Effect of Coulomb interaction with barrier carriers in the waveguide region on multiple quantum well laser inversion threshold

A A Karpova¹, G G Zegrya²

¹ ITMO University, Saint-Petersburg 197101, Russia
² Ioffe Institute, Saint-Petersburg 194021, Russia

va7059va@yandex.ru

Abstract. A mechanism of nonradiative recombination of nonequilibrium carriers in semiconductor quantum wells is suggested and discussed. For a studied Auger recombination process the energy of localized electron-hole pair is transferred to barrier carriers due to Coulomb interaction. It is shown that the Auger coefficient is a weak function of temperature and nonmonotonically depends on the quantum well width.

1. Introduction

Nowadays fiber-optic communication lines are considered to be the most promising environment for transferring large amounts of information over significant distances. The lasing wavelength of InGaAsP/InP multiple quantum well lasers is 1.3 – 1.55 micrometers and coincides with the second, the third and the fifth transparency windows of optical fiber, what makes them to be an actual research field of semiconductor optoelectronics.

To enhance the efficiency of device, it is important to understand the processes which might govern light emission. It is known, that the lifetime of electron confined in a quantum well depends on three processes such as radiative recombination, nonradiative Auger recombination of confined electrons and holes and nonradiative recombination of confined carriers interacting with electrons in the waveguide region. Thus, the last process should be considered as well if the threshold characteristics of lasers are analyzed.

2. Basic equations. Wave functions of carriers in quantum well and under the barrier

The analysis of present Auger recombination process starts with determining of carrier wave functions in quantum well and in waveguide region. For this purpose the four-band Kane model is used. The carrier wave function has following representation:

\[ \psi = \Psi_s |s\rangle + \Psi_p |p\rangle, \]  

where \( \Psi_s \) and \( \Psi_p \) are spinors, \( |s\rangle \) and \( |p\rangle \) are s- and p-type Bloch wave functions.

Near the \( \Gamma \) point the equations of the envelope functions \( \Psi_s \) and \( \Psi_p \) in spherical approximation can be represented in the form:
Here is Kane matrix element, $\tilde{\gamma}_1$, $\tilde{\gamma}_2 = \tilde{\gamma}_3$ – generalized Luttinger parameters, $\delta = \Delta_{so}/3$, $\Delta_{so}$ – spin-orbit splitting constant, $E_c$ and $E_v$ are the energies of the lower edge of the conduction band and the upper edges of valence band, $m$ is the mass of a free electron, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ – Pauli matrices.

The Fourier transformation of equation (2) makes it possible to obtain the energy spectra for electrons and holes. The spectrum for electrons has the form:

$$k^2 = \frac{\varepsilon}{\hbar^2 \gamma^2} \left( \varepsilon^2 + \varepsilon (2E_g + \Delta \delta) + (E_g + \Delta \delta)E_g \right).$$

The spectra for heavy, light and spin-split-off holes are given by equations (4) and (5) respectively:

$$E_{h} = \delta - \frac{\hbar^2 k^2}{2m},$$

$$E_{l,so} = -\frac{\delta}{2} - \frac{\hbar^2 k^2}{4} \left( m_{-1}^{-1} + m_{-1}^{-1} \right) + \left( 2\delta^2 + \left( \frac{\delta}{2} - \frac{\hbar^2 k^2}{4} \left( m_{-1}^{-1} - m_{-1}^{-1} \right) \right) \right)^{1/2}. \tag{5}$$

In equations (3) – (5) $k$ is quasimomentum of the carriers.

In the present work the energy of $\delta$ is set as a zero reference level for holes, electron energy $E$ is calculated from the lower edge of conduction band.

Let us consider a rectangular quantum well with width $a$, for which the coordinate $x$ is measured from its symmetry plane.

Wave functions of electrons in quantum well might be presented in the form:

$$\Psi_{sc} = A_1 \cos k_c x \eta + A_2 \sin k_c x \xi,$$

$$\Psi_{c} = i \hbar y \frac{1}{A_1} \left( k_c \sin k_c x \eta - \lambda_c \cos k_c x \xi \right) + i \hbar y \frac{1}{A_2} \left( -k_c \cos k_c x \eta - \lambda_c \sin k_c x \xi \right), \tag{6}$$

where $\eta = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ 1 \end{array} \right)$ and $\xi = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ -1 \end{array} \right)$.

Wave functions of electron under the potential barrier have the form:

$$\Psi_{sc}^{(1)} = \left[ \tilde{A}_1 \eta + \tilde{A}_2 \xi \right] \exp \left( -k_c \left( x - \frac{a}{2} \right) \right),$$

$$\Psi_{c}^{(1)} = \left[ i \hbar y \frac{1}{\tilde{A}_1} \left( \frac{\kappa_c \eta - \tilde{\lambda}_c q \xi}{i \eta} \right) + i \hbar y \frac{1}{\tilde{A}_2} \left( \frac{\kappa_c \xi - \tilde{\lambda}_c q \eta}{i \xi} \right) \right] \exp \left( -k_c \left( x - \frac{a}{2} \right) \right). \tag{7}$$

Wave functions of heavy holes in quantum well and under the potential barrier are given by equations (8) and (9) respectively:

$$\Psi_{h}(q, x) = H_1 \left( \begin{array}{c} q \cos k_h x \xi \\ -i k_h \sin k_h x \xi \end{array} \right) + H_2 \left( \begin{array}{c} q \sin k_h x \eta \\ i k_h \cos k_h x \eta \end{array} \right), \tag{8}$$

$$\Psi_{h} = H_1 \left( \begin{array}{c} q \xi \\ -i k_h \xi + q \eta \end{array} \right) \exp \left( -k_h \left( x - \frac{a}{2} \right) \right) + H_2 \left( \begin{array}{c} q \eta \\ -i k_h \eta + q \xi \end{array} \right) \exp \left( -k_h \left( x - \frac{a}{2} \right) \right). \tag{9}$$

Wave functions of light holes in quantum well and under the potential barrier have the form:

$$\Psi_{l}(q, x) = L_1 \left( \begin{array}{c} q k_l \sin k_l x \xi \\ -i q \cos k_l x \eta \end{array} \right) + L_2 \left( \begin{array}{c} q \sin k_l x \eta \\ -i k_l \cos k_l x \xi \end{array} \right), \tag{10}$$

$$\Psi_{l} = i \hbar y \left( k_l^2 + q^2 \right) \left[ L_1 \cos k_l x \eta + L_2 \sin k_l x \xi \right],$$
\[ \Psi_l = \left[ \mathcal{L}_1 \left( \frac{\kappa_i \eta - \tilde{\lambda}_i q_{\xi}}{-i q_{\xi} + i \tilde{\lambda}_i \kappa_i} \right) + \mathcal{L}_2 \left( \frac{-i \tilde{\lambda}_i \kappa_i \eta + i q_{\xi}}{-\tilde{\lambda}_i q_{\xi} + \tilde{\lambda}_i \kappa_i} \right) \right] \exp \left( -\frac{\kappa_i (x - a)}{2} \right), \]

\[ \Psi_{sl} = \left( \frac{i \hbar y (-\kappa_i^2 + q_{\xi}^2)}{E_g + \delta + U_c e^{-E_g}} \right) \left( \mathcal{L}_1 \eta + \mathcal{L}_2 \xi \right) \exp \left( -\kappa_i (x - a) \right). \]

In equations (6) – (11) \( k_i \) – \( x \)-component of carrier quasimomentum in quantum well, \( \kappa_i \) – magnitude of \( x \)-component of carrier quasimomentum under the barrier, \( i = c, h \),

\[ Z = \frac{\varepsilon \varepsilon + E_g + 2 \delta}{E_g + \varepsilon + 2 \delta} \]

\[ Z = \frac{\varepsilon \varepsilon + 2 \delta}{E_g + \varepsilon + 2 \delta} \]

\[ \lambda_c = \frac{\varepsilon \varepsilon + \varepsilon + 2 \delta}{\varepsilon + \varepsilon + 2 \delta} \]

\[ \tilde{\lambda}_c = \frac{\varepsilon \varepsilon + \varepsilon + 2 \delta}{\varepsilon + \varepsilon + 2 \delta} \]

\[ \tilde{\lambda}_l = \frac{\varepsilon \varepsilon + \varepsilon + 2 \delta}{\varepsilon + \varepsilon + 2 \delta} \]

\[ \lambda = \frac{\varepsilon \varepsilon + \varepsilon + 2 \delta}{\varepsilon + \varepsilon + 2 \delta}. \]

Boundary conditions for wave-function envelopes could be obtained with the use of probability flux conservation law and Kane equations, which might be integrated through interface:

\[ \left\{ \begin{array}{l}
 (E_g + \delta - E) \psi' - i \hbar y \nabla \psi' = 0, \\
 -E \psi' - i \hbar y \nabla \psi' + \frac{\hbar^2}{2m} \left[ \frac{\partial}{\partial y_1} + \frac{\hbar^2}{2m_1 \delta x_k} \left( \psi' \right) \right] + i \partial [\sigma \psi'] = 0.
\end{array} \right. \]

It is convenient to calculate energy of electrons in waveguide region from the lower edge of conduction band of wide-band material. The system of Kane equations for barrier electrons without taking into account spin-orbit interaction has the form:

\[ \left\{ \begin{array}{l}
 -E \psi' - i \hbar y \nabla \psi' = 0, \\
 (E - E_{gb}) \psi' - i \hbar y \nabla \psi' = 0,
\end{array} \right. \]

Wave functions of electrons in waveguide region are given in following form:

\[ \psi' = A e^{i k x} e^{i q y}, \]

\[ \psi' = A \left( \frac{i q}{E - E_{gb}} \right) e^{i q y} \psi'. \]

In equations (20) and (21) \( A = \frac{1}{\sqrt{V}} \) \( V \) is an arbitrary volume.

3. Auger recombination rate and coefficient

The probability of Auger recombination per unit time is calculated within first-order perturbation theory with respect to the electron-electron interaction:

\[ W_{l \rightarrow f} \left( \frac{2 \pi}{h} \right) M_{lf}^{2} \delta (E_f - E_l), \]

\[ M_{lf} = M_l - M_f. \]

To carry out a rate and coefficient estimation for the present Auger recombination process, it might be assumed, that \( M_l \gg M_{lf} \).

The matrix element of the electron-electron Coulomb interaction has the following form with use of Fourier representation:

\[ M_{l} = \frac{4 \pi e^2}{k_0} \int \frac{L_{a}(p) L_{a}(-p) \frac{dp}{p^2 + q^2}}{q_1 + q_2 - q_3 - q_4}, \]

\[ I_{ij}(p) = \int \psi_i^*(x) \psi_j(x) e^{ipx} dx, \]

\[ \delta_q = \left\{ \begin{array}{ll}
 1, & q = 0, \\
 0, & q \neq 0.
\end{array} \right. \]
In equations (24) – (26) $q$ is the momentum transferred in the plane of the quantum well during the Coulomb interaction.

For Auger recombination process with barrier electrons participation a more detailed matrix element has the form:

$$M_i = rac{4\pi e^2}{\kappa_0(q + (k_4 - k_1))} \int_{-a/2}^{a/2} \Psi_i^*(x)\Psi_2(x)A_1A_4e^{i(k_4 - k_1)}dx \delta(q_1 + q_2 - q_3 - q_4). \quad (27)$$

The Auger recombination rate has the following representation:

$$G = \frac{2\pi}{h} \sum_{k_1,k_2,k_3,k_4} \langle M^2 \rangle f_1f_2(1 - f_3)(1 - f_4)\delta(E_3 + E_4 - E_1 - E_2). \quad (28)$$

where $\langle M^2 \rangle$ – matrix element summed over the spin variables, $f_1$ и $f_2$ – Fermi distribution functions of the carriers in the initial state, $f_3$ и $f_4$ – Fermi distribution functions of the carriers in the final state.

Auger recombination coefficient $C$ is related to Auger recombination rate by the expression:

$$G = C n_b n_{QW}^2 P_{QW}^2. \quad (29)$$

$$n_{QW}^2 = \frac{m_c}{\pi h^2} e_n^\infty \left( \exp\left(\frac{E - \mu_n}{T}\right) + 1 \right)^{-1} dE, \quad (30)$$

$$P_{QW}^2 = \frac{m_h}{\pi h^2} e_p^\infty \left( \exp\left(\frac{E - \mu_p}{T}\right) + 1 \right)^{-1} dE. \quad (31)$$

$$n_{bp}^{2D} = \sqrt{\frac{4}{3\pi} N_c \tau_{bf}^{2D}(T) \left( \frac{T}{E_g} \right)^{3/4} \times \left( \int_0^\infty \frac{e^{3/2}d\varepsilon}{1 + \exp(\varepsilon + \xi_n - \eta_n)} - \int_0^\infty \frac{e^{3/2}d\varepsilon}{1 + \exp(\varepsilon + \xi_n + \phi_n - \eta_n)} \right)^{1/2} \quad (32)$$

where $\mu_n$ и $\mu_p$ are the quasi-Fermi levels for the electrons and holes, $N_c \tau_{bf}^{2D} = \frac{m_c^* e}{\pi h^2}$, $\phi_n$ is the electron potential energy at the half-distance between the neighboring quantum wells.

4. Results and discussion

The calculations of the studied Auger recombination rate and coefficient are carried out for a model structure In$_{0.53}$Ga$_{0.47}$As/InP. The following values of the structure are used in calculations: $E_g = 0.74\ eV$, $U_c = 0.22\ eV$, $U_p = 0.38\ eV$, $\Delta_{so} = 0.35\ eV$, $\kappa_0 = 13.94$, $m_c = 0.041m_0$, $m_{hh} = 0.45m_0$, $m_{lh} = 0.052m_0$.

Figure 1 presents the dependence of the Auger recombination rate $G$ on the quantum well width at temperature $T = 300\ K$.

It can be seen from figure 1, that Auger recombination rate soars at quantum well width approximately equal to 30 Å.

Figure 2 shows the dependence of the Auger recombination coefficient $C$ on the quantum well width at temperature $T = 300\ K$. 

---

4

Figure 1 – Dependence of the Auger recombination rate $G$ on the quantum well width $a$ at 300 K.

Figure 2 – Dependence of the Auger recombination coefficient $C$ on the quantum well width at temperature $T = 300$ K.
In figure 2 one can observe a conspicuous maximum at quantum well width approximately equal to 30 Å. It is the dependence of electron and hole wave functions overlap integral on quantum well width what makes the coefficient of Auger recombination process to be a non-monotonic function of quantum well width. For narrow quantum wells overlap integral is small owing to the long electron wave function tails in barrier region. After reaching the maximum value the overlap integral decreases owing to delocalization of electron and hole wave functions.

It can be seen from figure 2, that the Auger coefficient has an order of magnitude $10^{-14}$. It makes the inverse time of the present Auger process to have an order of magnitude $10^{10}$ with two-dimensional densities of confined holes and barrier electrons proportional to $10^{24}$:

$$\frac{1}{\tau_A} = \frac{G}{n_{QW}^2} = \frac{C_P^2n_b^2}{n_{QW}^2} \sim 10^{-14} \times 2 \times 10^{12} \times 10^{12} = 2 \times 10^{10},$$

$$\tau_A \sim \frac{1}{2 \times 10^{10}} = 5 \times 10^{-11} \text{ sec.}$$

This estimation means that the present Auger recombination process strongly affects the lifetime of nonequilibrium carriers in quantum wells and threshold current density. That process might compete with already known nonradiative Auger recombination processes in quantum wells.

Figure 3 represents the temperature dependence of the Auger process coefficient.

As it can be seen from figure 3, the Auger recombination coefficient changes negligibly with increasing temperature.
5. Conclusion
A new nonradiative Auger recombination process has been studied for quantum wells. The dependences of Auger recombination coefficient and rate on quantum well width at 300 K have been obtained. Also the temperature dependence of Auger recombination coefficient has been considered. It is shown that this process important for proper analyze of the multiple quantum well laser threshold characteristics.

References
[1] Zegrya G G, Polkovnikov A S 1998 JETP 86 815
[2] Polkovnikov A S, Zegrya G G 1998 Phys. Rev. B 58 4039
[3] Asryan L V, Gun'ko N A, Polkovnikov A S, Zegrya G G, Suris R A, Lau P K, Makino T 2000 Semicond. Sci. Tech. 15 1131