CHAPTER 3. Local exchange-correlational potential on particle-hole pairing in superconducting state in ZnO/(Zn,Mg)O quantum wells

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Abstract In this paper a theoretical studies of the space separation of electron and hole wave functions in the quantum well ZnO/(Zn,Mg)O are presented. For this aim the self-consistent solution of the Schrödinger equations for electrons and holes and the Poisson equations at the presence of spatially varying quantum well potential due to the piezoelectric effect and local exchange-correlation potential is found. The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density for electrons and holes the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions in addition. The shifts of the Hartree valence band spectrums and the conduction band spectrum with respect to the flat band spectrums as well as the Hartree-Fock band spectrums are found. An overlap integrals of the wave functions of holes and electrons with taking into account besides the piezoelectric effects the exchange-correlation effects in addition is greater than an overlap integral of Hartree ones. The Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles. It is found that an effective mass of heavy hole of Mg0.27Zn0.73O under biaxial strain is greater than an effective-mass of heavy hole of ZnO. It is calculated that an electron mass is less than a hole mass. It is found that the Bohr radius is greater than the localization range particle-hole pair, hence the excitons may be spontaneously created.

1 Introduction

There has been widely studied in the ultraviolet spectral range lasers based on direct wide-bandgap hexagonal wurtzite crystal material systems such as ZnO [1, 2, 3, 4, 5, 6]. Significant success has been obtained in growth ZnO quantum wells with (ZnMg)O barriers by scrutinized methods of growth [7, 8]. The carrier relaxation from (ZnMg)O barrier layers into a ZnO quantum well through time-resolved photoluminescense spectroscopy is studied in the paper [9]. The time of filling of particles for the single ZnO quantum well is found to be 3 ps [9].

In the paper we present a theoretical investigation of the intricate interaction of the electron-hole plasma with a polarization-induced electric fields. The confinement of wave functions has a strong influence on the optical properties which is observed with a dependence from the intrinsic electric field which is calculated to be 0.37 MV/cm [10], causing to the quantum-confined Stark effect (QCSE). In this paper we present the results of theoretical studies of the space separation of electron and hole wave functions by self-consistent solution of the Schrödinger equations for electrons and holes and the Poisson equations at the presence of spatially varying quantum well potential due to the piezoelectric effect and the local exchange-correlation potential.

In addition large electron and hole effective masses, large carrier densities in quantum well ZnO are of cause for population inversions. These features are comparable to GaN based systems [11, 12].

A variational simulation in effective-mass approximation is used for the conduction band dispersion and for quantization of holes a Schrödinger equation is solved with wurtzite hexagonal effective Hamiltonian [13] including deformation potentials [14]. Keeping in mind the above mentioned equations and the potential energies which have been included in this problem from Poisson’s equations we have obtained completely self-consistent band structures and wave functions.

So in this paper we present a self-consistent calculation an above mentioned equations in wurtzite ZnO quantum well taking into account the piezoelectric effect and the exchange-correlation potential for bandgap renormalization and engineering of localized Hartree-Fock wave functions. The energy shifts as well as the localization range of exchange-correlational wave functions with respect to Hartree energy shifts and Hartree localization range of wave functions require a scrutiny study.

We consider the pairing between oppositely charged particles with complex dispersion. The Coulomb interaction leads to the electron-hole bound states scrutiny study of which acquire significant attention in the explanations of superconductivity. If the exciton binding energy is grater than the localization range particle-hole pair, the excitons may be spontaneously created.

2 Theoretical study
2.1 Effective Hamiltonian

It is known [13, 15] that the valence-band spectrum of hexagonal würtzite crystal at the Γ point originates from the sixfold degenerate Γ15 state. Under the action of the hexagonal crystal field in würtzite crystals, Γ15 splits and leads to the formation of two levels: Γ1, Γ5. The wave functions of the valence band transform according to the representation Γ1 + Γ5 of the point group C6v, while the wave function of the conduction band transforms according to the representation Γ1.

<table>
<thead>
<tr>
<th>C6v</th>
<th>E</th>
<th>C2</th>
<th>2C3</th>
<th>2C6</th>
<th>3σv</th>
<th>3σ′v</th>
</tr>
</thead>
<tbody>
<tr>
<td>Γ1 + Γ5</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>C2</td>
<td>E</td>
<td>E</td>
<td>C3</td>
<td>C3</td>
<td>E</td>
<td>E</td>
</tr>
<tr>
<td>χ_0^0(g)</td>
<td>9</td>
<td>1</td>
<td>0</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>χ_0(g^2)</td>
<td>3</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>1/2 [χ_0^0(g) + χ_0(g^2)]</td>
<td>6</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>1/2 [χ_0^0(g) - χ_0(g^2)]</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
</tr>
</tbody>
</table>

An irreducible presentations for orbital angular momentum \( j \) may be built from formula

\[
χ_j(ϕ) = \frac{\sin(j + \frac{3}{2}ϕ)}{\sin\frac{3ϕ}{2}}, \tag{1}
\]

For the vector representational \( j = 1 \)

\[
χ_v(ϕ) = \frac{\sin\frac{3ϕ}{2}}{\sin\frac{ϕ}{2}} = 1 + 2\cosϕ. \tag{2}
\]

The direct production of two irreducible presentations of wave function and wave vector of difference \( κ - Γ \) expansion with taken into account time inversion can be expanded on

\[
p^κ : τ_v × τ_ψ = (Γ_1 + Γ_5) × (Γ_2 + Γ_5) = Γ_5 × Γ_5, \tag{3}
\]

for the square of wave vector

\[
[p^κ p^κ] : τ_v × τ_ψ = (2Γ_1 + Γ_5 + Γ_6) × (2Γ_1 + Γ_5 + Γ_6) = 4Γ_1 × Γ_1 + Γ_5 × Γ_5 + Γ_6 × Γ_6. \tag{4}
\]

In the low-energy limit the Hamiltonian of würtzite

\[
\hat{H}_0 = i(Δ_1 + Δ_2) + \Delta_1 J_x^2 + Δ_2 J_z^2 + \sqrt{2}Δ_3 (J_z σ_- + J_- σ_+), \tag{5}
\]

In the basis of spherical wave functions with the orbital angular momentum \( l = 1 \) and the eigenvalue \( m_l \) of its \( z \) component:

\[
|1, \zeta_1⟩ = \frac{1}{\sqrt{2}} (Y^1_1ψ(1/2)e^{-3iϕ/2}e^{-3iπ/4} + Y^1_{-1}ψ(-1/2)e^{3iϕ/2}e^{3iπ/4})
\]

\[
|2, \zeta_2⟩ = \frac{1}{\sqrt{2}} (±Y^0_1ψ(-1/2)e^{-iϕ/2}e^{-iπ/4} + Y^1_{-1}ψ(1/2)e^{iϕ/2}e^{iπ/4}) \tag{6}
\]

\[
|3, \zeta_3⟩ = \frac{1}{\sqrt{2}} (±Y^0_1ψ(1/2)e^{-iϕ/2}e^{-iπ/4} + Y^0_{-1}ψ(-1/2)e^{iϕ/2}e^{iπ/4}), \tag{7}
\]

the Hamiltonian may be transformed to the diagonal form indicating two spin degeneracy [16]:

\[
H_± = \begin{vmatrix}
F & K_t & ±iH_t & 1, \zeta_1 \\
K_t & G & Δ ± iH_t & 2, \zeta_2 \\
±iH_t & Δ ± iH_t & λ & 3, \zeta_3 \\
\end{vmatrix}. \tag{8}
\]
where \( F = \Delta_1 + \Delta_2 + \lambda + \theta \), \( G = \Delta_1 - \Delta_2 + \lambda + \theta \), \( \lambda = \lambda_x + \lambda_z \), \( \theta = \theta_x + \theta_z \), \( \lambda_e = \frac{h^2}{2m_0}(A_1k_x^2 + A_2k_z^2) \), \( \lambda_e = D_1\epsilon_{zz} + D_2(\epsilon_{xx} + \epsilon_{yy}) \), \( \theta_e = D_3\epsilon_{zz} + D_4(\epsilon_{xx} + \epsilon_{yy}) \), \( K_i = \frac{h^2}{2m_0}(A_1k_z^2) \), \( H_i = \frac{h^2}{2m_0}(A_2k_z^2) \), \( \Delta = \sqrt{\Delta_3} \), \( k_i^2 = k_i^2 + k_j^2 \).

From Kane model one can define the band-edge parameters such as the crystal-field splitting energy \( \Delta_{\nu} \), the spin-orbit splitting energy \( \Delta_{\partial} \), and the momentum-matrix elements for the longitudinal (\( e \parallel z \)) polarization: \( \Delta_{\nu} = \langle S|\hat{p}_z|Z \rangle \), \( \Delta_{\partial} = \langle S|\hat{\rho}_y|X \rangle \equiv \langle S|\hat{\rho}_y|Y \rangle \). Here we use the effective-mass parameters, energy splitting parameters, deformation potential parameters as in papers [14, 17, 18].

We consider a quantum well of width \( w \) in ZnO under biaxial strain, which is oriented perpendicularly to the growth direction (0001) and localized in the spatial region \(-2/3 < z < w/2\). In the ZnO/MgZnO quantum well structure, there is a strain-induced electric field. This piezoelectric field, which is perpendicular to the quantum well plane (i.e., in \( z \) direction) may be appreciable because of the large piezoelectric constants in wurtzite structures.

The transverse components of the biaxial strain are proportional to the difference between the lattice constants of the well and the barrier and depend on the Mg content \( x \):

\[
\Delta = 2.47 \text{ meV}, \quad \Delta_{\nu} = 3.8 \text{ meV}, \quad \Delta_{\partial} = 2.099 \text{ meV}.
\]

The physical parameters for ZnO are as follows. We take the effective-mass parameters [17]: \( A_1 = -2.743 \), \( A_2 = -0.393 \), \( A_3 = 2.377 \), \( A_4 = -2.069 \), \( A_5 = -2.051 \), \( A_6 = -2.099 \), \( m_z^+ = 0.329 m_0 \), where \( m_0 \) is the electron rest mass in the vacuum, the parameters for deformation potential [14]: \( D_1 = -3800 \text{ meV} \), \( D_2 = -3800 \text{ meV} \), \( D_3 = -800 \text{ meV} \), \( D_4 = 1400 \text{ meV} \), \( D_5 = -6860 \text{ meV} \), \( D_6 = -6260 \text{ meV} \) and the energy parameters at 300 K [17, 18]: \( E_z = 3400 \text{ meV} \), \( \Delta_{\nu} = 36.3 \text{ meV} \), \( \Delta_{\partial} = 0.63 \text{ meV} \), \( \Delta_{\theta} = 2.47 \text{ meV} \), \( \Delta_3 = 3800 \text{ meV} \), \( \Delta_6 = 3800 \text{ meV} \), \( \Delta_9 = 90 \text{ GPa} \) and \( \epsilon_{33} = 196 \text{ GPa} \), the permittivity of the host materials \( \kappa = 7.8 \).

### 2.2 ZnO/(Zn,Mg)O quantum well

We take the following wave functions written as vectors in the three-dimensional Bloch space:

\[
|\nu_{\zeta}, k_i \rangle = \sum_{m=1}^{3} \psi_{(1)}^{(m)}(i, \nu) \psi_{(Z)}(1, \zeta) \psi_{(1)}^{(m)}(i, \nu) \psi_{(1)}^{(m)}(i, \nu) \psi_{(1)}^{(m)}(i, \nu)
\]

The Bloch vector of \( \nu \)-type hole with spin \( \zeta \) is specified by its three coordinates \( \psi_{1}^{(1)}(m, \nu), \psi_{2}^{(1)}(m, \nu), \psi_{3}^{(1)}(m, \nu) \) in the basis \([1, \zeta], [2, \zeta], [3, \zeta]\) [16], known as spherical harmonics with the orbital angular momentum \( \ell = 1 \) and the eigenvalue \( m \) its \( z \) component. The envelope \( Z \)-dependent part of the quantum well eigenfunctions can be specified from the boundary conditions \( \psi_m(Z = 0) = \psi_m(Z = 1) = 0 \) of the infinite quantum well as

\[
\psi_m(Z) = \sqrt{\frac{2}{w}} \sin(\pi m Z),
\]

(11)

The hole wave function can be written as

\[
\psi_{\nu, \zeta, k_i}(r) = e^{i k_i r},
\]

(12)

The valence subband structure \( E_{\nu}^{(i)}(k_i) \) can be determined by solving equations system:

\[
\sum_{j=1}^{3} (H_{ij}^{(i)}(k_z) = -i \frac{\partial}{\partial z} + V(z) + \delta_{ij}E_{\nu}^{(i)}(k_i) \times \phi_{(i)}^{(j)}(z, k_i) = 0,
\]

(13)

where \( \phi_{(i)}^{(j)}(z, k_i) = \sum_{m=1}^{3} \psi_{(i)}^{(j)}(m, \nu) \psi_{(z)}(\nu) \), \( i = 1, 2, 3 \).

The wave function of electron of first energy level with accounts QCSE [19]:

\[
\Psi(r) = \frac{1}{\sqrt{A}} e^{i k R} \Psi(Z, \xi)[S]|\zeta\rangle,
\]

(14)

where

\[
\Psi(Z, \xi) = \begin{cases} 
\psi_1(Z, \xi) = C_1 e^{(\xi - \xi)(w Z)} \in (-\infty, 0), \\
\psi_2(Z, \xi) = C e^{i |k_0 w (Z - \frac{1}{2}) + \delta_0} e^{\xi e^{z \xi w(z - \frac{1}{2})}}, \in [0, 1], \\
\psi_2(Z, \xi) = C_2 e^{-(\xi + \xi w)(Z - 1)}, \in (1, \infty).
\end{cases}
\]

(15)
Figure 1. (Color online) For the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 4 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300 K: (a) conduction band energy; (b) valence band energy.

Figure 2. (Color online) For the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 4 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300 K: (a) Hartree screening potential; (b) Hartree-Fock screening potential.
\( |S\rangle = Y_0^0, \zeta_c = \pm 1/2. \)

From bond conditions \[19, 20\] \( \psi_1(Z, \xi)\rangle_{z=0} = \psi(Z, \xi)\rangle_{z=0}, \psi_2(Z, \xi)\rangle_{z=1} = \psi(Z, \xi)\rangle_{z=1}, \psi_3(Z, \xi)\rangle_{z=0} = \psi(Z, \xi)\rangle_{z=0}, \)

\( \psi_2(Z, \xi)\rangle_{z=1} = \psi_1(Z, \xi)\rangle_{z=1}, \)

where \( \Phi, \delta \)

One can find the functional, which is built in the form:

\[
J(\xi) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}.
\]

where \( H = H_c + V(z), \)

where \( H_c \) is a conduction band kinetic energy including deformation potential:

\[
H_c = E_g + \Delta_1 + \Delta_2 + \frac{\hbar^2}{2m^*_0} \left( k_x^2 + k_y^2 \right) + D_\epsilon \frac{\varepsilon_{xx} + \varepsilon_{yy}}{2}.
\]

The potential energies \( V(z) \) can look for as follows:

\[
V(z) = e\Phi^H(z) + \delta U_{c,v}(z) + \Phi_{xc}(z),
\]

\( \Phi_{xc}(z) \) is exchange-correlation potential energy which is found from the solution of three-dimensional Poisson's equation, using both an expression by Gunnarsson and Lundquist \[22\], and following criterions. At carrier densities \( 4 \times 10^{15} \text{ cm}^{-2} \), the criterion \( k_F > \sqrt{\hbar/} \text{ at a temperature } T = 0 \text{ K as } 1 > 0.1 \text{ has been carried. } k_F \) is Fermi wave vector. The criterion does not depend from a width of well. The ratio of Coulomb potential energy to the Fermi energy is \( r_F = E_C/E_F = 0.63 < 1. \) The problem consists of the one-dimensional Poisson's equation solving of which may be found Hartree potential energy and three-dimensional Poisson's equation which is separated on one-dimensional and two-dimensional equations by separated of variables using a criterion \[ \Psi_{\alpha,v,n}(k_F, z) \sin k_F \rho \ll 1, \] where \( \alpha = e, h. \) The three-dimensional Poisson's equation includes local exchange-correlation potential:

\[
\frac{d^2 \Phi_{e,h}}{d z^2} + \Delta_p \Phi_{e,h} = \frac{4\pi}{\kappa} (\rho_{e,h}^H(z; g)) + \rho_{e,h}^{xc}(r, r'),
\]

\[
\frac{d^2 \Phi_{e,h}^H}{d z^2} = \frac{4\pi}{\kappa} \rho_{e,h}^H(z; g),
\]

\[
\Delta_p \Phi_{e,h}^{xc} = \frac{4\pi}{\kappa} \rho_{e,h}^{xc}(r, r'),
\]

where

\[
\rho_{e,h}^H(z; g) = e \sum_{\nu,n,k_i} |\Psi_{e,h,v,n}(k_i, z)|^2 f_{n,\nu}(k_i; g),
\]

\[
f_{n,\nu}(k_i; g) = \frac{1}{e^{\left(\alpha + n + \frac{\nu}{2} + \sum_{j=0}^{n-1} \frac{\nu_j}{2} \right)} + 1} = \frac{1}{e^{\left(1 + r_F + g \sum_{j=0}^{n-1} \frac{\nu_j}{2} \right)} + 1}.
\]

The solution of equations system \(13, 17, 22\) as well as \(13, 17, 23\) does not depend from a temperature. Solving one-dimensional Poisson's equation \(23\) one can find screening polarization field and Hartree potential energy by substituting her in the Schrödinger equations. From Schrödinger equations wave functions and bandstructure are
found. The conclusive determination of screening polarization field is determined by iterating Eqs. (13), (17), (22) until the solutions of conduction and valence band energies and wave functions are converged:

\[ \Phi^H(z) = \Phi^H_0(z) + \Phi^H_e(z), \]

(27)

\[ e\Phi^H_0(z) = \frac{2\pi}{\kappa} \sum_{\nu,m,l} g_0 \int k_d k_r \{ \Psi_{\nu,m,l}^c[v,m] \Psi_{\nu,m,l}^h[v,m] \} f_{r,g}(k_r) \times \]

\[ \left( \frac{\cos \pi \frac{1}{2} (m+l)}{\pi^2 (m,l)^2} - \frac{\cos \pi \frac{1}{2} (m-l)}{\pi^2 (m,l)^2} \right), m \neq l, \]

\[ \left( \frac{\cos \pi \frac{1}{2} (m+l)}{\pi^2 (m,l)^2} + \frac{\cos \pi \frac{1}{2} (m-l)}{\pi^2 (m,l)^2} \right), m = l, \]

(28)

\[ e\Phi^H_e(z) = -\frac{2e^2}{\kappa} g_1 \int k_d k_r C^2 f_{1m}(k_r) \times \]

\[ \left( \frac{1-\cos(-k_d w+2\delta_0)}{2} \right) e^{\frac{z}{w}} w^{\frac{1}{2} (\nu+1)} \xi^2, \xi \in (-\infty, -w/2) \]

\[ \left( \frac{1-\cos(c_2 w+2\delta_0)}{2} \right) e^{-\frac{z}{w}} w^{\frac{1}{2} (\nu+1)} \xi^2, \xi \in \left( -w/2, w/2 \right) \]

(29)

where \( Z = \frac{z}{w} + \frac{1}{2}, \) \( g_0 \) and \( g_1 \) correspond to the degeneration of the \( v \) hole band and the first quantized conduction band, respectively, \( e \) is the value of electron charge, \( \kappa \) is the permittivity of a host material, and \( f_{r,g}(k_r), f_{1m}(k_r) \) are the Fermi-Dirac distributions for holes and electrons.

Exchange-correlation charge density may be determined as:

\[ \rho_{xc}^{\alpha}(r,r') = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} |\Psi_{\alpha,v,n}(k_l,\nu)|^2 \rho_{lm}(\rho - \rho') Y_{lm}(\frac{\rho - \rho'}{|\rho - \rho'|}), \]

(30)

using the expansion of plane wave

\[ \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \rho_{lm}(\rho) Y_{lm}(\frac{k_{\nu}}{|\rho|}) = e^{ik_{\nu} \cdot \rho} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(k_{\nu},\rho) R_{lm}(\frac{k_{\nu}}{|\rho|}) Y_{lm}(\frac{\rho}{|\rho|}). \]

(31)

At the condition \([\Psi_{\alpha,v,n}(k_{\nu},\nu) \sin k_{\nu} \rho] << 1\), the solution Eq. (24) may be found as follows

\[ \Phi_{xc}(xc) = \int_0^{\infty} \rho^0 \rho_{00}(\rho) \frac{1}{\rho} d\rho. \]

(32)

The solution the three-dimensional Poisson’s equation may be presented in the form:

\[ \Phi_{xc}(z) = \Phi^H(z) \Phi_{xc}(xc). \]

(33)

The complete potential which describes piezoelectric effects and local exchange-correlation potential in quantum well one can find as follows

\[ \Phi(z) = \Phi^H_0(z) + \Phi^H_e(z) + \Phi^H_0(z) \Phi_{xc}(xc) + \Phi^H_e(z) \Phi_{xc}(xc). \]

(34)

### 2.3 Uncertainty Heisenberg principle

The Heisenberg equation for a microscopic dipole \( \hat{p}_{p}^{v,\nu} = (\hat{b}_p \hat{a}_p) \) due to an electron-hole pair with the electron (hole) momentum \( p (-p) \) and the subband number \( v, \nu \) is written in the form:

\[ \frac{\partial \hat{p}_{p}^{v,\nu}}{\partial t} = \frac{i}{\hbar} [\hat{H}, \hat{p}_{p}^{v,\nu}]. \]

(35)

We assume a nondegenerate situation described by the Hamiltonian \( \hat{H} = \hat{H}_0 + \hat{V} + \hat{H}_{\text{int}}, \) which is composed of the kinetic energy of an electron \( \epsilon^c_{\nu}p \) and the kinetic energy of a hole \( \epsilon^h_{\nu}p \) in the electron-hole representation:

\[ \hat{H}_0 = \sum_{p} \epsilon^c_{\nu} \hat{a}_p^{\dagger} \hat{a}_p + \epsilon^h_{\nu} \hat{b}_p^{\dagger} \hat{b}_p. \]

(36)

where \( p \) is the transversal quasimomentum of carriers in the plane of the quantum well, \( \hat{a}_p, \hat{a}_p^{\dagger}, \hat{b}_p, \) and \( \hat{b}_p^{\dagger} \) are the annihilation and creation operators of an electron and a hole. The Coulomb interaction Hamiltonian for particles in the electron-hole representation takes the form:
The transverse effective masses for Mg depend on the wave vector $\nu$ and the subband number $\hat{a}$ unit vector of the vector potential of an electromagnetic wave, functions for an electron and a hole written in the form

$$V = \sum_{p,q,k} V^{\nu,V,\nu,V}_{p} \hat{a}_{p}^+ \hat{a}_{q}^+ \hat{a}_{-} \hat{a}_{+},$$

$$+ V^{\nu,V,\nu,V}_{p} \hat{b}_{p}^+ \hat{b}_{q}^+ \hat{b}_{-} \hat{b}_{+},$$

$$- 2 V^{\nu,V,\nu,V}_{p} \hat{a}_{p}^+ \hat{b}_{p}^+ \hat{b}_{q}^+ \hat{a}_{q}^+,$$

(37)

where

$$V^{\nu,V,\nu,V}_{p} = \frac{e^2}{\kappa A} \int_{-\omega/2}^{+\omega/2} dz \int_{-\omega/2}^{+\omega/2} dz' X_{\nu}(z) X_{\nu}(z') \frac{2\pi}{q} \times$$

$$e^{-q|z-z'|} X_{\nu}(z') X_{\nu}(z),$$

(38)

is the Coulomb potential of the quantum well, $\kappa$ is the dielectric permittivity of a host material of the quantum well, and $A$ is the area of the quantum well in the $xy$ plane.

The Hamiltonian of the interaction of a dipole with an electromagnetic field is described as follows:

$$\hat{H}_{\text{int}} = -\frac{1}{\kappa A} \sum_{V,\nu,\nu',p} (\mu_{p}^{\nu,\nu'}) \hat{b}_{p}^+ \hat{b}_{p}^+ E^* e^{i\omega t} +$$

$$(\mu_{p}^{\nu,\nu'}) \hat{a}_{p}^+ \hat{a}_{p}^+ E e^{-i\omega t},$$

(39)

where $\mu_{p}^{\nu,\nu'} = \langle \hat{b}_{-} \hat{a}_{p}^+ \rangle$ is a microscopic dipole due to an electron-hole pair with the electron (hole) momentum $p$ ($-p$) and the subband number $V_{\nu}$ ($V_{\nu}'$), $\mu_{p}^{\nu,\nu'} = \int d^3 r U_{\nu\sigma}^{\nu'} \epsilon_{p}^\nu U_{\nu\sigma}^{\nu'}$, is the matrix element of the electric dipole moment, which depends on the wave vector $k$ and the numbers of subbands, between which the direct interband transitions occur, $\epsilon$ is a unit vector of the vector potential of an electromagnetic wave, $\hat{b}$ is the momentum operator. Subbands are described by the wave functions $U_{j'(\sigma')k}$, $U_{\nu\sigma k}$, where $j'$ is the number of a subband from the conduction band, $\sigma'$ is the electron spin, $j$ is the number of a subband from the valence band, and $\sigma$ is the hole spin. We consider one lowest conduction subband $j' = 1$ and one highest valence subband $j = 1$. $E$ and $\omega$ are the electric field amplitude and frequency of an optical wave.

The polarization equation for the wurtzite quantum well in the Hartree–Fock approximation with regard for the wave functions for an electron and a hole written in the form [12, 23], where the coefficients of the expansion of the wave function of a hole in the basis of wave functions (known as spherical functions) with the orbital angular momentum $l = 1$ and the eigenvalue $m_{l}$ of its z component, depend on the wave vector can look for as follows:

$$\frac{d\hat{b}_{p}^{\nu,\nu'}}{d\tau} = -i \omega_{p}^{\nu,\nu'} \hat{b}_{p}^{\nu,\nu'} + i \Omega_{p}^{\nu,\nu'} (-1 + \hat{n}_{p}^{\nu} + \hat{n}_{p}^{\nu'}).$$

(40)

The transition frequency $\omega_{p}^{\nu,\nu'}$ and the Rabi frequency with regard for the wave function [12, 23] are described as

$$\omega_{p}^{\nu,\nu'} = \frac{1}{\hbar} (\epsilon_{\nu} + \epsilon_{\nu'} + \epsilon_{h\nu}).$$

(41)
Figure 4. (Color online) The transverse effective masses for Al$_{0.3}$Ga$_{0.7}$N under biaxial strain: (a) for the heavy hole; (b) for the light hole.

\[
\Omega_{p}^{\nu_{h} \nu_{e}} = \frac{1}{\hbar} (\mu_{p}^{\nu_{h} \nu_{e}} e^{-i\omega t}) + \sum_{q} V_{p}^{\nu_{h} \nu_{e} \nu_{h} \nu_{e}} \left( \frac{|-p|}{|-p-q|} \right) \rho_{p+q}, \tag{42}
\]

where \( e_{e,p}^{\nu_{e}}, e_{h,p}^{\nu_{h}} \) - Hartree-Fock energies for electron and holes,

\[
\begin{align*}
V_{p}^{\nu_{h} \nu_{e} \nu_{h} \nu_{e}} &= \frac{1}{2} e^{2} \frac{1}{\kappa} \frac{2\pi}{\pi} \int d\varphi \sum_{\alpha} g_{\alpha} \int dq \\
&\times \int d\xi \int d\xi^{'} \chi_{n_{1}}(\xi) \chi_{m_{1}}(\xi^{'}) \chi_{m_{2}}(\xi^{'}) \chi_{n_{2}}(\xi^{'}) \\
&\times e^{-q|\xi-\xi^{'}|} C_{p}^{i} [n_{1}, 1] V_{p}^{j} [m_{1}, 1] C_{Q_{1}}^{i} [n_{2}, 1] V_{Q_{1}}^{j} [m_{2}, 1], \\
&n_{1} = m_{1} = n_{2} = m_{2} = 1, \\
Q_{1} &= q + p.
\end{align*}
\tag{43}
\]

where \( \chi_{n_{i}}(\xi) \) is the envelope of the wave functions of the quantum well, \( V_{p}^{j} [m_{1}, 1] \) and \( C_{Q_{1}}^{i} [n_{2}, 1] \) are coefficients of the expansion of the wave functions of a hole and electron at the envelope part, \( \varphi \) is the angle between the vectors \( p \) and \( q \), and \( g_{\alpha} \) is a degeneracy order of a level.

Numerically solving this integro-differential equation, we can obtain the absorption coefficient of a plane wave in the medium from the Maxwell equations:

\[
\alpha(\omega) = \frac{\omega}{\kappa n c E} \text{Im} P, \tag{44}
\]

where \( c \) the velocity of light in vacuum, \( n \) is a background refractive index of the quantum well material,

\[
P = \frac{2}{A} \sum_{\nu_{h} \nu_{e} p} (\mu_{p}^{\nu_{h} \nu_{e}}) p_{p}^{\nu_{h} \nu_{e}} e^{-i\omega t}. \tag{45}
\]

The light absorption spectrum presented in the paper in Fig. 7, reflects only the strict TE (x or y) light polarization.

From Uncertainty Heisenberg principle:

\[
\Delta x \Delta p \geq \frac{\hbar}{2}, \tag{46}
\]

can be found the localization range particle-hole pair \( \Delta x \geq \frac{\hbar}{4m c} \).

Hence the Bohr radius is greater than the localization range particle-hole pair, and the excitons may be spontaneously created.
Figure 5. (Color online) For the quantum well ZnO/Mg_{0.27}Zn_{0.73}O with a width 4 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300 K, at a transverse wave vector $k_t = 2 \times 10^7$ cm$^{-1}$: (a) Square of Hartree wave functions; (b) Square of Hartree-Fock wave functions.

Figure 6. (Color online) For the quantum well ZnO/Mg_{0.27}Zn_{0.73}O with a width 4 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300 K: (a) Hartree charge density; (b) Hartree-Fock charge density.
Table 1. The localization range particle-hole pair $\Delta x$ in cm, exciton binding energy $Ry$ in meV carriers concentration $n = p$ in cm$^{-2}$, Bohr radius $a_B$ in cm.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>$Ry$</th>
<th>$n = p$</th>
<th>$a_B$</th>
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<tr>
<td>$5.58 \times 10^{-11}$</td>
<td>38.53</td>
<td>$4 \times 10^{12}$</td>
<td>$2.39 \times 10^{-7}$</td>
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Figure 7. (Color online) Absorption coefficient for the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 4 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300 K.

2.4 Results and discussions

We consider QCSE in strained wurtzite ZnO/Mg$_{0.27}$Zn$_{0.73}$O quantum well with width 4 nm, in which the barrier height is a constant value for electrons and is equal to $U_0 = 536.22$ meV. The theoretical analysis of piezoelectric effects and exchange-correlation effects is based on the self-consistent solution of the Schrödinger equations for electrons and holes in quantum well of width $w$ with including Stark effect and the Poisson equations. The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density for electrons and holes along the polarization field distribution the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions in addition. All calculations are performed at a temperature of 300 K.

We have calculated carriers population of the lowest conduction band and the both heavy hole and light hole valence band. Solving (13) for holes in the infinitely deep quantum well and finding the minimum of functional (17) for electrons in a quantum well with barriers of finite height, we can find the energy and wave functions of electrons and holes with respect to Hartree potential and exchange-correlational potential in a piezoelectric field at a carriers concentration $n = p = 4 \times 10^{12}$ cm$^{-2}$. The screening field is determined by iterating Eqs. (13), (17), (22) until the solution of energy spectrum is converged.

The dispersion of the renormalization band gap is presented in Fig. 1. We have found $E^H - E^{\text{Flat band}} = 20.72$ meV, $E^{HF} - E^H = 4.40$ meV, comparing the Hartree band gap with the flat band gap as well as the Hartree band gap with the Hartree-Fock band gap. Comparing $E^{HF}$ and $E^H$ and a shape of bedplate of quantum well for electrons which is presented in Fig. 2 as well as a same shape of bedplate of quantum well for holes one can see that an electron mass is less than a hole mass. The effective masses Mg$_{0.27}$Zn$_{0.73}$O under biaxial strain for the heavy holes and light holes are presented in Fig. 3. Both the effective mass of Mg$_{0.27}$Zn$_{0.73}$O under biaxial strain for the heavy hole and the effective mass of Al$_{0.3}$Ga$_{0.7}$N under biaxial strain for the heavy hole are presented in Fig. 4. From these Figures one can see that a mass of heavy hole of Mg$_{0.27}$Zn$_{0.73}$O is greater than a mass of heavy hole of Al$_{0.3}$Ga$_{0.7}$N. Comparing the effective mass of Mg$_{0.27}$Zn$_{0.73}$O under biaxial strain for the heavy hole with an effective-mass parameter $A_1 = -2.743$ one can conclude that an effective mass of heavy hole of Mg$_{0.27}$Zn$_{0.73}$O under biaxial strain is greater than an effective-mass of heavy hole of ZnO.

The squares of Hartree and Hartree-Fock wave functions for electrons, heavy holes and light holes are presented...
in Fig. 5. From Fig. 5 one can conclude that an overlap integrals of the wave functions of holes and electron taking into the account besides the piezoelectric effects the exchange-correlation effects in addition are greater than an overlap integrals of Hartree ones. Hartree charge density distribution and Hartree-Fock charge density distribution are presented in Fig. 6. Comparing charge density distributions presented in Fig. 6 one can conclude that Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles.

It is found that the localization range particle-hole pair $\Delta x \geq \frac{\hbar}{4m_c} \sim 5.58 \times 10^{-11}$ cm. Exciton binding energy is equal $R_y=38.53$ meV at carriers concentration $n = p = 4 \times 10^{12}$ cm$^{-2}$. Bohr radius is equal $a_B = 2.39 \times 10^{-7}$ cm.

If the Bohr radius is greater than the localization range particle-hole pair, the excitons may be spontaneously created.

3 Appendix

<table>
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<tr>
<th>$c_{1\sigma}$</th>
<th>$E_1$</th>
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<th>$E_3$</th>
<th>$E_4$</th>
<th>$E_5$</th>
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<tr>
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<td>0</td>
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<td>-1</td>
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</tbody>
</table>

where $k_{\pm} = k_x \pm i k_y$, $k_{p}^2 = k_x^2 + k_y^2$, $J_{\pm} = \frac{1}{\sqrt{2}}(J_x \pm i J_y)$, $2[J_xJ_{\pm}] = J_xJ_x \pm J_{\pm}J_{\pm}$, $\sigma_{\pm} = \frac{1}{2}(\sigma_x \pm \sigma_y)$.

4 Conclusions

In this paper theoretical studies of the space separation of electron and hole wave functions in the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O by the self-consistent solution of the Schrödinger equations for electrons and holes and the Poisson-equations at the presence of spatially varying quantum well potential due to the piezoelectric effect and local exchange-correlation potential are presented. The exchange-correlation potential energy is found from the solution of three-dimensional Poisson’s equation, using both an expression by Gunnarsson and Lundquist [22], and following criterions.

The criterion $k_x > \sqrt{\pi}/4$ at carrier densities $4 \times 10^{12}$ cm$^{-2}$, at a temperature $T=0 \ K$ is carried as $1 > 0.1$. The criterion does not depend from a width of well. The solution of equations system (13), (17), (23) as well as (13), (17), (22) does not depend from a temperature. The ratio of Coulomb potential energy to the Fermi energy is $r_\ast = E_C/E_F = 0.63 < 1$. The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density for electrons and holes along the polarization field distribution the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions in addition. The problem consists of the one-dimensional Poisson’s equation solving of which may be found Hartree potential energy and three-dimensional Poisson’s equation which is separated on one-dimensional and two-dimensional equations by separated of variables. At the condition that the ratio of wave function localization in the longitudinal $z$ direction on transversal in-plane wave function localization is less 1. We have compared the Hartree band gap with the flat band gap as well as the Hartree band gap with the Hartree-Fock band gap and have found $E^H_s - E^{H\text{lat band}}_s = 20.72$ meV, $E^{H\text{lat band}} - E^{H\text{flat band}}_s = 4.40$ meV. An overlap integrals of the wave functions of holes and electron taking into account besides the piezoelectric effects the exchange-correlation effects in addition is greater than an overlap integral of Hartree ones. The Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles. It is found that an effective mass of heavy hole of Mg$_{0.27}$Zn$_{0.73}$O under biaxial strain is greater than an effective mass of heavy hole of ZnO. It is calculated that an electron mass is less than a hole mass. It is found that the Bohr radius is greater than the localization range particle-hole pair, hence the excitons may be spontaneously created.

References


