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Threshold characteristics of semiconductor lasers under conditions of violation of electroneutrality in quantum wells

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Abstract. **The threshold characteristics of semiconductor lasers are studied theoretically when the electroneutrality in quantum wells is violated. It is shown that even with the infinitely large threshold concentration of the charge carriers of one sign in the wells, the minimum threshold concentration of the carriers of the opposite sign is nonzero. It is found that in InGaAs/GaAs/AlGaAs heterostructures emitting near the wavelength 1.044 μm, in a wide range of values of the electron concentration in the wells the threshold concentrations of free electrons and holes in the waveguide region are small, the contribution of the recombination current in the waveguide region to the total threshold current is negligible and in the case of a single quantum well, the threshold current density is virtually constant, i.e., the violation of electroneutrality in the InGaAs/GaAs/AlGaAs structures with a single quantum well has almost no effect on the threshold current. In the structures with two or three wells the violation of electroneutrality manifests itself much stronger and can lead to either a decrease or an increase in the threshold current.**

Keywords: *semiconductor lasers, heterostructures, quantum wells, recombination of charge carriers, carrier concentration, threshold current.*

1. Introduction

The development of methods for epitaxial heterostructure layer growth has made it possible to use nanoscale objects (quantum wells [1–7] and then quantum dots [8]) as an active region of semiconductor lasers. In calculating the threshold characteristics of heterostructure lasers it is generally assumed that the concentrations of electrons and holes in the active region are equal [9], i.e., it has a local electroneutrality. In fact, because of the differences between the electron and hole parameters (first of all, the parameters that control the electron and hole capture in a nanosized active region and the position of sub-bands or quantum-confinement levels in it), the carrier densities in the active region may be different, which means violation of electroneutrality.

In contrast to quantum dot lasers for which this problem has been studied in [10–12], the violation of neutrality in quantum wells has not been properly considered in the literature. The present work is devoted to a theoretical study of this issue. We consider the influence of the difference between electron and hole concentrations in the wells from each other on the threshold characteristics of the laser. We study theoretically the threshold current of a Fabry–Perot cavity planar injection laser structure containing one or more wells. Since the threshold current is determined by the processes of spontaneous radiative recombination both in the quantum wells and in the waveguide region (optical confinement layer, OCL), we study in detail the concentration of charge carriers in these regions.

2. Two-dimensional threshold concentrations of electrons and holes localised in quantum wells

The threshold concentrations $n^{\rm QW}$ and $p^{\rm QW}$ of electrons and holes in quantum wells are related to each other by the lasing condition, which can be written in the form [13, 14]:

$$N_{\rm QW}g^{\max}\left[1-\exp\left(-\frac{n^{\rm QW}}{N_{\rm c}^{\rm 2D}}\right)-\exp\left(-\frac{p^{\rm QW}}{N_{\rm v}^{\rm 2D}}\right)\right]=\beta+\alpha_{\rm int}, \quad (1)$$

where $N_{\rm QW}$ is the number of quantum wells in the active region; $g^{\max}$ is the maximum modal gain of the laser per quantum well {see expression (10) in [13] for $g^{\max}$}; $\beta = (1/L)\ln(1/R)$ are the losses associated with the radiation output from the resonator; L is the length of the resonator; R is the reflectivity of the mirrors; $\alpha_{\rm int}$ are the internal optical losses in the structure;

$$N_{\rm c}^{\rm 2D}=\frac{m_{\rm e}^{\rm QW}k_{\rm B}T}{\pi\hbar^2}, \qquad N_{\rm v}^{\rm 2D}=\frac{m_{\rm hh}^{\rm QW}}{m_{\rm e}^{\rm QW}}N_{\rm c}^{\rm 2D} \quad (2)$$

are the effective two-dimensional densities of the electron states in the conduction band and heavy hole states in the valence band in a quantum well; $m_{\rm e}^{\rm QW}$ and $m_{\rm hh}^{\rm QW}$ are the effective masses of electrons and heavy holes in the well; $k_{\rm B}$ is the Boltzmann constant; and T is the temperature.

In deriving (1) we assumed that the carrier concentrations (different for electrons and holes) do not change from one well to another. We also assumed that the internal optical losses $\alpha_{\rm int}$ do not depend on the number of quantum wells.

When the condition of electroneutrality in the quantum wells is fulfilled ($n^{\rm QW} = p^{\rm QW}$), the concentration of electrons and holes would be calculated directly from (1).

We consider in this paper the general case of neutrality violation in the quantum wells and, therefore, analyse the threshold characteristics of the laser as a function of the differences between the concentrations $n^{\rm QW}$ and $p^{\rm QW}$. Using

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Eqn (1) the threshold concentration of electrons can be expressed through the threshold concentration of holes in the quantum well as follows:

$$n^{\mathrm{QW}} = N_{\mathrm{c}}^{\mathrm{2D}} \ln\left[1 - \frac{\beta + \alpha_{\mathrm{int}}}{N_{\mathrm{QW}} g^{\max}} - \exp\left(-\frac{p^{\mathrm{QW}}}{N_{\mathrm{v}}^{\mathrm{2D}}}\right)\right]^{-1}. \tag{3}$$

Similarly, from (1) we can express p^{QW} through n^{QW}.

Equations (1) and (3) shows that the minimum threshold concentration of the electrons, $n_{\min}^{\mathrm{QW}}$, in the quantum well, required for lasing is not zero. It is determined from these expressions by tending p^{QW} to infinity, giving

$$n_{\min}^{\mathrm{QW}} = N_{\mathrm{c}}^{\mathrm{2D}} \ln\left(1 - \frac{\beta + \alpha_{\mathrm{int}}}{N_{\mathrm{QW}} g^{\max}}\right)^{-1}. \tag{4}$$

Similarly to $n_{\min}^{\mathrm{QW}}$, the minimum threshold concentration of holes, $p_{\min}^{\mathrm{QW}}$, at which the electron concentration becomes infinitely large, is also non-zero. The expression for $p_{\min}^{\mathrm{QW}}$ can be obtained directly either from (1) or from the condition when the denominator in the right-hand side of equation (3) vanishes; it is different from (4) only in that it includes $N_{\mathrm{v}}^{\mathrm{2D}}$ instead of $N_{\mathrm{c}}^{\mathrm{2D}}$, i.e., the difference in minimal concentrations of electrons and holes in the quantum well is due to the difference in their effective masses:

$$\frac{p_{\min}^{\mathrm{QW}}}{n_{\min}^{\mathrm{QW}}} = \frac{m_{\mathrm{hh}}^{\mathrm{QW}}}{m_{\mathrm{e}}^{\mathrm{QW}}}. \tag{5}$$

Thus, for the lasing condition (1) to be fulfilled at a minimum concentration of charge carriers of one sign, the concentration of charge carriers of the opposite sign should be infinitely high, which means an infinitely high level of pumping (i.e., infinitely high threshold current density, see Figs 5 and 7 below).

Lasing condition (1) can be written as

$$f_{\mathrm{n}} + f_{\mathrm{p}} - 1 = \frac{\beta + \alpha_{\mathrm{int}}}{N_{\mathrm{QW}} g^{\max}}, \tag{6}$$

where f_{n} and f_{p} are the filling factors (occupancies) of the states corresponding to the lower edges of the quantum-confinement sub-bands of electrons and heavy holes in the quantum well. They are expressed through n^{QW} and p^{QW} as follows [13–17]:

$$f_{\mathrm{n}} = 1 - \exp(-n^{\mathrm{QW}}/N_{\mathrm{c}}^{\mathrm{2D}}), \; f_{\mathrm{p}} = 1 - \exp(-p^{\mathrm{QW}}/N_{\mathrm{v}}^{\mathrm{2D}}). \tag{7}$$

Tending the concentration of the carriers of one sign to infinity means that the filling factor of the quantum-confinement sub-band edge of this type of carries tends to unity. In this case, the filling factor of the quantum-confinement sub-band edge of the carriers of opposite sign tends to the minimum value required for lasing,

$$f_{\min} = \frac{\beta + \alpha_{\mathrm{int}}}{N_{\mathrm{QW}}\, g^{\max}}. \tag{8}$$

Using (8), we can write equation (4) in the form

$$n_{\min}^{\mathrm{QW}} = N_{\mathrm{c}}^{\mathrm{2D}} \ln(1 - f_{\min})^{-1}. \tag{9}$$

Below we present the results of calculations for a laser heterostructure based on InGaAs/GaAs/AlGaAs. The active region of the structure contains one or more strained $\mathrm{In_{0.28}Ga_{0.72}As}$ quantum wells of thickness 80 Å each. The material of the broad (1.7 μm) waveguide region is GaAs, the material of the emitters is $\mathrm{Al_{0.3}Ga_{0.7}As}$. The effective masses of electrons and heavy holes in the quantum well are $m_{\mathrm{e}}^{\mathrm{QW}} = 0.059 m_0$ and $m_{\mathrm{hh}}^{\mathrm{QW}} = 0.361 m_0$ (calculated according to [18], m_0 is the free electron mass); the calculated wavelength is $\lambda_0 = 1.044\,\mu\mathrm{m}$; the length of the Fabry–Perot cavity is $L = 1.5$ mm; $R = 0.32$; $\beta = 7.6\ \mathrm{cm^{-1}}$; $\alpha_{\mathrm{int}} = 1\ \mathrm{cm^{-1}}$; $T = 300$ K; $g^{\max} = 49.1\ \mathrm{cm^{-1}}$; and $f_{\min} = 0.175$.

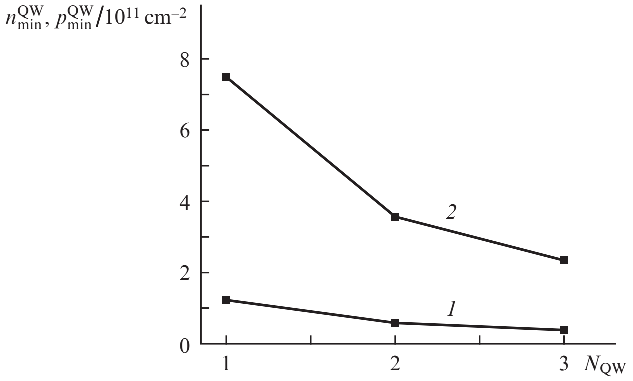

Figure 1. Minimum threshold concentrations of (*1*) electrons and (*2*) holes in the quantum wells vs. the number of wells.

Equations (4) and (5) show that $n_{\min}^{\mathrm{QW}}$ and $p_{\min}^{\mathrm{QW}}$ decrease with increasing N_{QW}. Figure 1 presents the dependence of the minimum concentrations on the number of quantum wells.

Figure 2 shows the threshold concentration of the holes in the quantum well as a function of the threshold concentration of the electrons for the structures with one, two and three quantum wells. For a structure with one quantum well $n^{\mathrm{QW}} = p^{\mathrm{QW}} = 1.36\times10^{12}\ \mathrm{cm^{-2}}$, with two wells – $1.14\times10^{12}\ \mathrm{cm^{-2}}$, with three wells – $1.08\times10^{12}\ \mathrm{cm^{-2}}$.

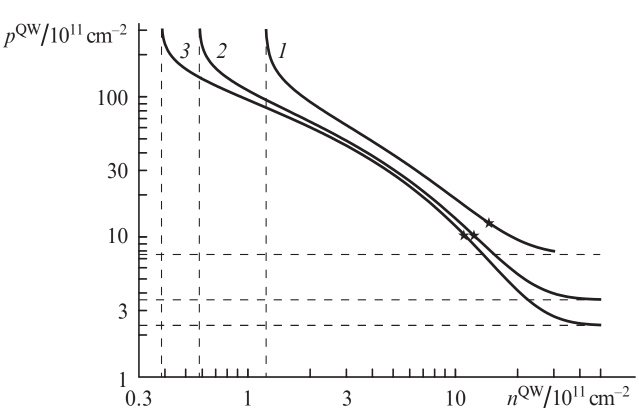

Figure 2. Threshold concentration of holes in the quantum well as a function of the threshold electron concentration for the structures with (*1*) one, (*2*) two and (*3*) three wells. Vertical dashed lines show $n_{\min}^{\mathrm{QW}}$, horizontal – $p_{\min}^{\mathrm{QW}}$. Asterisks show the points corresponding to electroneutrality in the wells ($n^{\mathrm{QW}} = p^{\mathrm{QW}}$).

3. Three-dimensional threshold concentrations of free electrons and holes in the waveguide region

Three-dimensional concentrations of free electrons, $n_{\rm th}^{\rm OCL}$, and holes, $p_{\rm th}^{\rm OCL}$, in the waveguide region at the lasing threshold are expressed through the threshold values of two-dimensional electron and hole concentrations in the quantum well as follows [13, 14]:

$$n_{\rm th}^{\rm OCL} = n_1^{\rm OCL}\left[\exp(n^{\rm QW}/N_{\rm c}^{\rm 2D}) - 1\right],$$

$$p_{\rm th}^{\rm OCL} = p_1^{\rm OCL}\left[\exp(p^{\rm QW}/N_{\rm v}^{\rm 2D}) - 1\right], \qquad (10)$$

where

$$n_1^{\rm OCL} = N_{\rm c}^{\rm 3D}\exp[-(\Delta E_{\rm c} - \varepsilon_{\rm n})/k_{\rm B}T];$$

$$p_1^{\rm OCL} = N_{\rm v}^{\rm 3D}\exp[-(\Delta E_{\rm v} - \varepsilon_{\rm p})/k_{\rm B}T]; \qquad (11)$$

$\Delta E_{\rm c}$ and $\Delta E_{\rm v}$ are the offsets of the conduction and valence bands at the heterojunction between the waveguide region and the quantum well; $\varepsilon_{\rm n}$ and $\varepsilon_{\rm p}$ are the energies of the lower edges of the quantum-confinement sub-bands of electrons and heavy holes in the quantum well (measured from the bottom of the well);

$$N_{\rm c}^{\rm 3D} = 2\left(\frac{m_{\rm e}^{\rm OCL}k_{\rm B}T}{2\pi\hbar^2}\right)^{3/2}, \quad N_{\rm v}^{\rm 3D} = 2\left(\frac{m_{\rm hh}^{\rm OCL}k_{\rm B}T}{2\pi\hbar^2}\right)^{3/2} \qquad (12)$$

are the effective bulk densities of states in the conduction band and the valence band in the waveguide region; and $m_{\rm e}^{\rm OCL}$ and $m_{\rm hh}^{\rm OCL}$ are the effective masses of electrons and heavy holes in the waveguide region.

Using equations (3), (10) and (8) we can express the threshold concentration of electrons in the waveguide region through the threshold concentration of holes in this region:

$$n_{\rm th}^{\rm OCL} = n_1^{\rm OCL}\left[\left(\frac{p_{\rm th}^{\rm OCL}}{p_{\rm th}^{\rm OCL} + p_1^{\rm OCL}} - f_{\rm min}\right)^{-1} - 1\right]. \qquad (13)$$

Similarly, we can express $p_{\rm th}^{\rm OCL}$ through $n_{\rm th}^{\rm OCL}$.

When $n^{\rm QW}$ tends to $n_{\rm min}^{\rm QW}$, the concentration of free electrons also becomes minimal ($n_{\rm th}^{\rm OCL} \to n_{\rm th\,min}^{\rm OCL}$), and $p_{\rm th}^{\rm OCL} \to \infty$; in this case,

$$n_{\rm th\,min}^{\rm OCL} = n_1^{\rm OCL}\frac{f_{\rm min}}{1 - f_{\rm min}}. \qquad (14)$$

When $p^{\rm QW} \to p_{\rm min}^{\rm QW}$, the concentration of free holes also tends to its minimum value ($p_{\rm th}^{\rm OCL} \to p_{\rm th\,min}^{\rm OCL}$), and $n_{\rm th}^{\rm OCL} \to \infty$. The expression for $p_{\rm th\,min}^{\rm OCL}$ is obtained by substituting $n_1^{\rm OCL}$ by $p_1^{\rm OCL}$ in (14). As can be seen from (14) and (11), the difference in the minimum concentration of free electrons and holes is caused not only by the difference in their effective masses, but also in energies $\Delta E_{\rm c} - \varepsilon_{\rm n}$ and $\Delta E_{\rm v} - \varepsilon_{\rm p}$.

Thus, when the concentration of the charge carriers of one sign in the quantum well is minimal, the concentration of the carriers of that sign in the waveguide region is also minimal, and the concentrations of the carriers of opposite charge in the quantum well and in the waveguide region are infinitely high (Figs 2 and 3). This means that strong violation of electroneutrality in the quantum wells should lead to such violation of neutrality in the waveguide region.

Figure 3 shows threshold concentrations of free electrons and holes in the waveguide region as functions of the two-dimensional concentration of electrons in the quantum well for the structures with one, two and three wells. In the calculations we used the following parameters: $\Delta E_{\rm c}$ = 166.6 meV, $\Delta E_{\rm v}$ = 117.7 meV (calculated according to [18]), $\varepsilon_{\rm n}$ = 41.6 meV and $\varepsilon_{\rm p}$ =10.7 meV. The number of quantum wells ($N_{\rm QW}$) does not enter explicitly into expressions (10) and, thus, the curve in Fig. 3a describes the dependence of $n_{\rm th}^{\rm OCL}$ on $n^{\rm QW}$ for all three structures under consideration – the difference between the structures is only in the position of the initial points $n_{\rm min}^{\rm QW}$ on this curve.

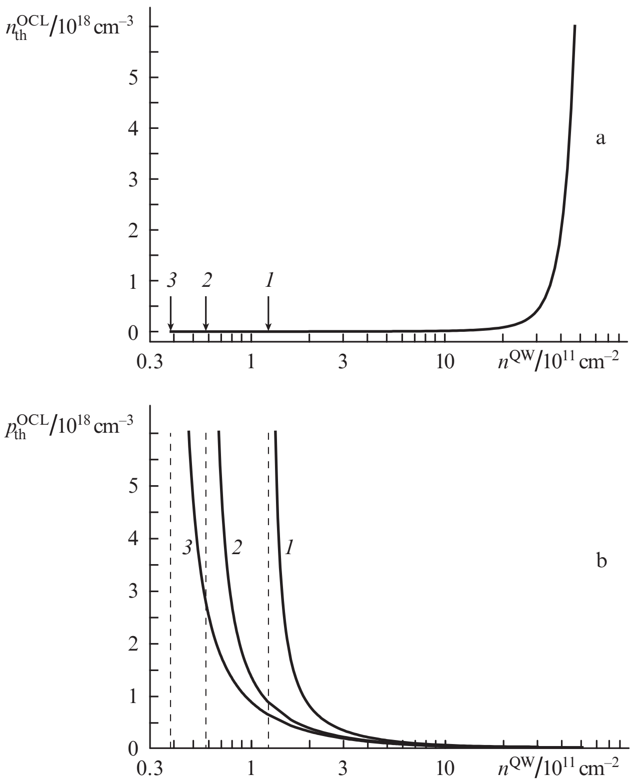

Figure 3. Threshold concentrations of (a) free electrons and (b) holes in the waveguide region as functions of the two-dimensional concentration of electrons in the quantum well for structures with (*1*) one, (*2*) two and (*3*) three wells. Vertical dashed lines in Fig. 3b correspond to the values of $n_{\rm min}^{\rm QW}$ shown by arrows in Fig. 3a.

4. Threshold current

The threshold current density $j_{\rm th}$ is equal to the sum of current densities of spontaneous radiative recombination in the quantum wells and waveguide region at the lasing threshold:

$$j_{\rm th} = j_{\rm th}^{\rm QW} + j_{\rm th}^{\rm OCL} = eN_{\rm QW}B_{\rm 2D}n^{\rm QW}p^{\rm QW} + ebB_{\rm 3D}n_{\rm th}^{\rm OCL}p_{\rm th}^{\rm OCL}, \quad (15)$$

where e is the electron charge; b is the width of the waveguide region; $B_{\rm 2D} = 2.51\times10^{-4}$ cm^2 s^{-1}, $B_{\rm 3D} = 2.04\times10^{-10}$ cm^3 s^{-1} are the spontaneous radiative recombination coefficients in two-dimensional (quantum well) and three-dimensional (waveguide) regions for the laser structure under consideration here (expressions for B_{2D} and B_{3D} are given in [19]).

As can be seen from (15), j_{th}^{QW} is found by multiplying the number of quantum wells and the concentrations of electrons and holes in each well at the lasing threshold. The dependence of the product $n^{QW}p^{QW}$ on n^{QW} [recall that p^{QW} is a function of n^{QW}, see (1) or (3)], i.e., on the extent of violation of electroneutrality in the quantum well is shown in Fig. 4 for structures with one, two and three wells. As can be seen from Fig. 4, the product $n^{QW}p^{QW}$ increases dramatically at both small and large values of n^{QW}. Indeed, for small n^{QW} (when $n^{QW} \to n_{min}^{QW}$) the concentration of holes $p^{QW} \to \infty$ (Fig. 2) and, therefore, the product $n^{QW}p^{QW} \to \infty$. When n^{QW} increases infinitely, the hole concentration tends to a constant ($p^{QW} \to p_{min}^{QW}$, see Fig. 2), i.e., again $n^{QW}p^{QW} \to \infty$. The dependence of $n^{QW}p^{QW}$ on n^{QW} has a local maximum between two local minima. However, in a structure with one well, the product $n^{QW}p^{QW}$ changes slightly when the concentration of electrons changes by more than an order of magnitude – from 1.5×10^{11} to 2.2×10^{12} cm^{-2}. With increasing number of quantum wells, the local maximum becomes more pronounced, but its magnitude decreases.

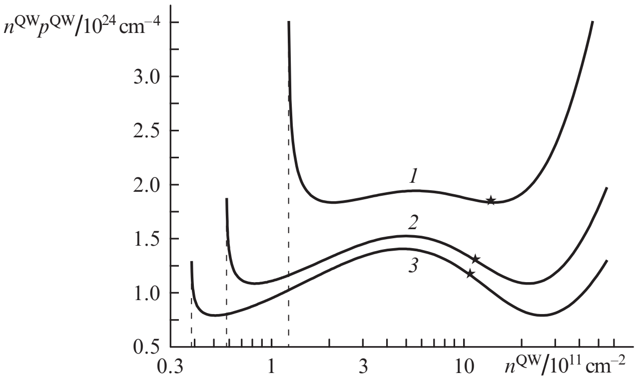

Figure 4. Dependence of the product $n^{QW}p^{QW}$ on the concentration of electrons in the quantum well for structures with (*1*) one, (*2*) two and (*3*) three wells. Asterisks show the points corresponding to the case $n^{QW} = p^{QW}$. Vertical dashed lines show the values of n_{min}^{QW} [see (4) or (9)].

The dependence of the recombination current density in the quantum wells, j_{th}^{QW}, on the electron density in the wells at the lasing threshold is shown in Fig. 5 for structures with one, two and three wells. The dependence of j_{th}^{QW} on n^{QW} basically repeats the dependence of $n^{QW}p^{QW}$ on n^{QW} (Fig. 4). The only difference is that the local maximum of j_{th}^{QW} increases with increasing number of quantum wells, which is caused by the presence of the multiplier N_{QW} in the expression for j_{th}^{QW} (15). It follows from Fig. 5 that in a single-well structure the recombination current density in the well at the lasing threshold remains virtually unchanged over a wide range of electron concentrations, i.e., independent of the presence or absence of electroneutrality in the well. Such a weak dependence of j_{th}^{QW} is explained by the compensation for the increase in the concentration of carriers of one sign by the fall of the concentration of carriers of opposite sign. In the limiting case of very strong violation of neutrality, when the concentration of carriers of one type is close to its minimum value, and the concentration of carriers of opposite charge is greatly increased, there is a significant increase in j_{th}^{QW}. In contrast to the single-well structure, in structures with two and especially three wells the value of j_{th}^{QW} is significantly more sensitive to the relationship between the concentrations of electrons and holes in the quantum wells. As can be seen from Fig. 5, the point of electroneutrality ($n^{QW} = p^{QW}$) is located on a dropping section of the curve, i.e., j_{th}^{QW} decreases when undergoing transition from a small positive surface charge of the well, $e\,(p^{QW} - n^{QW})$, to a negative one.

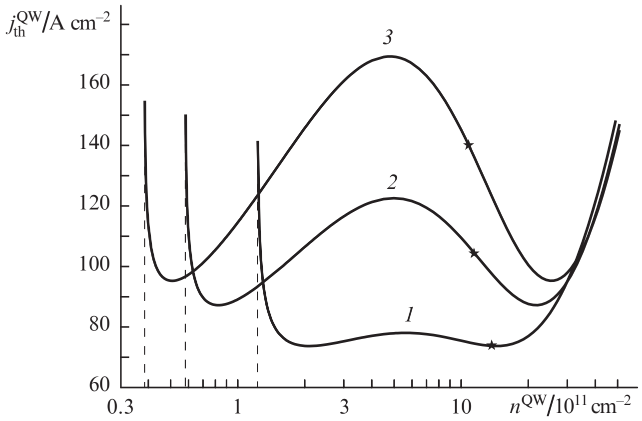

Figure 5. Dependence of the recombination current density in the quantum wells on the electron concentration in the well at the lasing threshold for structures with (*1*) one, (*2*) two and (*3*) three wells. Asterisks show the points corresponding to the case $n^{QW} = p^{QW}$. Vertical dashed lines show the values of n_{min}^{QW}.

For structures with one, two and three wells, Fig. 6 shows the dependence of the recombination current density j_{th}^{OCL} in the waveguide region on the electron concentration in the wells at the lasing threshold. One can see that in all three structures j_{th}^{OCL} is low and almost unchanged over a wide range of n^{QW} values, which increases with increasing number of quantum wells. Let us indicate a range of n^{QW} values, within which $j_{th}^{OCL} \leqslant 5$ A cm^{-2} and, therefore, the contribution of the recombination current in the waveguide region to j_{th} [see (15)] is negligible: 2.3×10^{11}–1.3×10^{12} cm^{-2} (structure

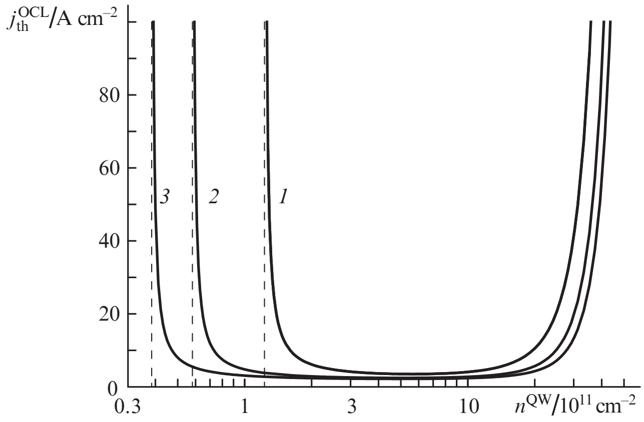

Figure 6. Recombination current density in the waveguide region as a function of the concentration of electrons in the well at the lasing threshold for the structures with (*1*) one, (*2*) two and (*3*) three wells. Vertical dashed lines show the values of n_{min}^{QW}.

with one well), 1×10^{11}–1.9×10^{12} cm^{-2} (structure with two wells), 6×10^{10}–2.1×10^{12} cm^{-2} (structure with three wells).

In our model, as can be seen from (10) and (13), violation of electroneutrality takes place not only in the quantum wells, but also in the waveguide region. A small contribution of the recombination current density in the waveguide region into $j_{\rm th}$ allows one to ignore the violation of electroneutrality in it within above-indicated ranges of concentrations of electrons in the quantum wells. Outside these concentration ranges, $j_{\rm th}^{\rm OCL}$ drastically increases, which is due to a sharp increase in the concentration of free carriers of one type in the waveguide region. In the case of such a strong violation of neutrality in the waveguide region, self-consistent consideration is required of the problem of the spatial profile of the electric field (i.e., band bending) in the laser structure, which takes into account both the charge of free carriers in this region and of two-dimensional carriers localised in the quantum wells, which is beyond the scope of this article.

The dependence of the threshold current density on the threshold concentration of electrons in the quantum wells for structures with one, two and three wells is shown in Fig. 7. One can see that in the middle range of the $n^{\rm QW}$ values, the dependence $j_{\rm th}(n^{\rm QW})$ repeats the dependence $j_{\rm th}^{\rm QW}(n^{\rm QW})$ (Fig. 5); the higher the $N_{\rm QW}$ in this region of the $n^{\rm QW}$ values, the higher the $j_{\rm th}$. However, at low and high values of $n^{\rm QW}$ there occurs a sharp increase in $j_{\rm th}$, due to the contribution of the recombination current in the waveguide region $j_{\rm th}^{\rm OCL}$; the greater the $N_{\rm QW}$ at such values of $n^{\rm QW}$, the lower the $j_{\rm th}$.

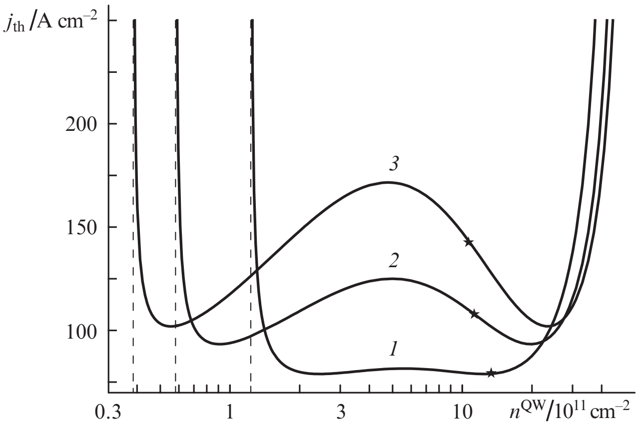

Figure 7. Threshold current density as a function of the threshold concentration of electrons in the well for structures with (*1*) one, (*2*) two and (*3*) three wells. Asterisks show the points corresponding to the case $n^{\rm QW} = p^{\rm QW}$. Vertical dashed lines show the values of $n_{\rm min}^{\rm QW}$.

5. Conclusions

We have theoretically investigated the threshold characteristics of semiconductor lasers under conditions of violation of electroneutrality in the quantum wells. It is found that in the heterostructures based on InGaAs/GaAs/AlGaAs (λ = 1.044 μm), the threshold concentrations of free electrons and holes in the waveguide region are small in a wide range of values of the electron concentration in the wells.

It is shown that violation of electroneutrality in InGaAs/GaAs/AlGaAs structures with a single well has almost no effect on the threshold current in a wide range of carrier concentrations in the well. In structures with two or three wells, violation of electroneutrality manifests itself much stronger and can lead to either a decrease or an increase in the threshold current.

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