xc,h}(z) = \frac{de_{xc}}{dn_h}. \quad (9)$$

In general case, the form of the expression for e_{xc} is unknown. In case of a neutral electron-hole plasma, $n_e(z) = n_h(z) = n(z)$ and for the exchange-correlation energy $\varepsilon_{xc} = e_{xc}/n$, we use the formula proposed in [6]:

$$\varepsilon_{xc} = \frac{1}{2} \frac{a + br_s}{c + dr_s + r_s^2}, \quad (10)$$

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

CALCULATION RESULTS AND DISCUSSION

Nonlinear Schrödinger equations (2) and (3) for electrons and holes were solved numerically. Calculations for two silicon surfaces were carried out. For the calculations, we used the following parameters [1, 2]: $g_e = 2$, $m_{z,e} = 0.918m_0$, $m_{d,e} = 0.19m_0$, $m_{z,h} = 0.53m_0$, and $m_{d,h} = 0.53m_0$ for a (100) surface and $g_e = 6$, $m_{z,e} = 0.258m_0$, $m_{d,e} = 0.358m_0$, $m_{z,h} = 0.53m_0$, and $m_{d,h} = 0.53$ for a (111) surface (m_0 is the free electron mass). In the $\text{SiO}_2/\text{Si}/\text{SiO}_2$ structure, the QW depths are 3.2 and 5 eV for electrons and holes, respectively [2].

Figure 1 shows the results of calculations for the silicon (100) surface at the equilibrium density of electron-hole pairs of $N = 0.43$ and the QW widths of $d = 1$. The QW depths for charge carriers are much larger than the values

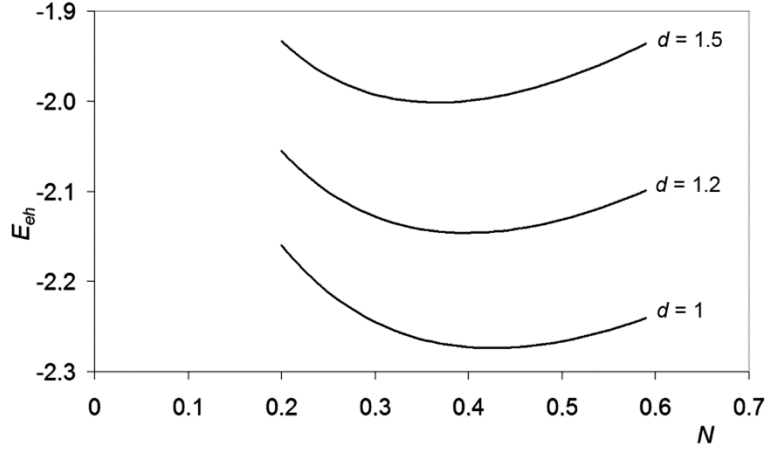


Fig. 2. Dependence of the energy of an electron-hole pair on the two-dimensional density of electron-hole pairs.

of the lower energy levels, so the wave functions of electrons and holes coincide and they are indistinguishable in Fig. 1. We note that the QW depths decrease by an amount of the order of Ry_{ex} due to the exchange-correlation interaction. In general, an EHL has local electroneutrality and therefore, the image potential caused by a strong difference in the dielectric permittivities of silicon and silicon oxide can be neglected. In an external electric field, the neutrality of the EHL is violated, and the image forces will strongly influence the EHL properties [2].

Figure 2 shows the dependence of the electron-hole pair energy E_{eh} on the two-dimensional density of pairs N for the silicon (100) surface for various values of the QW widths d . It is seen that as d increases, the equilibrium density and energy decrease. The formation of an EHL is possible, if it is stable with respect to the decay into free excitons, i.e., if the electron-hole pair energy equal to $-E_{eh}$ is greater, than the exciton binding energy. For $d > a_{ex}$, the binding energy of an exciton in a QW is close to the binding energy of a three-dimensional exciton. It follows from the results presented in Fig. 2 that the binding energy of the EHL with respect to the decay into excitons is of the order of Ry_{ex} or it is larger, then this value, which greatly exceeds the binding energy of a three-dimensional EHL. With increasing QW width, the binding energy decreases. We note that the three-dimensional charge carrier densities $n \approx N/d$ are close to the value of the equilibrium density in a three-dimensional liquid.

Figure 3 shows the calculated (the solid line) and experimental [2] (the triangles) dependences of the equilibrium density (in the units $r_{s,2D} = 1/(\pi N)^{1/2}$) on the QW width. The calculations and experiments were performed for the silicon (100) surface. It can be seen that the theory gives a fairly satisfactory agreement with the experimental results.

It is well known that the presence of the conduction band degeneracy leads to an increase in the equilibrium density and binding energy of a three-dimensional EHL. A similar phenomenon is observed in a quasi-two-dimensional EHL. The results of calculations for the silicon (111) surface (Fig. 4) showed that the binding energy increases by about 1.4 times and the equilibrium density increases by more than 2 times in comparison with the density for the silicon (100) surface. The increase in the binding energy and equilibrium density is mainly due to the decrease in the longitudinal kinetic energy of electrons (the first term in Eq. (6)). For the silicon (111) surface, the equilibrium density of electron-hole pairs $N_{eq} = 4 \cdot 10^{12} \text{ cm}^{-2}$ for $d = 1$ and the equilibrium density decreases with increasing QW width. We also note that the three-dimensional densities of charge carriers are much larger than the densities in the three-dimensional EHL.

An analytical expression for the energy of a quasi-two-dimensional EHL was obtained in [7]. Comparison of the results obtained in the present paper with the analytical results [7] at $d = 1$ for the silicon (100) and (111) surfaces showed that the difference in the equilibrium density is insignificant (several percent), whereas the energy differs by

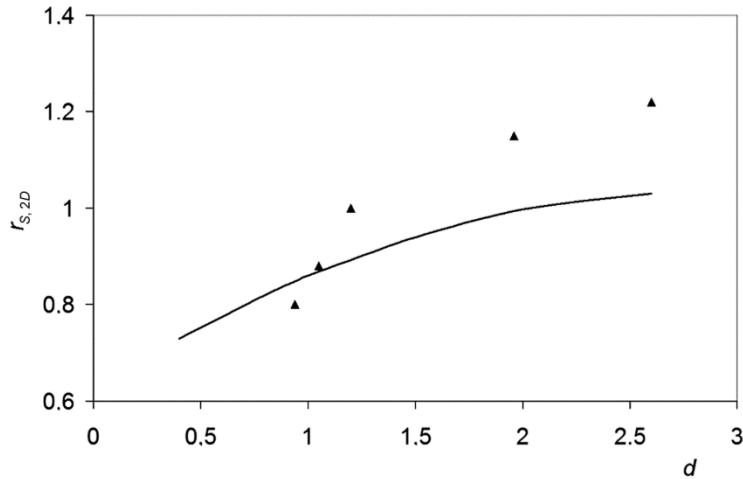


Fig. 3. Dependence of the parameter $r_{s,2D}$ on the QW width. Solid line – the numerical calculation, triangles – the experiment [2].

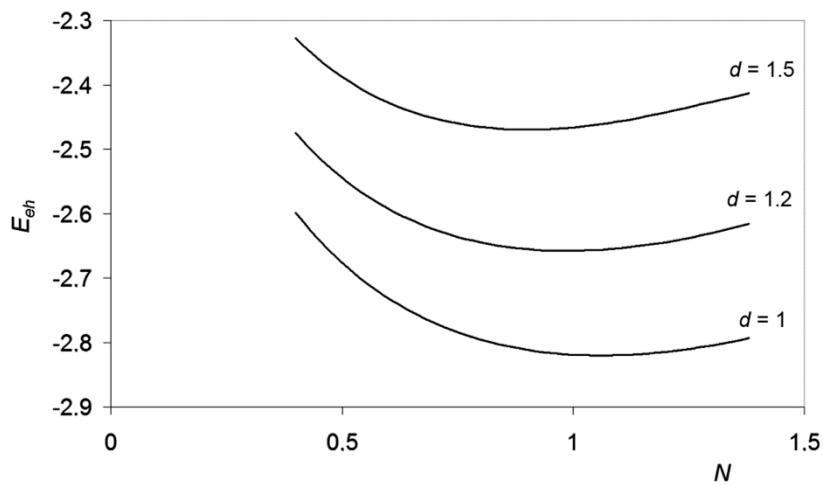


Fig. 4. Dependence of the electron-hole pair energy on the two-dimensional density of electron-hole pairs.

about 1.5 times. The difference in energy is mainly due to the fact that in this paper, the energy was counted off from the energy levels of electrons and holes in an empty well.

CONCLUSIONS

In this paper, the density functional theory is used to calculate the EHL energy and find the equilibrium density of electron-hole pairs in the $\text{SiO}_2/\text{Si}/\text{SiO}_2$ quantum well. Nonlinear Schrödinger equations for electrons and holes were solved numerically. Calculations were carried out for the silicon (100) and (111) surfaces. The largest binding energy and equilibrium density of electron-hole pairs were obtained for the silicon (111) surface. It is shown that the binding

energy of the EHL with respect to the decay into excitons can be greater than Ry_{ex} , which is much higher than the binding energy in a three-dimensional EHL. Calculations have been carried out for quantum wells of various widths and it is found that with increasing QW width, the binding energy and equilibrium density decrease. A satisfactory agreement between the calculated values of the equilibrium density and the experimental results [2] for the silicon (100) surface was obtained. Also good agreement was found between the results of numerical calculations and the results of analytical calculations given in [7].

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