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High-Temperature Electron-Hole Liquid in Diamond Films

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***Abstract*—Using the density functional theory we find the energy and the equilibrium density of the electron-hole liquid in diamond films. The local density approximation is used to account for exchange and correlation energy. In diamond films, electron-hole liquid is multi-component and contains electrons, and heavy, light, and spin-orbit split holes. The nonlinear Kohn-Sham equations for electrons, and heavy, light, and spin-orbit split holes are solved numerically. We find that wave functions of electrons and holes strongly overlap, so the contribution of the Coulomb interaction to the energy of electron-hole liquid is small. The exchange-correlation potentials in the center of the quantum well have a value of the order excitonic Rydberg. The energy of electron-hole pair is calculated for (111) diamond films. It is well known that in diamond crystals, the critical electron-hole liquid temperature of 170 K is observed. We show that the critical temperature of the electron-hole liquid in diamond films can reach 260 K.**

Keywords—diamond films, electron-hole liquid.

I. INTRODUCTION

It is well known that in many semiconductors, excitons condense into an electron-hole liquid (EHL) [1]. The highest critical EHL temperature of 170 K is observed in diamond crystals [2, 3]. A review of the current state of research on the properties of quasi-two-dimensional EHL is given in [4]. Recently, there have been reports of EHL formation in quantum wells. Using the density functional theory, we have developed a model that well explains the experimental results for EHL in Si/SiO_2 and SiGe/Si quantum wells [5]. In this work, we use the density functional theory to study the properties of EHL in diamond films.

II. TEORETICAL MODEL

To calculate the EHL energy, we use the model proposed in [6]. In diamond films, EHL is multi-component and contains electrons, and heavy, light, and spin-orbit split holes. The total energy for an electron-hole system is written as

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

where T_i is the kinetic energy (i = e, hh, hl, so); E_c is the electrostatic energy; U_i is the external potential; E_{xc} is the exchange-correlation energy; n_e, n_{hh}, n_{hl}, and n_{so} are the densities of electrons and heavy, light, and spin-orbit split holes, respectively; and $n_h = n_{hh} + n_{hl} + n_{so}$.

In the exciton system of units, the Kohn-Sham equations are given by

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

where μ is the reduced mass; $V_{eff,i}(z) = \delta_i \cdot V_c(z) + V_{xc,i}(z) + U_i(z)$ with δ_e = 1 and δ_k = –1 for k = hh, hl, so; $V_c(z)$ is the electrostatic potential; and $V_{xc,i}(z)$ is the exchange-correlation potential.

Electrostatic potential is:

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

Confinement potentials are given by

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

where d is the film thickness, $\Delta_e = \Delta_{hh} = \Delta_{hl} = 0$ and $\Delta_{so} = 0.066$.

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Exchange-correlation potentials are written as

$$V_{xc,e}(z) = \frac{d(n_e \varepsilon_{xc})}{dn_e},$$
$$V_{xc,hh}(z) = \frac{d(n_h \varepsilon_{xc})}{dn_{hh}},$$
$$V_{xc,hl}(z) = \frac{d(n_h \varepsilon_{xc})}{dn_{hl}}, \quad (5)$$
$$V_{xc,hl}(z) = \frac{d(n_h \varepsilon_{xc})}{dn_{so}}.$$

Here the following approximation formula is used for ε_{xc}:

$$\varepsilon_{xc} = \frac{1}{2} \frac{a + br_s}{c + dr_s + r_s^2} \quad (6)$$

where $r_s = (3/(4\pi n))^{1/3}$, a = -4.83, b = -5.09, c = 0.016, and d = 3.05.

When only the lowest subbands are occupied, the carrier densities of are given by

$$n_e(z) = N_e \psi_e^2(z),$$
$$n_{hh}(z) = N_{hh} \psi_{hh}^2(z),$$
$$n_{hl}(z) = N_{hl} \psi_{hl}^2(z), \quad (7)$$
$$n_{so}(z) = N_{so} \psi_{so}^2(z)$$

where N_e, N_{hh}, N_{hl}, N_{so} are the two-dimensional densities of the charge carrier.

The energy per electron–hole pair is:

$$E_{eh} = -E_e - E_{hh} + E_t / N. \quad (8)$$

The hole densities are determined from equations:

$$N_e = N_{hh} + N_{hl} + N_{so} = N, \quad (9)$$

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

III. Results

The nonlinear Schrödinger equations (2) are solved numerically. We assume for simplicity that $U_e = U_{hh} = U_{hl} = = U_{so} = U$.

Calculations have shown that the lowest energy of EHL is achieved in (111)-oriented diamond films. For this film, we use the following parameters: g_e = 6, $m_{z,e}$ = 0.46m_0, $m_{d,e}$ = = 0.56m_0, $m_{z,hh}$ = 0.57m_0, $m_{d,hh}$ = 0.57m_0, $m_{z,hl}$ = 0.32m_0, $m_{d,hl}$ = = 0.32m_0, $m_{z,so}$ = 0.39m_0, $m_{d,so}$ = 0.39m_0, and Δ_{so} = 0.066 m_0 (m_0 is free electron mass).

Fig. 1 shows the potentials and wave functions for a quantum well with d = 1 and U =1. For these values, the equilibrium density is N = 0.92. In our chosen model, the effective potentials of light and heavy holes coincide. One can see that the wave functions of electrons and holes strongly overlap, so the contribution of the Coulomb interaction to the energy of EHL is small (about 1 percent). From the results presented in Fig. 1, one can see that the exchange-correlation potentials in the center of the quantum well have a value of the order Ry_{ex}.

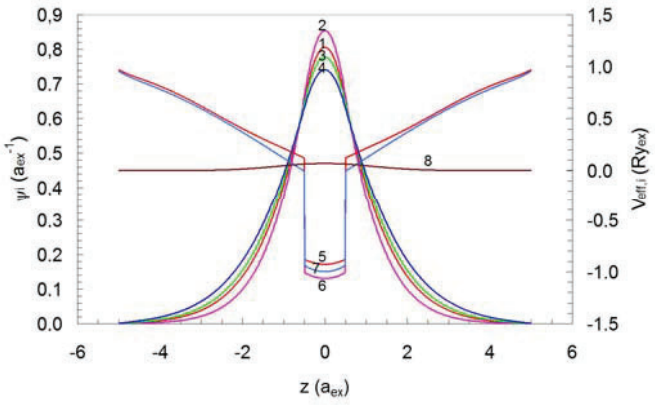

Fig. 1. Potentials and wavefunctions for electrons and holes. U = 1, d = 1, N_e = 0.92 N_{hh} = 0.43, N_{hl} = 0.25, and $N_{so} \approx$ 0. 24. 1 – ψ_e, 2 – ψ_{hh}, 3 – ψ_{hl}, 4 – ψ_{so}, 5 – $V_{eff,e}$, 6 – $V_{eff,hh}$, 7 – $V_{eff,so}$, 8 – V_c.

Fig. 2 shows the energy as function of the density for a quantum well with a width d = 1. The minimum energy is achieved at $N \approx$ 1.1, with $N_{hh} \approx$ 0.72, $N_{hl} \approx$ 0.26, and $N_{so} \approx$ 0.12. We see that the energy can drop to as low as E_{gs} = -2.37. This energy is significantly less than the energy of a three-dimensional EHL [3]. The critical temperature of EHL may be described by an empirical relationship $T_c = 0.1\ |E_{gs}|/k_B$. Using this relationship for diamond films, we obtain T_c = 260K.

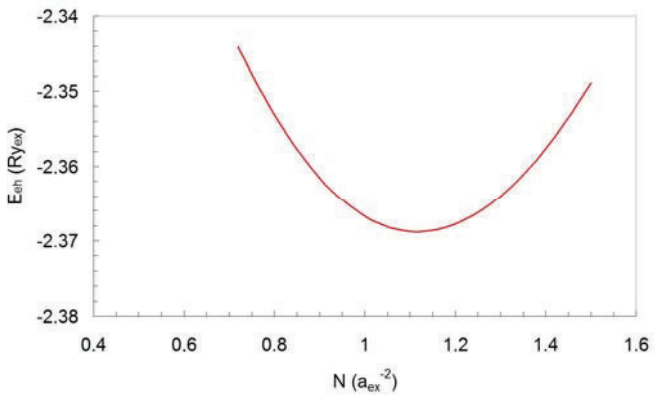

Fig. 2. The energy per electron-hole pair as function of the density for (111) diamond films. $U = 20$, $d = 1$.

IV. Conclusion

In summary, numerical results have been obtained for the energy and equilibrium density of EHL in diamond films. We have shown that the critical temperature of EHL in (111) diamond films can reach 260 K.

Acknowledgment

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