Features of luminescence in semiconductor quantum wires in external electric and magnetic fields

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The interband optical transitions in quantum wires in a model of a parabolic potential in an electric and magnetic field directed perpendicular to the nanowire axis are studied theoretically. The frequency dependences of the luminescence intensity of light are calculated when the interaction of carriers with a rough surface and with long-wave acoustic oscillations is taken into account. Graphs of the dependence of the luminescence half-width on the wire radius are obtained and a comparison with the experiment is made.
Key words: interband optical transitions, nanowires, luminescence, absorption, rough surface.

In nanosystems, due to the effect of size quantization, additional channels of spontaneous luminescence, absorption of electromagnetic waves, do not exist in bulk materials. Dimensionally bounded quantum systems (quantum wells, quantum wires, nanotubes) are of scientific interest, since only in them the scattering processes of carriers on a rough surface are clearly manifested [1], which (for example, in narrow QWs) can fully determine the optical properties [2], [3], transport phenomena in quantum systems. Interband luminescence was experimentally studied in quantum wells, InGaAs / AlGaAs [4], InGaAs / AlGaAs [5]. In recent years, the optical properties of semiconductor quantum wires of the type ZnO, GaN, CdS, InP, and GaAs in which scattering processes of carriers on a rough surface are very active have been intensively studied [6]. The optical properties of the QW Ge were investigated in [7] over a wide range of the radius of the nanowire ($R = 100\dot{A}, 250\dot{A}, 1100\dot{A}$). The attractiveness and relevance of research is due to the fact that in singularities of quantum systems at the bottom of each dimension-quantized conduction band (valence band), singularities arise in the density of electronic states. It is this circumstance it leads to specific features of the frequency dependences of luminescence and the absorption coefficient of an electromagnetic wave, as compared with two-dimensional systems. It is important to note that a noticeable effect of size quantization on the optical properties of quantum wires is possible at large radii of nanosystems ($R \geq 10^3\dot{A}$). [8]

The intensity of band-band luminescence in quantum wires (in the parabolic potential model) in transverse electric and uniform magnetic fields was investigated in this article. Note that the description of kinetic properties in the parabolic potential model is fully justified [9] and is now often used [11]. In the study of optical characteristics in condensed media, the balance equation method is used. The change in the energy U of the electromagnetic field per unit time in the lowest approximation in the electron-photon interaction is determined by the relation [12]:

$$\frac{dU}{dt} = \hbar\Omega\{(1+N)W_l - W_p\} \tag{1}$$

$\hbar\Omega$ is the photon energy, N is the number of photons per unit volume, and $N\hbar\Omega$ determines the energy of the electromagnetic field per unit volume.

According to (1), the increasing of the energy of the electromagnetic field (the first term) is naturally associated with luminescence processes, and the decrease (the second term) is determined by the absorption of light. The luminescence intensity is determined through the Fourier transform of the correlation function of the product of momentum operators [12]

$$W_l = \frac{2\pi e^2}{m_0^2 \hbar\Omega V}\int_{-\infty}^{\infty} dt\, e^{-i\Omega t}\langle(\hat{P}(t)\vec{e})(\hat{P}\vec{e})\rangle \tag{2}$$

$$\hat{P}(t) = e^{\frac{it\hat{H}}{\hbar}}\hat{P}e^{-\frac{it\hat{H}}{\hbar}}$$

Here: H is the Hamiltonian of the quantum system under investigation in the absence of an electromagnetic field of frequency Ω of polarization $\vec{e}$, m_0 is the mass of a free electron, and V is the volume of the quantum system under study. Since we further we consider the interaction of carriers with long-wave acoustic vibrations and take into account scattering of carriers on a rough surface of the nanostructure, then $\langle ... \rangle$ in (2) describes the averaging with an equilibrium density matrix.

In what follows we investigate the spontaneous emission of a weak electromagnetic wave associated with the quantum transitions of an electron from the conduction band to the valence band. In this case, the expression for the intensity (2) in the representation of the second quantization is determined by the relation:

$$W_l = \frac{4\pi e^2}{\hbar\Omega V}\left|\frac{\vec{P}_{cv}\vec{e}}{m_0}\right|^2 \sum_{\alpha\beta\alpha_1\beta_1} \langle\alpha|\beta\rangle\langle\beta_1|\alpha_1\rangle\, I_1 \qquad (3)$$

where

$$I_1 = \int_{-\infty}^{\infty} dt\, e^{-i\Omega t}\langle a_\alpha^{c+}(t) a_\beta^{v}(t) a_{\beta_1}^{v+} a_{\alpha_1}^{c}\rangle$$

Here the following notation is introduced: $a_\alpha^{i+}\left(a_\beta^{i+}\right)$ are the creation (annihilation) operators for electrons in the state α in the ith zone, $\vec{P}_{cv}$ is the matrix element of the momentum operator on the Bloch wave functions of the electron in the conduction band and in valence band, $\langle\alpha|\beta\rangle$a matrix element on the smoothed wave functions of the conduction band ($\langle\alpha|$) and the valence band ($|\beta\rangle$).

$$\hat{a}^i(t) = e^{\frac{it\hat{H}}{\hbar}}\hat{a}e^{-\frac{it\hat{H}}{\hbar}} \qquad (4)$$

If $\hat{V}$ is the interaction operator of an electron with acoustic phonons and (or) with a rough surface $\hat{H}_i = \hat{H}_i^0 + \hat{V}$, $\hat{H}_i^0|\alpha^i\rangle = E_i|\alpha^i\rangle$, then according to [13]

$$a_\alpha^{+c}(t) = \sum_{\alpha_2} a_{\alpha_2}^{+}\langle\alpha_2\left|e^{i\frac{t}{\hbar}\hat{H}c}\right|\alpha\rangle,$$
$$a_\beta^{v} = \sum_{\beta_2}\langle\beta\left|e^{-i\frac{t}{\hbar}\hat{H}_V}\right|\beta_2\rangle a_{\beta_2}^{v} \qquad (5)$$

Taking into account (5), relation (3) can be written in the following form:

$$W_l = \frac{4\pi e^2}{\hbar\Omega V}\left|\frac{\vec{P}_{cv}\vec{e}}{m_0}\right|^2 \sum_{\alpha\beta\alpha_1\beta_1}\langle\alpha|\beta\rangle\langle\beta_1|\alpha_1\rangle\, I_l(\Delta) \qquad (6)$$

$$I_2 = \int_{-\infty}^{\infty} dt\, e^{-i\Omega t} n_{\alpha_1}^{(c)}\left(1 - n_{\beta_1}^{(v)}\right)\left\{\left\langle\alpha_1\left|e^{\frac{it\widehat{H^c}}{\hbar}}\right|\alpha\right\rangle\left\langle\beta\left|e^{-\frac{it\widehat{H^v}}{\hbar}}\right|\beta_1\right\rangle\right\}$$

$n_\alpha^c\left(n_\beta^v\right)$ — the equilibrium distribution functions of electrons (holes) in the dimension-quantized conduction band (in the valence band) of the nanosystem under study, $\{\ldots\}$ — describes the averaging over the free-field system and (or) averaging over the realization of the random process [14].

Further calculations are carried out using the relaxation time approximation [13], when

$$\left\langle\alpha_1\left|e^{\frac{it\hat{H}^c}{\hbar}}\right|\alpha\right\rangle = \delta_{\alpha_1\alpha}e^{\frac{it\varepsilon_\alpha^c}{\hbar}}e^{-\Gamma_\alpha^c|t|}$$
$$\left\langle\beta\left|e^{\frac{it\hat{H}^v}{\hbar}}\right|\beta_1\right\rangle = \delta_{\beta\beta_1}e^{-\frac{it\varepsilon_\beta^v}{\hbar}}e^{-\Gamma_\alpha^v|t|} \qquad (7)$$

$\varepsilon_\alpha^c(\varepsilon_\beta^c)$- the electron energy in the conduction band (in the valence band) in the stateα; $2\Gamma_\alpha^c(2\Gamma_\beta^v)$ determines the quantum-mechanical probability of scattering of carriers in the c-band (in the v-band) or on long-wave acoustic vibrations [3] or on a rough surface [2]. In the approximations considered above, the intensity of spontaneous luminescence (6) takes the final form:

$$W_l = \frac{4\pi e^2}{\hbar\Omega V}\left|\frac{\vec{P}_{cv}\vec{e}}{m_0}\right|^2 \sum_{\alpha\beta}|\langle\alpha|\beta\rangle|^2 \int_{-\infty}^{\infty} dt\, e^{-i\Omega t} n_\alpha^c I_3$$
$$I_3 = \left(1 - n_\beta^v\right)\frac{2\left(\Gamma_\alpha^c + \Gamma_\beta^c\right)}{\left(\Gamma_\alpha^c + \Gamma_\beta^c\right)^2 + \frac{1}{\hbar^2}\left(\varepsilon_\alpha^c - \varepsilon_\beta^v - \hbar\Omega\right)^2} \qquad (8)$$

As an example, we investigate spontaneous band-band luminescence in semiconductor quantum wires (in the parabolic potential model) in the presence of transverse electric $\vec{E}$ and homogeneous magnetic $\vec{H}$ fields. In the case under consideration, the Hamiltonian for an electron in the conduction band of mass m_e in the Landau gauge $\vec{A}(-Hy, 0{,}0)$can be written as:

$$\hat{H}_e^0 = \frac{1}{2m_e}\left\{\left[\hat{p}_x - \frac{eHy}{c}\right]^2 + \hat{p}_y^2 + \hat{p}_z^2\right\} + \frac{m_e\omega_e^2(y^2 + z^2)}{2} + eEz \qquad (9)$$

Here $\hbar\omega_e$ is the energy of size quantization, which is simply related to the potential energy ΔE_c at the boundary of a quantum wire of radius : $\omega_e = \frac{1}{R}\left[\frac{2\Delta E_c}{m_e}\right]^{1/2}$. In the case under consideration, $\vec{H}$ is directed perpendicular to the nanowire axis $\left(\vec{H} \parallel Oz, \vec{H} \parallel \vec{E}\right)$.

In what follows, for simplicity, we consider the scattering of an electron on a rough surface [14] and the interaction of electrons with long-wave acoustic vibrations [13]. In this case

$$\Gamma_\alpha^c = \frac{1}{|k_x|}\gamma \qquad (13)$$

Here we introduce the following notation: E_1 – is the deformation potential constant for an electron, v is the speed of sound in a nanostructure with density ρ, ${\gamma_0}^{1/3}$ which determines the fluctuation height.

где $\gamma = \gamma_1(1+\delta^2)^{\frac{5}{4}} + \gamma_2(1+\delta^2)\left[\frac{1}{2}\left(1 + \frac{1}{\sqrt{1+\delta^2}}\right) + \gamma_3\right]$

$$\gamma_1 = \frac{E_1^2 k_0 T m_e^2 \omega_e}{2\pi\hbar^4 \rho v^2}, \gamma_2 = \frac{2 m_e \gamma_0 \omega_e^2}{\hbar R^2},$$
$$\gamma_3 = \frac{2\Delta}{\hbar\omega_e}, \delta = \frac{\hbar\omega_c}{\hbar\omega_e}$$

As follows directly from (13), the interaction of an electron with a rough surface (the second term in Eq. (13)) depends essentially on the radius of the quantum wire $\left(\propto \frac{1}{R^4}\right)$, and, therefore, it must be taken into account when studying kinetic phenomena in nanowires with For typical semiconductor GaAs (($m_e = 0.06 m_0, m_v = 0.4 m_0, E_1 = 10\ eV,\ \Delta E_c = 0.255$ эВ, $\rho = 5.4\ ^{g}/_{cm^3}, v = 3 \cdot 10^5\ ^{cm}/_{s}$) for ${\gamma_0}^{1/3} = 20$ Å (for such values of γ_0 the mobility reaches large experimental values $\left(\mu \sim 3 \cdot 10^4\ ^{cm^2}/_{V \cdot s}\right)$. the scattering of electrons by the rough surface can be neglected if $R > 5 \cdot 10^2$Å. In this case $\gamma \sim \frac{1}{R}$, that means that it depends much less on the size of the nanostructure. From the explicit form of γ, it follows that with increasing magnetic field strength γ increases In the transverse electric field, the electrons "cling" to the surface of the quantum wire, which leads to a noticeable increase in the scattering of particles on a rough surface (the growth of the second term in Eq. (13) as E increases).

$$W_l = W_0 \sum_{\alpha\beta} |\langle 0_c | 0_v \rangle|^2 \frac{n_e n_v}{k_0 T} \left(\frac{2\hbar}{\omega_f (m_e^* + m_v^*)} \right)^{\frac{1}{2}} I_l(\Delta) \quad (14)$$

where

$$I_l(\Delta) = \int_{-\infty}^{\infty} dx\, e^{-\beta\hbar\omega_f x} \frac{1}{1 + x\left[\frac{\Delta}{\hbar\omega_f} + x\right]^2}$$

$$W_0 = \frac{2\pi e^2}{\Omega S} \left| \frac{\vec{P}_{cv} \vec{e}}{m_0} \right|^2$$

$$\omega_f = \left[\frac{\hbar\gamma^2}{2\mu^*}\right]^{1/3}, \frac{1}{\mu^*} = \frac{1}{m_e^*} + \frac{1}{m_v^*}, \Delta = -\hbar\Omega + E_g^*, \beta = \frac{1}{k_0 T},$$

$$\Delta_{cv} = \frac{(eER)^2}{4}\left(\frac{1}{\Delta E_c} + \frac{1}{\Delta E_v}\right)$$

$$|\langle 0_c | 0_v \rangle|^2 = 4\left[\frac{R_e R_v R_e^0 R_v^0}{(R_e^2 + R_v^2)(R_e^{02} + R_v^{02})}\right] e^{-\frac{e^2 E^2 R^4}{(R_e^{02} + R_v^{02})}\left(\frac{1}{\Delta E_c} + \frac{1}{\Delta E_v}\right)^2}$$

$$R_e^2 = \frac{\hbar}{m_e \Omega_e}, \quad R_e^{02} = \frac{\hbar}{m_e \omega_e}$$
$$R_v^2 = \frac{\hbar}{m_v \Omega_v}, \quad R_v^{02} = \frac{\hbar}{m_v \omega_v}$$

$n_e(n_v) = \frac{N_e}{L_x}\left(\frac{N_v}{L_x}\right)$ – is the linear concentration of electrons (holes) in a quantum wire, $E_g^* = E_g + \frac{1}{2}(\hbar\omega_e + \hbar\Omega_e + \hbar\omega_v + \hbar\Omega_v) - \Delta_{cv}$, S the width of the forbidden band of the investigated nanostructure in external fields, S-section of the control gear.

Figure 1 shows the frequency dependence of the luminescence intensity (in relative units) ($E = 0, T = 40\ K$). Curves 1-5 were obtained for $\xi = 2, 3, 5, 7, 10$ respectively $\left(R = 10^2 \xi\ \text{Å}\right)$. As follows directly from Fig. 1, the half-width of the line of spontaneous luminescence with increasing radius of the nanowire decreases. The insertion in Fig. 1 shows the dependence of the half-width of the luminescence intensity line $I\ (\Delta)$ on the radius of the quantum wire. Therefore, for small radius of a quantum wire ($\xi < 4$), the half-width decreases sharply with increasing R. It is in such nanosystems that scattering of carriers on a rough surface is the dominant scattering mechanism and $\omega_f \sim R^{-\frac{8}{3}}$. For $R = 200\text{Å}, 500\text{Å}, 700\text{Å}$ the half-width of the emission line ΔI is equal to $\Delta I = 10.17\ \text{meV}, 2.4\ \text{meV}, 1.9\ \text{meV}$. As R grows, the effect of scattering of carriers on a rough surface by the luminescence intensity decreases, and the half-width of the emission line is determined by the interaction charged particles with long-wave acoustic vibrations $\left(\Delta I \propto R^{-2/3}\right)$ and, consequently, weakly depends on the size of the nanostructure under study. It is precisely this dynamics of the change in the half-width of the band-band luminescence line from R that was experimentally observed in the study of the magnetooptics of quantum wires [15]. As the radius of the QW decreases, the width of the forbidden band increases by $\frac{1}{2}(\hbar\omega_e + \hbar\omega_v)$what naturally leads to the fact that the maximum of the band-band luminescence shifts to the high-frequency region of the spectrum.

As the radius of the nanowire decreases, the energy of size quantization in the bands $\left(\hbar\omega_e, \hbar\omega_v \propto \frac{1}{R}\right)$, increases, which leads to a decrease in the number of size-quantized levels in the parabolic potential well $\Delta E_c (\Delta E_v)$. The latter circumstance may be the reason for the decrease in the number of peaks of the interband absorption of a weak electromagnetic wave. It was such a dynamics of the change in the spectrum of the interband absorption of light that was observed in Ge nanowires with a change in the radius of the quantum system from 10^2 to $1.1 \cdot 10^3\ \dot{A}$ [7].

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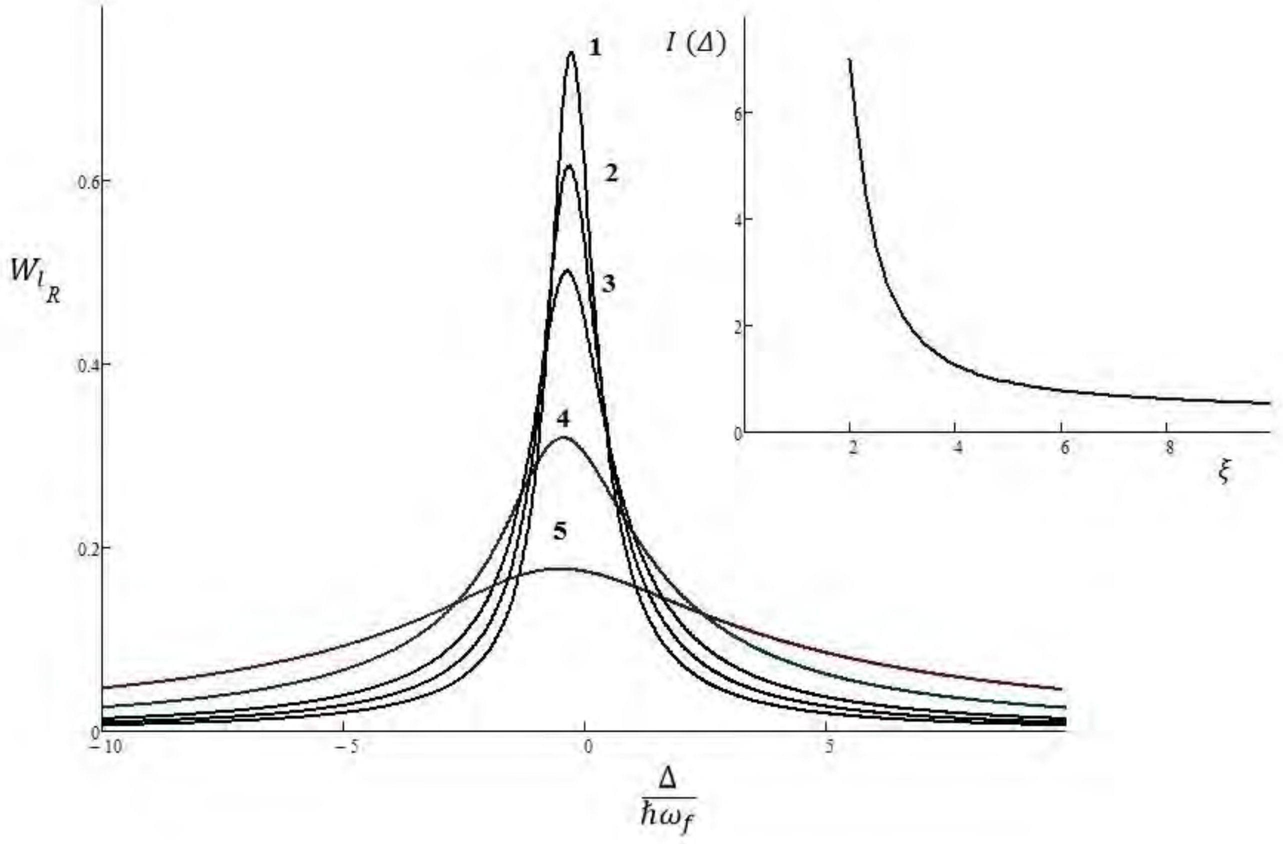

Fig.1 Frequency dependence of luminescence intensity (in relative units) ($E = 0, T = 40\ K$)