Diffusion-drift model of injection lasers with double heterostructure

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Abstract. This paper introduces the diffusion-drift model for numerical analysis of dynamical processes in injection lasers. The model takes into account the laser’s structural features, the mechanisms of spontaneous and stimulated recombination. The numerical simulation of injection lasers with a double heterostructure has been made. The simulation results allowed to determine the validity limits for the proposed model.

1. Introduction
The paper is devoted to the problem of the simulation of physical processes in semiconductor laser structures. This problem is one of the urgent problems of modern semiconductor optoelectronics. It was considered in [1], [2], [3].

Currently the dynamics of processes in injection lasers is described by the kinetic equations which connect the concentration of charge carriers with the density of pumping current and the density of photons in the active region of the laser and are formulated as below [4], [5], [6]:

\[ \frac{dn}{dt} = \frac{j}{eD} - \frac{n}{\tau_s} - \frac{v_g n_{ph} g(n, n_{ph})}{\tau_s}; \]  
\[ \frac{dn_{ph}}{dt} = -\frac{n_{ph}}{\tau_f} + \frac{\beta n}{\tau_s} + \frac{v_g n_{ph} g(n, n_{ph})}{\tau_s}, \]

where \( n \) is the concentration of mobile charge carriers in the active region of the laser; \( n_{ph} \) is the concentration of photons; \( j \) is the density of the pumping current; \( t \) is the time; \( e \) is the electron charge; \( D \) is the characteristic size of the active region of the laser; \( g(n, n_{ph}) \) is the optical gain coefficient; \( \beta \) is the fraction of spontaneous emission that falls in the laser mode; \( \tau_s \) is the time of spontaneous radiative recombination; \( \tau_f \) is the photon lifetime in the active region of the laser; \( v_g \) is the photon speed in the active region of the laser.

The kinetic equations represent a system of ordinary differential equations and do not take into account the following factors that can be important for analyzing the characteristics of the laser structures [7], [8]:

- the difference in the distribution of electron and hole concentrations by coordinates in the active region of the laser (the kinetic equations are derived on the assumption that electrons and holes concentrations are equal within the active region of the laser);
- uneven spatial distributions of charge carrier and photon concentrations in the active region;
• the features of spatial distribution of current density;
• the influence of peripheral regions on the laser characteristics;
• the impossibility of the transient analysis in the injection laser in the fixed voltage on contacts mode (only the fixed injection current mode was researched).

The aim of this work was to develop the physical and topological model of semiconductor laser structures which would consider the above factors.

2. Mathematical methods

This model was derived on the basis of the semiconductor fundamental equations system in diffusion-drift approximation [9] and the kinetic equations for lasers [4], [5], [6], which can be written as follows:

\begin{equation}
\nabla (\varepsilon \cdot \nabla \varphi) = \frac{e}{\varepsilon_0} (n - p - N);
\end{equation}

\begin{equation}
\frac{dn}{dt} = \nabla \left[ \mu_n \left( -n\nabla (\varphi + V_n) + \varphi_i \nabla n \right) \right] - \frac{\sqrt{np-n_i^2}}{\tau_s} - v_g g \cdot n_{ph};
\end{equation}

\begin{equation}
\frac{dp}{dt} = \nabla \left[ \mu_p \left( p\nabla (\varphi - V_p) + \varphi_i \nabla p \right) \right] - \frac{\sqrt{np-n_i^2}}{\tau_s} - v_g g \cdot n_{ph};
\end{equation}

\begin{equation}
\frac{dn_{ph}}{dt} = -\frac{n_{ph}}{\tau_f} + \frac{g\sqrt{np-n_i^2}}{\tau_s} + v_g g \cdot n_{ph};
\end{equation}

\begin{equation}
g = \begin{cases} 
  g(n, p, n_{ph}) > 0, & E_{p\text{in}} - E_{p\text{p}} \geq E_C - E_V, \\
  0, & E_{p\text{in}} - E_{p\text{p}} < E_C - E_V,
\end{cases}
\end{equation}

where \( n, p \) are electron and hole concentrations; \( \mu_n, \mu_p \) are electron and hole mobilities; \( N \) is the effective impurity concentration; \( n_i \) is the intrinsic concentration; \( \varphi \) is the electrostatic potential; \( \varphi_T \) is the temperature potential; \( V_n, V_p \) are heterostructure potentials in the conduction and valence bands; \( \varepsilon \) is the dielectric constant of a semiconductor; \( \varepsilon_0 \) is the dielectric constant of vacuum; \( g \) is the optical gain coefficient; \( E_{p\text{in}}, E_{p\text{p}} \) are electron and hole imrefs; \( E_C, E_V \) are levels of the bottom of the conduction band and the top of the valence band.

The boundary conditions for the fixed voltage on contacts which were used for solving the system of equations (3) – (7) can be written as follows:

- on the ohmic contacts:

\begin{align*}
\varphi &= \varphi_i \ln \frac{N}{2} + \sqrt{\left( \frac{N}{2} \right)^2 + n_i^2} + U(t); \\
n &= \frac{N}{2} + \sqrt{\left( \frac{N}{2} \right)^2 + n_i^2}; \\
p &= -\frac{N}{2} + \sqrt{\left( \frac{N}{2} \right)^2 + n_i^2}; \\
n_{ph} &= 0,
\end{align*}

\( N \) is the effective impurity concentration; \( n_i \) is the intrinsic concentration; \( \varphi_i \) is the intrinsic potential; \( U(t) \) is the voltage on contacts; \( \sqrt{\left( \frac{N}{2} \right)^2 + n_i^2} \) is the Fermi level.
where $U$ is the voltage on the contact;

- on Schottky’s contact:

$\varphi = \varphi_r \ln \left( \frac{N}{2} + \sqrt{\left( \frac{N}{2} \right)^2 + n_i^2} \right) + U(t) - \varphi_0; \quad (12)$

$n = \left( \frac{N}{2} + \sqrt{\left( \frac{N}{2} \right)^2 + n_i^2} \right) \exp \left( - \frac{\varphi_0}{\varphi_r} \right); \quad (13)$

$p = \left( \frac{N}{2} + \sqrt{\left( \frac{N}{2} \right)^2 + n_i^2} \right) \exp \left( \frac{\varphi_0}{\varphi_r} \right); \quad (14)$

$n_{ph} = 0, \quad (15)$

where $\varphi_0$ is the contact-potential difference of Schottky’s junction;

- on the boundaries which are free from contacts:

$\frac{\partial \varphi}{\partial \xi} = 0; \quad (16)$

$\frac{\partial n}{\partial \xi} = 0; \quad (17)$

$\frac{\partial p}{\partial \xi} = 0; \quad (18)$

$\frac{\partial n_{ph}}{\partial \xi} = 0, \quad (19)$

where $\xi$ is the surface normal.

The boundary conditions for the fixed current density are similar to (9) – (19), the equation (8) is replaced by the following expression:

$$\frac{\partial \varphi}{\partial \xi} = \frac{j}{e} + \mu_e \left( \varphi_r \frac{\partial n}{\partial \xi} - n \frac{\partial V_n}{\partial \xi} \right) - \mu_p \left( \varphi_r \frac{\partial p}{\partial \xi} - p \frac{\partial V_p}{\partial \xi} \right) \bigg|_{n_{ph}} \div \left( \mu_e n + \mu_p p \right). \quad (20)$$

The proposed model does not consider the dimensional quantization of the energy spectrum of the charge carriers. Therefore it cannot be used for the simulation of laser structures with narrow quantum wells.

The photon lifetime in the active region of the laser $\tau_f$ is determined by the optical loss and the parameters of the resonator mirrors.

The optical gain coefficient $g$ is considered to be one of the key parameters of injection lasers. The optical gain coefficient depends on the charge carrier and photon concentrations in the active region of the laser is traditionally defined by the models introduced in [5], [6]. In the proposed system of equations (3) – (7) the optical gain coefficient value $g(n, p, n_{ph})$ is defined similarly by the
expressions given in [5], [6]. In these expressions the generalized concentration of the charge carriers that implies the equality \( n = p \) in the active region of the laser, is replaced by the expression \( \sqrt{np - n^2} \) for taking into account the influence of electron, hole and photon concentrations. The expression being considered determines the degree of the electron and hole concentrations deviation from the equilibrium values more accurately.

In contrast to the kinetic equations, the system of equations (3) – (7) allows to investigate the changes of spatial distributions of electron, hole and photon concentrations in the active and peripheral regions of the laser. Thus, transient processes analysis is possible at a set pumping current or at a specified voltage on contacts in accordance with the boundary conditions used. It is important to use the heterostructure potential and profiles of dopant spatial distributions as a data source for the equations (3) – (7) in view of the injection lasers structures huge variety. It allows obtaining the results on the laser numerical simulation taking into account the various structural and topological features thereby expanding the scope of the proposed model validity. The numerical solution of the equation system (3) – (7) was performed using the finite difference method. The solution of the appropriate stationary problem was performed using the Newton’s method in order to obtain the initial condition [9]. The system of equations used for the calculation of the initial conditions can be written as follows:

\[
\nabla (e \cdot \nabla \phi) = \frac{e}{E_0} (n - p - N); \tag{21}
\]

\[
\nabla \left[ \mu_n (-n \nabla (\phi + V_n) + \phi \nabla n) \right] = \frac{\sqrt{np - n^2}}{\tau_s} + v_g n_p n_h; \tag{22}
\]

\[
\nabla \left[ \mu_p (p \nabla (\phi - V_p) + \phi \nabla p) \right] = \frac{\sqrt{np - n^2}}{\tau_s} + v_g n_p n_h; \tag{23}
\]

\[
n_p n_h = \frac{\beta \sqrt{np - n^2}}{\tau_s \left( \frac{1}{\tau_f} - v_g n_h \right)}; \tag{24}
\]

\[
g = \begin{cases} 
  g(n, p, n_p, n_h) > 0, & E_{F_n} - E_{F_p} \geq E_c - E_v, \\
  0, & E_{F_n} - E_{F_p} < E_c - E_v.
\end{cases} \tag{25}
\]

3. Simulation results and discussion

Figures 1 – 3 show the results of the simulation of the double heterostructure laser \( n^+ - Al_{0.3}Ga_{0.7}As/i-GaAs/p^+ - Al_{0.3}Ga_{0.7}As \) with the active region width of 50 nm, the photon lifetime in the resonator is \( \tau_f = 3 \) ps, the time of spontaneous radiative recombination is \( \tau_s = 4 \) ns, the proportion of spontaneous emission getting in the laser mode is \( \beta = 10^4 \) for the pulse of the pumping current density with the duration of \( \tau_p = 100 \) ps and the amplitude of \( j = 10^8 \) A/cm\(^2\).

The results shown in figure 1(a) were obtained by solving the kinetic equations. Figures 1(b–d) and figure 2 show the results obtained using the proposed model. The time dependences of the electron, hole and photon concentrations are shown for various cross-sections of the active region of the double heterostructure laser in figure 1(b–d).

Figure 2 shows that electron and hole concentrations in the active region of the laser are distributed irregularly. It explains the irregularity of the photon concentration distribution within the active region, which is presented in figure 3. That is the reason why, as it is seen in figure 1, the quantitative discrepancy of results obtained by solving the kinetic equations (figure 1(a)) and the system of
equations (3) – (7) (figure 1(b–d)) for individual cross-sections of the laser active region is more than 50%.

**Figure 1.** The results of the numerical simulation of the transient process in the double heterostructure laser obtained by solving the kinetic equations (a) and the equations of the proposed model for the central (c) and peripheral (b, d) cross-sections of the active region.

**Figure 2.** The electron and hole concentrations in the double heterostructure laser in the moments of reaching the first maximum (a) and the first minimum (b) in the central cross-sections of the active region.

The kinetic equations for the laser were formulated under the following assumption: when the density of the pumping current is above the threshold value, the optical gain coefficient $g$ undergoes periodic changes only over time in the course of the transient process. The numerical simulation results obtained using the proposed model (3) – (7) confirm the possibility of periodic changes of the
laser optical gain coefficient values both in time and by coordinate. It allows analyzing the transient processes in the laser structures taking into account this effect.

![Graphs](image_url)

**Figure 3.** The photon density in the moments of reaching the first maximum (a) and the current pulse rear front (b)

### 4. Conclusion

The comparative analysis of the obtained results allows to conclude that the kinetic equations with the accepted assumptions can be used for the simulation of transient processes in injection lasers if the problem doesn’t require the consideration of non-uniformity of the spatial distributions of electron, hole and photon concentrations in the active and peripheral regions, non-uniformity of the laser optical gain coefficient by coordinates, characteristics of laser structure, its band diagram, spatial distribution of current density.

If all these factors (or some of them) have to be considered according to the problem of simulation or if it is needed to explore the transient processes in the laser for a set voltage pulse (not a current pulse) on the external contacts, it is advisable to use more accurate models, in particular, the equation system considered in this research.

The proposed approach allows to ensure the adequacy of the results of the laser structures simulation and to improve the accuracy of the calculation of the laser’s characteristics.

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