Impact of quantum dots on III-nitride lasers: a theoretical calculation of threshold current densities

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We present a theoretical study on the gain and threshold current density of III-nitride quantum dot (QD) and quantum well (QW) lasers with a comprehensive theory model. It is found that at transparency condition the injection current density of QD lasers is about 120 times lower than QW lasers in III-nitrides, while in III-arsenide it is about 15 times. It means that using QDs in III-nitride lasers could be 8 times more efficient than in III-arsenide. This significant improvement in III-nitrides is due to their large effective-masses and the large asymmetry of effective-masses between valence bands and conduction bands. Our results reveal the advantages of using QD for low threshold laser applications in III-nitrides.

1. Introduction

III-nitride semiconductor lasers have a broad range of applications, such as optical communications, high-brightness white lighting and material processing. However, the threshold current densities ($J_{th}$) of III-nitrides lasers are usually quite high. For example, InGaN quantum well (QW) lasers have typical $J_{th}$ of values of 1–4 kA cm$^{-2}$, or even higher. Indeed, the imperfections in crystal growth and electrode fabrication could play important roles in the large $J_{th}$ values, whereas other factors in III-nitrides should also be taken into accounts, i.e., the large effective-masses of carriers ($m^*_{vc}$ in conduction bands and $m^*_{val}$ in valence bands) and their large asymmetry ($m^*_{vc}/m^*_{val} > 1$).

As known, under parabolic approximation assumptions for band structures, the density of states ($\rho(E)$) in three dimensional (3D) bulks ($\rho_{3D} \propto m^{3/2}$) and two dimensional (2D) QWs ($\rho_{2D} \propto m^*$) increase with effective-masses of carriers. Large densities of states result in a slow increasing of quasi Fermi levels, and thus higher threshold of injected carriers for lasing. Most importantly, in semiconductors that have a large asymmetry of effective-masses ($m^*_{vc}/m^*_{val}$), normally the quasi Fermi level of holes ($E_F$) is above the top of valence band, so the quasi Fermi level of electrons ($E_F$) has to rise above the bottom of conduction band to satisfy Bernard-Duraffourg condition ($E_{cm} - E_{ci} > E_F$). Consequently, semiconductors with a large $m^*_{vc}/m^*_{val}$ value would need a higher injection carrier density $N_i$ to reach transparency condition (with the gain $g = 0$) and would require a higher injection threshold to reach lasing conditions than the ones with symmetric effective-masses ($m^*_{vc}/m^*_{val} = 1$).

There are mainly two ways to overcome the effective-mass asymmetry in order to realize lasers with low threshold currents. One is to relax the effective-mass asymmetry, usually by decreasing $m^*_{val}$ in valence bands via strain-induced band-mixing effects. The other way is to change the dimensionality of active layers, such as using 2D QWs or 1D quantum wires. Nevertheless, even in the 1D and 2D structures with strain engineering, the $m^*_{vc}/m^*_{val}$ effects still exist, through the effective-mass-related density of states. Whereas, zero-dimensional quantum dots (QDs) are expected to terminate the effect of $m^*_{vc}/m^*_{val}$ with a $\delta$-function-like density of states that has no direct relation with effective-masses, and thus lasers made with QDs can exhibit extremely low lasing thresholds. Therefore, given the large effective-masses and their large asymmetry of $m^*_{vc}/m^*_{val}$ in III-nitrides, applying QDs to low threshold lasing applications should be more important and more advantageous than in other material systems, such as in III-arsenide, which has relatively smaller effective-masses and smaller asymmetry of $m^*_{vc}/m^*_{val}$ (much closer to 1).

In this work, we perform detailed theoretical calculations on the modal gain and threshold current densities of ridge-type InGaAs QD and QW lasers with a comprehensive theory model, which includes the strain and polarization fields in active layers, k·p method for band structures, the non-uniform optical-mode distribution in laser structures and inhomogeneities of carrier distributions. We find that at transparency conditions, the required current density for lasing in QD lasers is 118 times smaller than in QW lasers. In addition, the threshold current densities of InGaAs lasers are also calculated and the improvement of InGaAs QD lasers over InGaAs QW lasers is only 15 times at transparency condition. The different improvement of using QDs over QWs between InGaN and InGaAs lasers is expected to be due to the different effective-masses and different $m^*_{vc}/m^*_{val}$ values. These results show that III-nitride QDs could be more advantageous than III-arsenide QDs for low threshold laser applications.

2. Calculation models

The In$_x$Ga$_{1-x}$N QDs are formed on a 0.5 nm thick wetting layer with a density $N_{QD} = 5 \times 10^{10}$ cm$^{-2}$ and are surrounded by In$_x$Ga$_{1-x}$N barriers. The indium composition $x$ and $y$ are set to be 0.2 and 0.02, respectively. The QDs have truncated hexagonal pyramid shape, with top width $a = 3$ nm, basal width $b = 6$ nm and height $h = 2$ nm [see Fig. 1(a)]. In order to compare the InGaN QD lasers with InGaN QW lasers, In$_x$Ga$_{1-x}$N/In$_x$Ga$_{1-x}$N QWs with a well thickness $L_{QW} = 1.6$ nm are employed. Here the specific $L_{QW}$ value is chosen to have the same ground-state transition energy as QDs.
Laser structures are assumed to be grown on c-plane GaN templates, with a 300 nm thick waveguiding layer sandwiched between two AlGaN cladding layers. The lower cladding layer is 600 nm thick and the upper one is 500 nm thick. Then a 200 nm thick GaN layer is capped at the top and a 2 μm-wide ridge is formed by etching down to the bottom of the top cladding layer [see Fig. 1(b)]. In the waveguiding layer [Fig. 1(c)], there are 20 periods of active layers (QD or QW layers, the period length is set as 7 nm), followed by a 20 nm thick AlGaN stop layer. The optical-mode distribution $|E(x, z)|^2$ of transverse electrical field $E(x, z)$ over the laser cross-section is obtained by solving Maxwell’s equations, as shown in Fig. 1(b). The optical confinement factor of the $i$th active layer is calculated by

$$\Gamma_{iQD} = \frac{\int dx \int_{z_i}^{z_i+h_{QD}} dz |E|^2 N_{2D_{QD}} V_{QD}}{\int dx dz |E|^2 h_{QD}},$$

for QD lasers, and

$$\Gamma_{iQW} = \frac{\int dx \int_{z_i}^{z_i+L_{QW}} dz |E|^2}{\int dx dz |E|^2},$$

for QW lasers, where $V_{QD}$ and $h_{QD}$ are the QD’s volume and height, respectively. Note that $y$-axis is along the ridge direction and $z$-axis is along sample’s growth direction.

Figure 1(d) presents the calculated optical confinement factor ($\Gamma$) of each active layer, from which we can see that the optical confinement factors show a strong non-uniformity for active layers at different positions: the most-outside layers have $\Gamma$ values of only about a half of the central layer. Thus, in order to have a meaningful analysis of lasers with multi active layers, the non-uniformity of optical confinement factors in the waveguiding layer has to be taken into accounts.

3. Calculation methods

The strain distribution of QDs is obtained by minimizing the elastic strain energy.$^{24}$ For the band structures and wavefunctions of both QDs and QWs, an effective-mass Hamiltonian based on single band envelope approximation is applied for electrons and a $6 \times 6$ Hamiltonian matrix derived from k-p theory is applied for holes.$^{25,26}$ The material gains of a single QD-layer and QW-layer are calculated respectively by

$$g_{QD}(\hbar \omega) = \frac{C_0}{V_{QD}} \sum_{n,m,u} \int dE \left| \vec{e} \cdot \mathbf{P}_{nm}^0 \right|^2 \times \left[ f(E_{cm}^u) - f(E_{vn} - E_{ct}) \right] - D_n(E - (E_{cm}^v - E_{vn})) L_\gamma(E - \hbar \omega),$$

and

$$g_{QW}(\hbar \omega) = \frac{C_0}{L_{QW}} \sum_{m,n} \int k_x dE_n \left| \vec{e} \cdot \mathbf{P}_{nm}^0 \right|^2 \times \left[ f(E_{cm}^u(k_x, k_z)) - f(E_{vn}(k_x, k_z) - E_{cn}(k_x, k_z)) \right] L_\gamma(E - \hbar \omega),$$

where $C_0 = \frac{\pi \hbar^2}{\eta e^2 \varepsilon \gamma m_{QD}}$, index $\eta$ denotes spin-up and spin-down states of electrons in conduction bands, index $m$ denotes sub-bands in conduction bands, index $n$ denotes sub-bands in valence bands, $E_{cm}^u$ is the energy level of the $m$th sub-band in conduction bands, $E_{vn}$ is the energy level of the $n$th sub-band in valence bands, $\left| \vec{e} \cdot \mathbf{P}_{nm}^0 \right|^2$ is the momentum matrix element, $f$ is the Fermi–Dirac distribution function defined as

$$f(E - E_f) = \frac{1}{1 + \exp \left( \frac{E - E_f}{k_B T} \right)},$$

the lineshape function $L_{\gamma}$ is defined as

$$L_{\gamma}(E - \hbar \omega) = \frac{\gamma / \pi}{(E - \hbar \omega)^2 + \gamma^2}$$

to account for the homogeneous broadening, and

$$D_n(E - E') = \frac{1}{\sqrt{2 \pi \sigma^2}} \exp \left[ - \frac{(E - E')^2}{2 \sigma^2} \right]$$

to account for the inhomogeneous broadening. The inhomogeneous broadening is also included in the calculation of quasi Fermi levels $E_{cm}^u$ in conduction bands and $E_{vn}^u$ in valence bands, by using the carrier density relations...
$$n_{QD}^{3D} = 2N_{QD}^{3D} \sum_n \int dE \rho_{\alpha}(E - E_{cm}) f(E - E_{ct})$$
$$+ \frac{m^*_n \hbar^2}{\pi \hbar^2} \ln \left(1 + \exp \left( \frac{E_{ct} - E_{wly}}{k_B T} \right) \right), \quad (8)$$
$$p_{QD}^{3D} = N_{QD}^{3D} \sum_n \int dE \rho_{\alpha}(E - E_{vn}) [1 - f(E - E_{ct})]$$
$$+ \frac{m^*_n \hbar^2}{\pi \hbar^2} \ln \left(1 + \exp \left( \frac{E_{wly} - E_{vn}}{k_B T} \right) \right), \quad (9)$$

for QD lasers, and

$$n_{QW}^{3D} = 2N_{QW}^{3D} \sum_n \int dE \rho_{\alpha}(E - E_{cm}(k_x, k_y))$$
$$\times f(E_{cm}(k_x, k_y) - E_{ct}), \quad (10)$$
$$p_{QW}^{3D} = \sum_n \int dE \rho_{\alpha}(E - E_{vn}(k_x, k_y))$$
$$\times [1 - f(E_{vn}(k_x, k_y) - E_{ct}), \quad (11)$$

for QW lasers, where \(m^*_n\) (\(m^*_h\)) is the effective-mass of electrons (holes), \(E_{wly}\) (\(E_{wly}^h\)) is the ground-state energy of electrons (holes) in the 0.5 nm thick wetting layer and \(n^2_{3D}\) is the surface density of electrons (holes) per active layer. The factor “2” in Eqs. (8) and (10) accounts for two different spin states in conduction bands, since the single band envelope approximation is applied to electrons. The factor “2” disappears in Eqs. (9) and (11) because two spin states have already been considered in the 6 × 6 Hamiltonian for valence bands. The radiative current density is calculated with

$$J_{rad} = eL_{eff} \int r^{spop}(\omega) d\omega,$$  
(12)

where \(L_{eff}\) is the effective thickness of active layers (\(L_{eff} = L_{QW}\) for QW lasers and \(L_{eff} = N_{QD}^{3D} L_{QD}\) for QD layers) and \(r^{spop}\) is the spontaneous emission rate per unit volume per unit energy interval (s⁻¹ cm⁻³ eV⁻¹). with

$$r^{spop}_{QD}(\omega) = \frac{n^2_{3D} \omega^3}{\pi^2 \hbar^2} \frac{C_0}{L_{QD}^{2D}} \sum_{n,m} \int dE |\hat{e} \cdot \vec{P}_{nm}|^2$$
$$\times f(E_{cm}^n - E_{ct})[1 - f(E_{vn} - E_{ct})]$$
$$\times D_{\gamma}(E - (E_{cm}^n - E_{vn}))L_{\gamma}(E - h\omega), \quad (13)$$

for QD lasers, and

$$r^{spop}_{QW}(\omega) = \frac{n^2_{3D} \omega^3}{\pi^2 \hbar^2} \frac{C_0}{L_{QW}^{2D}} \sum_{n,m} \int dE |\hat{e} \cdot \vec{P}_{nm}|^2$$
$$\times f(E_{cm}^n - E_{ct})$$
$$\times [1 - f(E_{vn}(k_x, k_y) - E_{ct})]$$
$$\times \int dE \rho_{\alpha}(E - (E_{cm}^n - E_{vn}(k_x, k_y)) - E_{vn}(k_x, k_y))$$
$$L_{\gamma}(E - h\omega), \quad (14)$$

for QW lasers.

In calculations, we use the material parameters recommended by Ref. 29 and we set \(T = 300\) K. The homogeneous broadening parameter \(\gamma\) is set as 5 meV, corresponding to a dephasing time of about 0.1 ps. 30 For the inhomogeneous broadening parameters, we assume \(\sigma_c = 10\) meV, \(\sigma_v = 2.5\) meV, and thus \(\sigma = \sqrt{\sigma_c^2 + \sigma_v^2} = 10.31\) meV, which corresponds to a full-width-at-half-maximum value of 24.2 meV (2√2 ln 2 \(\sigma_c\)), just in between the values used in Refs. 28 and 31. The same broadening parameters are used in both QD lasers and QW lasers for simplicity.

4. Results and discussion

Figures 2(a) and 2(b), respectively, show the modal gain spectra (\(\Gamma g\)) of QD and QW lasers with a single active layer under varying injection levels, where the single active layer is assumed to be located at the center of the waveguiding layer and the optical confinement factors take the highest values that are shown in Fig. 1(d). Since we purposely have set the QW thickness \(L_{QW} = 1.6\) nm to match with the ground-state transition energy of QDs, the gain peaks of QDs and QWs are located at the same energy range. One big difference between the gain spectra of QDs and QWs is that the peak modal gain of QDs is much lower than QWs [see Fig. 2(c)], because of the limited volume of the active-region in QD lasers. Another difference is that QW lasers require a much higher injection level to have a positive gain, which is due to the much larger density of states of QWs than QDs. The large effective-masses of carriers and large effective-mass asymmetry in...
III-nitride require even higher carrier injection density to have $\Gamma g > 0$ in InGaN QW lasers.

Figure 3 shows the dependence of peak modal gains on radiative current densities for multi-active-layer lasers. The peak modal gains are taken from the maximum gain point in the gain spectra shown in Fig. 2. From Fig. 3 we see that the transparency current density (when peak modal gain in QD lasers ($J_{\text{th}}^{\text{QD}} = 1.8 \text{ A cm}^{-2}$) is 118 times lower than that in QW lasers ($J_{\text{th}}^{\text{QW}} = 212 \text{ A cm}^{-2}$) for the single-active-layer case.

Based on results shown in Fig. 3, the lasing threshold current densities $J_{\text{th}}$ at different loss levels ($\Gamma g_{\text{th}}$) are calculated and shown in Fig. 4(a), with red closed-circles for InGaN QD lasers ($J_{\text{th}}^{\text{QD}}$) and red open circles for InGaN QW lasers ($J_{\text{th}}^{\text{QW}}$). Here the numbers of active layers have been optimized to obtain the lowest $J_{\text{th}}$ values. It can be seen that, within the studied loss levels (i.e., $\Gamma g_{\text{th}} < 20 \text{ cm}^{-1}$), lasers with InGaN QDs could give much lower threshold values than that with InGaN QWs. The improvement factor that is defined as $J_{\text{th}}^{\text{QW}} / J_{\text{th}}^{\text{QD}}$ is shown in Fig. 4(b) as red open circles, from which we can see that $J_{\text{th}}^{\text{QD}}$ is more than 100 times lower as compared with $J_{\text{th}}^{\text{QW}}$ at transparency condition. Even at a loss level of 20 cm$^{-1}$, $J_{\text{th}}^{\text{QD}}$ is still several times lower than $J_{\text{th}}^{\text{QW}}$.

As mentioned above, besides the effect of the lower dimensionality of QDs that results in a smaller active-region volume than QW lasers, another reason for the large improvement on $J_{\text{th}}$ of QD lasers over QW lasers in III-nitrides would be the large effective-masses and the large asymmetry between $m_{v}^*$ and $m_{c}^*$. In order to have a direct comparison with material systems that have relatively smaller effective-masses and smaller $m_{v}^*/m_{c}^*$, we perform similar calculations for III-arsenide lasers.

The III-arsenide laser structures are assumed to be grown on (001) GaAs templates. Being grown on a 0.5 nm thick wetting layer, In$_{0.2}$Ga$_{0.8}$As QDs have a truncated pyramid shape, with a top width of 6 nm, a basal width of 12 nm, a height of 2 nm and a density of $5.0 \times 10^{10} \text{ cm}^{-2}$ (the same as above InGaN QDs). These In$_{0.2}$Ga$_{0.8}$As QDs are capped with In$_{0.02}$Ga$_{0.98}$As barriers. The thickness of the corresponding In$_{0.2}$Ga$_{0.8}$As/In$_{0.02}$Ga$_{0.98}$As QWs is set as 2.8 nm to have the same ground-state transition energy (1.35 eV) as In$_{0.2}$Ga$_{0.8}$As QDs. A 2-μm-wide ridge structure is used with a 360 nm thick waveguiding layer, in which 10 periods of active layers are embedded with a period length of 30 nm.

The calculated threshold current densities of InGaAs lasers are also shown in Fig. 4(a) as blue circles. It is seen that the $J_{\text{th}}$ of InGaAs QW lasers [blue open circles in Fig. 4(a)] is about 2 times lower than InGaN QW lasers [red open circles in Fig. 4(a)] for a fixed loss level, which is due to the smaller effective-masses and smaller effective-mass asymmetry ($m_{v}^*/m_{c}^*$) in III-arsenide compared with those in III-nitrides, i.e., ($m_{v}^*/m_{c}^*$)$_{\text{III-arsenide}} < (m_{v}^*/m_{c}^*)_{\text{III-nitride}}$. However, the $J_{\text{th}}$ of QD lasers in InGaN and InGaAs looks quite similar to each other, as the influence of different effective-masses has been suppressed or eliminated by the strong quantum confinement in QDs. As a result, the threshold improvement $J_{\text{th}}^{\text{QW}} / J_{\text{th}}^{\text{QD}}$ from QW lasers to QD lasers in III-nitrides is larger than in III-arsenide, as shown in Fig. 4(b). For example, at transparency conditions, the improvement with InGaN is 118 times while it is only 15 times with InGaAs, which means using InGaN QDs could be 8 times more efficient than InGaAs QDs [Fig. 4(c)]. Furthermore, the reduced injection carrier density within InGaN QD lasers will in turn suppress carrier leakages and other non-radiative recombinations such as Auger recombination. These results reveal that using QDs in III-nitride lasers for low threshold applications is more advantageous than in other material systems.
5. Conclusions

In summary, we theoretically investigated the threshold current densities of III-nitride lasers with QDs and QWs in a comprehensive theoretical picture. It was found that using QDs instead of QWs for III-nitride lasers could give a large improvement on threshold current densities. At transparency condition, the improvement in III-nitride lasers could be 118 times, which, however, is only 15 times with III-arsenide. This is mainly due to the large effective-masses of carriers ($m^*_e$ and $m^*_h$) and the large asymmetry between the effective-masses in valence bands and conduction bands ($m^*_e/m^*_h$) in III-nitrides. Our results emphasize the importance of using QDs in III-nitride for low threshold laser applications, which could be 8 times more efficient than in III-arsenide.

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