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To cite this article: Z N Sokolova et al 2016 J. Phys.: Conf. Ser. 740 012002

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Theory of operating characteristics of a semiconductor quantum well laser: Inclusion of global electroneutrality in the structure

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Abstract
A model for calculating the operating characteristics of semiconductor quantum well (QW) lasers is presented. The model exploits the condition of global electroneutrality, which includes the charge carriers both in the two-dimensional (2D) active region (QW) and bulk waveguide region (optical confinement layer – OCL). The charge of each sign in the OCL is shown to be significantly larger than that in the QW. As a result of this, (i) the global electroneutrality condition reduces to the condition of electroneutrality in the OCL and (ii) the local electroneutrality in the QW can be strongly violated, i.e., the 2D electron and hole densities in the QW can significantly differ from each other.

1. Introduction
The stimulated emission in contemporary semiconductor lasers is generated in a low-dimensional active region, which is surrounded by a wider band gap bulk waveguide region (optical confinement layer – OCL) [1, 2]. In such structures, electrons and holes are first injected from the cladding layers into the OCL and then captured into the active region [3] (figure 1).

In [4], the operating characteristics of semiconductor QW lasers were calculated with a proper account for noninstantaneous capture of charge carriers. In calculations, we assumed the local electroneutrality in QWs, i.e., equality of the 2D electron and hole densities in QWs to each other.

In this work, the operating characteristics of a semiconductor QW laser are calculated exploiting the condition of global electroneutrality, which includes the charge carriers both in the active region (QWs) and OCL. This condition thus presents the equality of the total charge of electrons to that of holes – see equation (10) below. The charge of each sign in the OCL is shown to be significantly larger than that in the QW. As a result of this, (i) the global electroneutrality condition reduces to the condition of electroneutrality in the OCL and (ii) the local electroneutrality in the QW can be strongly violated, i.e., the 2D electron and hole densities in the QW can significantly differ from each other.
Figure 1. A schematic of a semiconductor laser with a quantum-confined active region.

2. Theoretical model
To calculate the laser characteristics, the following set of steady-state rate equations is used [4]:

For free electrons in the bulk OCL \( \frac{b(\partial n^{\text{OCL}}/\partial t)}{e} = 0 \),

\[
\frac{j}{e} + N_{\text{QW}} \frac{n^{\text{QW}}}{\tau_{n,\text{esc}}} - N_{\text{QW}} v_{\text{n,capt,0}} (1 - f_n) n^{\text{OCL}} - b B_{2D} n^{\text{OCL}} p^{\text{OCL}} = 0
\] (1)

For free holes in the OCL \( \frac{b(\partial p^{\text{OCL}}/\partial t)}{e} = 0 \),

\[
\frac{j}{e} + N_{\text{QW}} \frac{p^{\text{QW}}}{\tau_{p,\text{esc}}} - N_{\text{QW}} v_{\text{p,capt,0}} (1 - f_p) p^{\text{OCL}} - b B_{2D} n^{\text{OCL}} p^{\text{OCL}} = 0
\] (2)

For electrons confined in the QW \( \frac{\partial n^{\text{QW}}}{\partial t} = 0 \),

\[
v_{\text{n,capt,0}} (1 - f_n) n^{\text{OCL}} - \frac{n^{\text{QW}}}{\tau_{n,\text{esc}}} - B_{2D} n^{\text{QW}} p^{\text{QW}} - v_g g^{\text{max}} (f_n + f_p - 1) \frac{N}{S} = 0
\] (3)

For holes confined in the QW \( \frac{\partial p^{\text{QW}}}{\partial t} = 0 \),

\[
v_{\text{p,capt,0}} (1 - f_p) p^{\text{OCL}} - \frac{p^{\text{QW}}}{\tau_{p,\text{esc}}} - B_{2D} n^{\text{QW}} p^{\text{QW}} - v_g g^{\text{max}} (f_n + f_p - 1) \frac{N}{S} = 0
\] (4)

And for photons in the lasing mode \( \frac{\partial N}{\partial t} = 0 \),

\[
v_g N_{\text{QW}} g^{\text{max}} (f_n + f_p - 1) N - v_g (\beta + \alpha_{\text{int}}) N = 0
\] (5)

The following quantities are the unknowns in equations (1)-(5): \( n^{\text{OCL}} \) and \( p^{\text{OCL}} \) are the free electron and hole densities in the OCL, \( n^{\text{QW}} \) and \( p^{\text{QW}} \) are the 2D densities of electrons and holes confined in each of the QWs, \( N \) is the number of photons in the stimulated emission, \( f_n \) \( (f_p) \) is the occupancy of the lower (upper) edge of the electron (hole) quantum-confinement subband in the QW. The occupancies \( f_n \) and \( f_p \) are expressed in terms of the 2D electron and hole densities \( n^{\text{QW}} \) and \( p^{\text{QW}} \) as follows [7, 8]:
\[ f_n = 1 - \exp \left\{ -\frac{n_{n,\text{QW}}}{N_{c,\text{QW}}} \right\}, \quad f_p = 1 - \exp \left\{ -\frac{p_{p,\text{QW}}}{N_{v,\text{QW}}} \right\} \]  
(6)

where \( N_{c,v,\text{QW}} = \frac{m_{c,hh,\text{QW}}}{h^2} \) are the 2D effective densities of states in the conduction and valence bands in the QW, \( m_{c,hh,\text{QW}} \) are the electron and hole effective masses in the QW, and the temperature \( T \) is measured in units of energy.

The following parameters enter into equations (1)-(5): \( j \) is the injection current density, \( e \) is the electron charge, \( N_{\text{QW}} \) is the number of identical (of the same material composition and width) QWs, \( \tau_{\text{n,esc}} \) and \( \tau_{\text{p,esc}} \) are the thermal escape times of electrons and holes from a QW to the OCL, \( v_{n,\text{capt},0} \) and \( v_{p,\text{capt},0} \) are the capture velocities of electrons and holes into an empty (at \( f_n = 0 \) and \( f_p = 0 \) ) QW measured in units of cm/s, \( b \) is the thickness of the OCL, \( B_{3D} \) and \( B_{2D} \) are the spontaneous radiative recombination coefficients for the bulk (OCL) and 2D (QW) regions measured in units of cm\(^3\)/s and cm\(^2\)/s, respectively – see [5] and [6] for the expressions for \( B_{3D} \) and \( B_{2D} \); \( v_g \) is the group velocity of light, \( g_{\text{max}} \) is the maximum gain in each QW, \( S = WL \) is the cross-section of the junction, \( W \) is the lateral size of the device, \( L \) is the Fabry-Pérot cavity length, \( \beta = (1/L)\ln(1/R) \) is the mirror loss, \( R \) is the facet reflectivity, and \( \alpha_{\text{int}} \) is the coefficient of internal optical loss in the structure.

The thermal escape times of electrons and holes from the QW into the OCL are [4, 9]:

\[ \tau_{\text{n,esc}} = \frac{1}{v_{n,\text{capt},0}(1-f_n)} N_{c,\text{QW}}^{2D}, \quad \tau_{\text{p,esc}} = \frac{1}{v_{p,\text{capt},0}(1-f_p)} N_{v,\text{QW}}^{2D} \]  
(7)

Where

\[ n_1 = N_{c}^{3D} \exp \left\{ -\frac{\Delta E_c - \varepsilon_{n,\text{QW}}}{T} \right\}, \quad p_1 = N_{v}^{3D} \exp \left\{ -\frac{\Delta E_v - \varepsilon_{p,\text{QW}}}{T} \right\} \]  
(8)

and \( N_{c,v}^{3D} = 2 \frac{m_{c,v}^{\text{OCL}}}{h^2} \) are the 3D effective densities of states in the conduction and valence bands in the OCL, \( m_{c,v}^{\text{QW}} \) are the electron and hole effective masses in the OCL, \( \Delta E_{c,v} \) are the conduction and valence band offsets at the heterointerface of the QW and OCL, and \( \varepsilon_{n,\text{QW}} \) (\( \varepsilon_{p,\text{QW}} \)) is the energy of the lower (upper) edge of the electron (hole) subband in the QW.

The velocities \( v_{n,\text{capt},0} \) and \( v_{p,\text{capt},0} \) of electron and hole capture from the OCL into an empty QW are the characteristics of the QW; they thus depend on the QW width and depth, i.e., on the material compositions of the QW and surrounding layers. The capture velocity can be significantly different in different laser structures. In [10], we determined the value of the electron capture velocity in the laser structure similar to the one used here as an example for our calculations (see below).

The total capture velocities \( v_{n,\text{capt}} \) and \( v_{p,\text{capt}} \) are defined as [4]

\[ v_{n,\text{capt}} = v_{n,\text{capt},0}(1-f_n), \quad v_{p,\text{capt}} = v_{p,\text{capt},0}(1-f_p). \]  
(9)

The condition of global electroneutrality for the OCL and QW is written as follows:

\[ e \left( N_{QW} n_{n,\text{QW}}^0 + bn_{\text{OCL}} \right) = e \left( N_{QW} p_{p,\text{QW}}^0 + bp_{\text{OCL}} \right) \]  
(10)

The set of equations (1)-(5), added by equation (10), was solved numerically for an InGaAs/GaAs/AlGaAs laser structure containing a single strained In\(_{0.28}\)Ga\(_{0.72}\)As QW of 80 Å width. The
material of the OCL of thickness \( b = 1.7 \, \mu m \) was GaAs, the material of the cladding layers was \( \text{Al}_{0.3}\text{Ga}_{0.7}\text{As} \). The lasing wavelength was 1.044 \( \mu m \). The Fabry-Pérot cavity length \( L = 1.5 \, \text{mm} \), the stripe width \( W = 100 \, \mu m \), the mirror reflectivity \( R = 0.32 \), the mirror loss \( \beta = 7.6 \, \text{cm}^{-1} \), the temperature \( T = 300 \, \text{K} \), the coefficient of internal optical loss \( \alpha_{\text{int}} = 1 \, \text{cm}^{-1} \) (in this work, \( \alpha_{\text{int}} \) is assumed to be independent of the injection current). The maximum modal gain in the QW \( g_{\text{max}} = 49.1 \, \text{cm}^{-1} \). The following values were used for the electron and hole capture velocities \[ v_{n,\text{capt},0} = 4 \times 10^5 \, \text{cm/s} \text{ and } v_{p,\text{capt},0} = 4 \times 10^5 \, \text{cm/s} \].

### 3. Discussion of laser characteristics

The following characteristics were calculated versus the injection current density \( j \) (up to \( j = 75 \, \text{kA/cm}^2 \)): i) electron and hole densities in the QW, \( n_{\text{QW}} \) and \( p_{\text{QW}} \) (figure 2), ii) electron and hole densities in the OCL, \( n_{\text{OCL}} \) and \( p_{\text{OCL}} \) (figure 4), iii) stimulated recombination current density in the QW, \( j_{\text{stim}} \), and spontaneous recombination current density in the OCL, \( j_{\text{spon}} \) (figure 8), and iv) output optical power (figure 9).

The above listed characteristics, calculated using the global electroneutrality condition \((10)\), were compared with those calculated using the condition of local electroneutrality in the QW

\[ e \, n_{\text{QW}} = e \, p_{\text{QW}}. \tag{11} \]

As seen from figure 2, the electron and hole densities in the QW, calculated using the global electroneutrality condition \((10)\), differ significantly.

However, the product \( n_{\text{QW}} \, p_{\text{QW}} \), calculated with the use of the condition \((10)\), remains virtually constant with increasing injection current (figure 3).

The electron and hole densities in the OCL are shown in figure 4.

As seen from figure 5, the charge of each sign in the OCL is significantly larger than that in the QW,

\[ ebn_{\text{OCL}} \gg eN_{\text{QW}} \, n_{\text{QW}}, \quad ebp_{\text{OCL}} \gg eN_{\text{QW}} \, p_{\text{QW}} \tag{12} \]

**Figure 2.** Electron (1) and hole (2) densities in the QW against injection current density calculated using the global electroneutrality condition.

**Figure 3.** Product of electron and hole densities in the QW against injection current density calculated using the global electroneutrality condition.
In view of inequalities (12), the condition (10) of global electroneutrality reduces to the condition of electroneutrality in the OCL, i.e., i.e., to the equality of the free electron and hole densities in the OCL (figure 4, curves 1 and 2),

\[ n^{OCL} = p^{OCL} \]  \hspace{1cm} (13)

In contrast, the electron and hole densities in the OCL, calculated using the condition (11) of local electroneutrality in the QW, differ considerably (figure 4, curves 3 and 4).

Using in (13) expressions (A27) and (A28) of [4] for \( n^{OCL} \) and \( p^{OCL} \) and considering high injection current densities, the following relationship can be derived:

\[ v_{n,\text{capt},0}(1-f_n) = v_{p,\text{capt},0}(1-f_p) \]  \hspace{1cm} (14)

which is the equality of the total capture velocity of electrons to that of holes at high injection currents.

It follows from (14) that, at equal electron and hole capture velocities into an empty QW \( (v_{n,\text{capt},0} = v_{p,\text{capt},0}) \) and no matter what is their common value, \( f_n = f_p \); in the laser structure considered here, \( f_n = f_p = 0.588 \) (figure 6). If, however, \( v_{n,\text{capt},0} \neq v_{p,\text{capt},0} \) then, as seen from (14), the level occupancies \( f_n \) and \( f_p \) tend to different constant values with increasing injection current (figure 7).

The spontaneous radiative recombination current density in the OCL calculated using the expression

\[ j_{\text{spon}}^{OCL} = ebB_{3DN}^{OCL} n^{OCL} p^{OCL} \]  \hspace{1cm} (15)

is shown in figure 8 as a function of the injection current density (curves 1 and 2). The spontaneous recombination in the OCL is a parasitic processes, which reduces the quantum efficiency and output optical power of the laser. As seen from the figure, \( j_{\text{spon}}^{OCL} \), calculated using the global electroneutrality condition (curve 1), is lower than \( j_{\text{spon}}^{OCL} \), calculated using the local electroneutrality condition in the QW (curve 2).
Figure 6. Electron (1, 3) and hole (2, 4) level occupancies in the QW against injection current density: (1, 2) - using the global electroneutrality condition; (3, 4) - using the local electroneutrality condition in the QW. The electron and hole capture velocities into an empty QW \( v_{n,capt,0} = v_{p,capt,0} = 4 \times 10^5 \text{ cm/s} \).

Figure 7. Electron (1) and hole (2) level occupancies in the QW against injection current density calculated using the global electroneutrality condition. The electron and hole capture velocities into an empty QW \( v_{n,capt,0} = 10^6 \text{ cm/s} \) and \( v_{p,capt,0} = 5 \times 10^5 \text{ cm/s} \).

Figure 8. Spontaneous recombination current density in the OCL (1, 2) and stimulated recombination current density in the QW (3, 4) against injection current density: (1, 3) - using the global electroneutrality condition; (2, 4) - using the local electroneutrality condition in the QW.

Figure 9. Optical power of the laser against injection current density (light-current characteristic): (1) - using the global electroneutrality condition, (2) - using the local electroneutrality condition in the QW.

The current density of stimulated radiative recombination in the QW,

\[
\dot{j}_{\text{stim}} = e v_g (\beta + \alpha_{\text{int}}) \frac{N}{S}
\]

is also shown in figure 8. The current density of stimulated recombination, calculated using the global electroneutrality condition (curve 3), is higher than that, calculated using the local electroneutrality condition in the QW (curve 4).
The output optical power $P$ against injection current density,

$$P(j) = \frac{\hbar \omega}{e} S j_{\text{stim}}(j) \frac{\beta}{\beta + \alpha_{\text{int}}} \quad (17)$$

is shown in figure 9. The calculation using the global electroneutrality condition (curve 1) gives higher values of the power as compared to that, which uses the local electroneutrality condition in the QW (curve 2).

4. Conclusions
A model for calculating the operating characteristics of semiconductor QW lasers has been presented. The model exploits the condition of global electroneutrality, which includes the charge carriers both in the 2D active region (QW) and bulk waveguide region (OCL). The charge of each sign in the OCL has been shown to be significantly larger than that in the QW. As a result of this, (i) the global electroneutrality condition reduces to the condition of electroneutrality in the OCL and (ii) the local electroneutrality in the QW can be strongly violated, i.e., the 2D electron and hole densities in the QW can significantly differ from each other. The product of the 2D electron and hole densities in the QW, however, remains virtually constant with increasing injection current.

The use of the global electroneutrality condition gives higher values of the power than the use of the local electroneutrality condition in the QW.

Acknowledgments
This work was supported by the federal program of the Ioffe Institute. Z. N. Sokolova is grateful for the hospitality of MEPhI during her visit supported by the Competitiveness Program of National Research Nuclear University MEPhI. L. V. Asryan acknowledges the U.S. Army Research Office (Grant No. W911NF-13-1-0445) for support of this work.

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