Carrier and Photon Analyses of Photonic Microlasers by Two-Dimensional Rate Equations

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Abstract—In photonic crystal (PC) microlasers with point defect cavities, effective carriers are reduced by the leakage to outside of the defect, surface recombination, spatial carrier hole burning, and Auger recombination. To estimate these effects, we calculated carrier and photon behavior by solving two-dimensional rate equations in space and time domains. The result clearly shows these effects and their dependence on cavity structure, pump area, and so on. Compared with that for the microdisk laser, higher threshold values are estimated for PC microlasers. However, a comparably low threshold density and a high efficiency are expected for the quasi-periodic PC microlaser, because the hole burning by the whispering gallery mode of this cavity suppresses the carrier leakage.

Index Terms—Carrier diffusion, finite-difference time-domain (FDTD), microdisk, microlaser, photonic crystal (PC), quasi-periodic photonic crystal (QPC), rate equation, surface recombination velocity, whispering gallery mode.

I. INTRODUCTION

SEMICONDUCTOR photonic microlasers are expected to realize the low threshold lasing due to their small cavities and the high-efficiency and high-speed operation due to the enhanced spontaneous emission rate by the Purcell effect [1]–[4]. Compared with microdisk lasers (MDLs) surrounded by air [4]–[7] and vertical-cavity surface-emitting lasers (VCSELs) with one-dimensional Bragg mirrors [8], [9], photonic crystal (PC) lasers [10]–[12] with point defect cavities are more advantageous for the ultimate reduction in cavity size by using the photonic bandgap (PBG). Because of this reason, a very low threshold [13] and the strong Purcell effect [14] have been demonstrated, and a cavity quantum electrodynamic effect (e.g., strong coupling of the cavity with a quantum dot) has been expected [15]–[17]. On the other hand, quasi-periodic photonic crystals (QPCs) [18]–[20], which have high order rotational and line symmetries, are other candidates for the ultrasmall cavity. Recently, we have demonstrated the lasing action in a QPC microlaser [20]. However, most of these devices are composed of a III–V semiconductor slab, a hole array, and a hole-missing defect cavity. Therefore, part of carriers inside the defect cavity leak out by the diffusion and are lost by the

surface recombination at sidewalls of holes. This process results in a higher threshold and lower efficiency. The estimation of such useless carriers is an important issue, but has never been discussed yet. In general, rate equations for carriers and photons are used for analyzing lasing characteristics [2], [21], [22]. However, the simple analysis cannot precisely model complex structures of PCs and QPCs. In this work, we performed the finite-difference rate equation analysis with two-dimensional (2-D) cavity models and laser mode profiles. The behavior of carriers and photons including carrier diffusion, surface recombination, spatial hole burning, and Auger recombination were investigated in detail, and the threshold and internal efficiency in these microlasers were estimated. As the first step of this kind of analysis, we employed four sample models of microcavities with a fixed cavity Q factor and spontaneous emission factor. This means that we neglected the unique behavior of spontaneous emission such as the thresholdless lasing and the Purcell effect. We also ignored the thermal heating, which is important for estimating the continuous wave lasing condition but requires a large computational task for getting self-consistent results.

In the next section, we first explain the fundamental formulas and parameters used in the analysis. Then, in Section III, we present some calculated results of carrier distributions and lasing characteristics. In Section IV, we show the dependence on surface recombination velocity, carrier diffusion constant, and cavity Q factor. Finally, in Section V, we discuss the internal quantum efficiency and the effective surface recombination velocity including the carrier leakage effect, and summarize the advantages and disadvantages of each structure.

II. FORMULAS AND PARAMETERS

Rate equations for the carrier density $N(x, y; t)$ and the photon density $S(t)$ (number of photons divided by the volume of active region) with respect to positions x and y and time t are expressed as [21], [22]

$$\frac{dN}{dt} = \frac{P}{\hbar\omega} - \Gamma_z G S |E|^2 A_m - \frac{N}{\tau_c} + D \nabla^2 N \quad (1)$$

$$\begin{aligned} \frac{dS}{dt} = & \int_{\text{Act.}} \Gamma_z G S |E|^2 dx dy \\ & + \frac{C}{\Gamma_{xy}} \int_{\text{Act.}} \frac{N |E|^2}{\tau_{sp}} dx dy - \frac{S}{\tau_{ph}} \end{aligned} \quad (2)$$

where $P(x, y; t)$ is the pump power density, $\hbar\omega$ the pump energy, $G(N)$ the gain coefficient, A_m the effective modal area, $\tau_c(x, y; t)$ the carrier lifetime, $\tau_{sp}(x, y; t)$ the spontaneous emission lifetime, τ_{ph} the photon lifetime, D the carrier diffusion

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constant, and C the spontaneous emission factor. $E(x, y; t)$ is the electric field distribution of the laser mode, which is normalized as

$$\iint_{\text{Cavity}} |E|^2 dx dy = 1 \quad (3)$$

where E is determined by the cavity structure, namely, the refractive index distribution. More accurately, E is slightly changed by the gain, absorption, and carrier-induced index change, which are dependent on N . However, in cavities discussed in this paper, the mode is strongly influenced and almost determined by the very large index difference between the semiconductor and air. Therefore, we can consider E to be independent of time t in the rate equations. Γ_z and Γ_{xy} are confinement factors of E^2 into the active region. Even though the infinite uniformity is assumed in the perpendicular direction (z direction) in the 2-D analysis, the penetration of E^2 from the semiconductor slab to air in actual devices reduces the modal gain. Γ_z is used to express this reduction. The boundary condition at the edge of holes is expressed as

$$e_0 N v_s = -e_0 D \nabla N \quad (4)$$

where e_0 is the electron charge and v_s is the surface recombination velocity.

In the computation procedure, cavity models are assigned in the 2-D space divided by the small unit cell. The position (x, y) is expressed by the discrete coordinate (i, j) and the cell size Δx and Δy as $(i\Delta x, j\Delta y)$, respectively. The time t is expressed by the step number n and the unit time Δt as $n\Delta t$. N and S are denoted as $N_{i,j}^n$ and S^n , respectively, and derivatives in (1) and (2) are expressed in finite different formulas. Since E is independent of N and S , $E_{i,j}$ is calculated by the so-called finite-difference time-domain (FDTD) method before the rate equation analysis. Thus, (1) and (2) are solved against the pumping condition expressed by $P_{i,j}^n$, and dynamic behavior of $N_{i,j}^n$ and S^n after any time steps are obtained. The lasing threshold is estimated from the photon density at the steady state.

In overall calculations in this paper, we modeled the GaInAsP slab with compressively strained quantum wells (CS-QWs) [21]. In the FDTD analysis, a standard equivalent modal index of the slab of 2.73 was used for the background medium, and those of holes were set to 1.0. In the rate equation analysis, uniform circular photopumping at a wavelength of $0.98 \mu\text{m}$ with a diameter of $2R_{ex}$ was considered. Γ_z was set to 0.079 as a typical value for the slab with CS-QWs. On the other hand, Γ_{xy} was directly obtained by the FDTD analysis. A_m is given by $4/E_{\text{max}}$, where E_{max} is the maximum electric field determined by (3). The gain $G(N)$ was approximated by the logarithmic function $G_0(c/n_g) \ln(N/N_0)$, where c is the light velocity in vacuum, n_g the group index, and N_0 the transparent carrier density. For the CS-QWs, we set $G_0 = 1500 \text{ cm}^{-1}$, $n_g = 3.5$, and $N_0 = 1.5 \times 10^{18} \text{ cm}^{-3}$. The carrier lifetime τ_c has relation $\tau_c^{-1} = \tau_{nr}^{-1} + \tau_{sp}^{-1}$ with the nonradiative recombination lifetime τ_{nr} and the spontaneous emission lifetime τ_{sp} . Since the surface recombination is taken into account in (4), τ_{nr}^{-1} only includes the Auger recombination $C_A N^2$, where the Auger coefficient C_A was set to $2.5 \times 10^{-29} \text{ cm}^6 \text{ s}^{-1}$. The

Fig. 1. Cavity models and electric field distributions $E^2 (= E_x^2 + E_y^2)$ of laser modes, which are calculated by FDTD method. (a) MDL. (b) QPC. (c) PC-H2. (d) PC-H1.

spontaneous emission rate is given by $\tau_{sp}^{-1} = BN$, where B was set to $2.0 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$. The photon lifetime τ_{ph} was fixed to 2.23 ps, which corresponds to a cavity Q factor of 3000 at a wavelength of $1.55 \mu\text{m}$ and additional internal loss $\alpha_i = 5 \text{ cm}^{-1}$. The average threshold carrier density $\bar{N}_{th}$ is approximated as

$$\bar{N}_{th} = N_0 \exp\left(\frac{n_g}{c\Gamma_z G_0 \tau_{ph}}\right). \quad (5)$$

Substituting above values into (5), $\bar{N}_{th}$ is calculated to be $2.4 \times 10^{18} \text{ cm}^{-3}$. In the first part of the calculation, the spontaneous emission factor C and the diffusion constant D were fixed to be 0.1 and $2 \text{ cm}^2 \text{ s}^{-1}$, respectively, as standard values of GaInAsP microlasers [4], [12], [21], [23]. For the estimation of threshold power $p_{th} = P_{th}(\pi R_{ex}^2)d$, the total thickness d of CS-QWs was set to 20 nm. The cell size Δx and Δy were 15 nm in both the FDTD and rate equation analyses. Δt in the FDTD analysis was as short as 0.025 fs due to the fast oscillation of lightwaves, while it was 100 fs for the slower behavior of carriers and photons in rate equations.

III. CARRIER DENSITY DISTRIBUTIONS AND LASING CHARACTERISTICS

As examples of microlasers, we modeled a MDL of $1.77 \mu\text{m}$ diameter, 12-fold symmetric QPC [20] (the lattice constant $a = 585 \text{ nm}$ and the hole diameter $2r = 420 \text{ nm}$) with the seven-hole-missing defect, triangular lattice PC ($a = 435 \text{ nm}$ and $2r = 240 \text{ nm}$) with the seven-hole-missing defect (H2 defect) and PC with the single defect (H1 defect), as shown in Fig. 1. In the FDTD analysis, whispering gallery modes (WGMs) in the MDL (resonant wavelength $\lambda = 1.575 \mu\text{m}$) and in the QPC ($1.753 \mu\text{m}$), a Fabry–Perot like mode in the PC-H2 ($1.663 \mu\text{m}$), and a dipole mode in the PC-H1 ($1.489 \mu\text{m}$) were obtained by the selective excitation of these wavelengths. Although other various modes are formed in the QPC and the PC-H2, we chose them as examples here.

Fig. 2. Carrier distributions above threshold ($p \sim 2p_{th}$). (a) MDL. (b) QPC. (c) PC-H2. (d) PC-H1. From right to left, $2R_{ex} = 0.9 \mu\text{m}$, $2.1 \mu\text{m}$, and $4.2 \mu\text{m}$.

Fig. 2 shows carrier density distributions above threshold for $2R_{ex} = 0.9 \mu\text{m}$, $2.1 \mu\text{m}$, and $4.2 \mu\text{m}$. When the whole area of the MDL is uniformly pumped, the spatial hole burning occurs at the disk edge where the WGM is localized, and many carriers remain at the center, as shown in Fig. 2(a). When $2R_{ex}$ is reduced to $0.9 \mu\text{m}$ (similar situation to a current injection device with center posts), the hole burning becomes clearer. On this condition, direct pumping of the laser mode decreases, and the compensation of the hole burning by the carrier diffusion is not sufficient. In addition, the Auger recombination is enhanced at the center due to the high carrier density. In the QPC, the behavior of carriers is similar to that in the MDL, as shown in Fig. 2(b). The carrier loss by the surface recombination at holes is not so serious, compared with the hole burning. In other words, the carrier leakage to outside of the defect is blocked by the hole burning. In the PCs, the hole burning mainly occurs at the cavity center where their modes are localized, as shown in Figs. 2(c) and (d). Therefore, larger carrier leakage than in the QPC is expected. The detail of this matter will be discussed in Section V.

Fig. 3(a) shows log-log plots of lasing characteristics for $2R_{ex} = 2.1 \mu\text{m}$. The unclear kink at threshold is due to the large C factor assumed here. In the PCs and the QPC, the carrier leakage reduces the photon density of spontaneous emission below threshold. Fig. 3(b) shows the threshold power p_{th} versus $2R_{ex}$ characteristics. Each microlaser has its optimum pump diameter for threshold reduction. In the MDL, the optimum diameter is comparable to the disk diameter, because the WGM is directly excited on this condition. A low p_{th} of $30 \mu\text{W}$ is calculated for the uniformly pumped $1.77\text{-}\mu\text{m}$ -diameter MDL. This value roughly agrees to a measured value of $24 \mu\text{W}$ for the $1.7\text{-}\mu\text{m}$ -diameter MDL [4]. In the QPC and the PCs, $2R_{ex}$ larger than the modal diameter increases the useless excitation and threshold, but a too small $2R_{ex}$ also increases the threshold due to the strong hole burning and Auger recombination. As a result, optimum diameters are the same as or slightly larger than effective cavity diameters. This condition minimizes the carrier leakage, while keeping the direct pumping of the mode. For the QPC, PC-H2, and PC-H1, minimum threshold values of 48, 52, and $42 \mu\text{W}$ are calculated with optimum $2R_{ex} \sim 2.0, 1.5,$

Fig. 3. Lasing characteristics for (a) $2R_{ex} = 2.1 \mu\text{m}$ and (b) p_{th} versus $2R_{ex}$ characteristics. Cross, circle, square, and triangle denote MDL, QPC, PC-H2, and PC-H1, respectively.

and $0.8 \mu\text{m}$, respectively. Thus far, a threshold irradiated power of 0.2 mW was reported for PC-H1 with $2R_{ex} = 3 \mu\text{m}$ [13]. This value is converted to an effective threshold of $70 \mu\text{W}$ by considering a reasonable pump efficiency of 0.33 [7]. This value also roughly agrees to the calculated value of $90 \mu\text{W}$ for $2R_{ex} = 3 \mu\text{m}$, as shown in Fig. 3(b). The small difference should be caused by the different structural parameters (Q factor, material gain, etc.) and different experimental condition (intensity profile of pump light, etc.). The higher threshold values for these lasers than that for the MDL are due to the carrier leakage. However, the QPC maintains the low threshold for larger $2R_{ex}$. This means that the threshold density P_{th} in the QPC is lower than those of the PCs. It can be explained by the blocking effect of the carrier leakage. However, p_{th} in the QPC is still higher than that of the MDL. One essential factor is the Q factor, which is fixed for all lasers in this calculation. Previously, we observed in three-dimensional FDTD calculation that the QPC cavity ideally has over seven times higher Q than that of the MDL [7]. As will be shown in Section IV, such a high Q allows a p_{th} lower than that of the MDL.

IV. STRUCTURAL DEPENDENCE

In this section, we discuss the dependence of the threshold p_{th} on the surface recombination velocity v_s , diffusion constant D , and cavity Q . As a sample structure, we select QPC here. As shown in Fig. 4, smaller v_s reduces p_{th} , but this reduction is saturated due to the carrier leakage. The typical v_s for the GaInAsP system is $1.2 \times 10^4 \text{ cm/s}$, and it can be reduced to $0.7 \times 10^4 \text{ cm/s}$ by the CH_4 plasma irradiation [24]. Even if v_s is further reduced, p_{th} is not improved so significantly. Fig. 5 shows the p_{th} versus D characteristics. The dependence absolutely changes for different $2R_{ex}$. A smaller D suppresses the carrier leakage and the surface recombination, while accelerating the hole burning. Normally, the former factor is dominant. However, when $2R_{ex}$ is too small, the hole burning becomes serious and p_{th} increases for smaller D . Fig. 6 shows the p_{th} versus Q factor characteristics. For any $2R_{ex}$, p_{th} decreases with Q , but the decrease is saturated when Q is higher than 6000. It is influenced by the internal loss α_i assumed. The experimental Q factor of the MDLs is typically 3000. If $Q \sim 10000$ and $2R_{ex} = 2.1 \mu\text{m}$ (nearly equal to the defect diameter) are

Fig. 4. p_{th} versus v_s characteristics for QPC.

Fig. 5. p_{th} versus D characteristics for QPC.

realized for the QPC, p_{th} will be lower than that of the MDL. As mentioned in Section III, we can practically expect such a high Q and low threshold.

V. EFFECTIVE SURFACE RECOMBINATION VELOCITY

The threshold density P_{th} is approximately related with the average threshold carrier density $\bar{N}_{th}$ as

$$\eta \frac{P_{th}}{\hbar\omega} = B\bar{N}_{th}^2 \quad (6)$$

Fig. 6. p_{th} versus Q factor characteristics for QPC. Cross plots are for MDL.

TABLE I
SUMMARY OF EFFECTIVE CAVITY DIAMETER, THRESHOLD, EFFICIENCY,
AND EFFECTIVE SURFACE RECOMBINATION VELOCITY

	MDL	QPC	PC-H2	PC-H1
$2R_{eff}$ [μm]	1.77	1.83	1.26	0.63
p_{th1} [μW]	23	27	19	12
p_{th2} [μW]	30	48	52	42
η [%]	48	36	25	21
ξ [%]	29	20	18	20
ζ [%]	23	44	57	59
v_{eff} [cm/s]	1.2×10^4	3.2×10^4	5.1×10^4	5.3×10^4

where η is the internal quantum efficiency, which is defined as the ratio of carriers effectively contributing to the lasing. In the QPC and the PCs, η is reduced by the radiative recombination not coupled to the laser mode, Auger recombination, carrier leakage to outside of the defect, and surface recombination. Let us define ξ and ζ as ratios of carriers for the former two factors and for the latter two factors, respectively. They satisfy the relation

$$\eta + \xi + \zeta = 1. \quad (7)$$

For the QPC and the PCs, we first consider here the effective circular cavities like the MDL, which internally touch with the innermost holes. The diameter $2R_{eff}$ of the effective cavity is $1.83 \mu m$ for the QPC, $1.26 \mu m$ for the PC-H2, and $0.63 \mu m$ for the PC-H1. We first assume that effective cavities are surrounded by air with no surface recombination at the boundary ($v_s = 0$ cm/s). Then, the following relation is obtained:

$$(1 - \xi') \frac{P_{th1}}{\hbar\omega} = B\bar{N}_{th}^2 \quad (8)$$

where the prime indicates ξ without carrier leakage and surface recombination. The threshold density P_{th1} in this situation is calculated by the rate equation analysis assuming the uniform pumping ($2R_{ex} = 2R_{eff}$). As shown in Table I, the corresponding p_{th1} is roughly proportional to the cavity area πR_{eff}^2 .

Next, we assume full cavity models including outside of the defect and also assume an actual surface recombination velocity

of $v_s = 1.2 \times 10^4$ cm/s. Then, P_{th2} and corresponding p_{th2} are calculated. As shown in Table I, p_{th2} is considerably higher than p_{th1} . To explain this, we define the effective surface recombination velocity v_{eff} , which includes the total effect by the surface recombination and the carrier leakage. Then

$$\frac{P_{th2}}{\hbar\omega} = \frac{P_{th1}}{\hbar\omega} + v_{eff} \frac{2\pi R_{eff}}{\pi R_{eff}^2} \bar{N}_{th} = \frac{B\bar{N}_{th}^2}{1 - \xi'} + \frac{2v_{eff}\bar{N}_{th}}{R_{eff}}. \quad (9)$$

The second term of (9) shows the effective surface recombination. Since ζ denotes the ratio of carrier loss by the effective surface recombination, the following relation is obtained:

$$\zeta \frac{P_{th2}}{\hbar\omega} = \frac{2v_{eff}\bar{N}_{th}}{R_{eff}}. \quad (10)$$

From (9) and (10)

$$(1 - \xi')(1 - \zeta) \frac{P_{th2}}{\hbar\omega} = B\bar{N}_{th}^2. \quad (11)$$

By comparing (6) and (11), we obtain

$$\eta = (1 - \xi')(1 - \zeta) = 1 - \xi'(1 - \zeta) - \zeta. \quad (12)$$

Thus, from (7) and (12)

$$\xi = \xi'(1 - \zeta). \quad (13)$$

Table I summarizes η , ξ , ζ , and v_{eff} calculated by the above-mentioned procedure. In the MDL, η is higher than in other cavities due to the low ζ . The calculated v_{eff} is almost the same as the assumed v_s . This means that approximations of (5) and (6) are well consistent with the rate equation analysis. On the other hand, in the QPC, PC-H2, and PC-H1, η is 0.75 times, 0.52 times, and 0.44 times smaller than in the MDL, respectively, due to the carrier leakage. The relatively high value for the QPC is attributed to the low ζ arising from the above-mentioned blocking of the carrier leakage. In general, the decrease in R_{eff} increases v_{eff} . Therefore, it increases ζ more rapidly by the relation of (10). There are no significant differences of ζ between PC-H2 and PC-H1. This may be caused by assumed modal profiles for these cavities, both of which are localized at the defect center. As a result, v_{eff} is 2.7 times, 4.2 times, and 4.4 times larger than v_s in the QPC, PC-H2, and PC-H1, respectively. The relatively higher threshold p_{th2} in the QPC is simply arising from the larger defect size. If the defect size of the QPC is reduced by adjusting the lattice and hole size, p_{th2} will be lower than those of PCs. Fig. 7 shows the relation between v_{eff} , v_s and p_{th2} in the MDL and the QPC. In the MDL, v_{eff} always equals to v_s . On the other hand, in the QPC, a large difference is observed between v_{eff} and v_s . When v_s is very large, most of carriers are lost only at innermost holes around the defect by the surface recombination. Therefore, the carrier leakage cannot be a dominant factor, and the QPC and the PCs behave like MDLs. When v_s is sufficiently small, the surface recombination at innermost holes decreases, and the carrier leakage expands the difference between v_{eff} and v_s .

Fig. 7. Relation among v_{eff} , v_s , and $p_{\text{th}2}$. (a) MDL. (b) QPC.

VI. CONCLUSION

We performed the 2-D laser rate equation analysis, which was combined with the FDTD mode analysis, and observed the behavior of carriers and photons in photonic microlasers. Since the surface recombination and the carrier diffusion are precisely taken into account, distribution of the gain and absorption and the special hole burning can be quantitatively evaluated. Moreover, these results are obtained in time domain. Therefore, this method is applicable to the dynamic calculation of laser characteristics [14]. In the calculated results, the MDL having no carrier leakage to the outer space showed the lowest threshold. Compared with PCs, the QPC showed a relatively low threshold density and a high efficiency due to the blocking of the carrier leakage by the WGM. To achieve a lower threshold and higher efficiency in PCs and the QPC, suppression of the carrier leakage by separating the defect area from the PC or QPC area will be an important issue.

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