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Shyh-Jer Huang and Shun-Tung Yen

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Shyh-Jer Huang and Shun-Tung Yen

Department of Electronics Engineering, National Chiao Tung University, Hsinchu, Taiwan 30050, Republic of China

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The optical properties of modulation-doped InGaN/GaN laser diodes are theoretically studied with the effects of electron spillover from quantum wells considered. We use a six-band model including the strain effect for calculating valence band states. The continuous subbands are treated by a dense discretization for the electrons spilling from the quantum wells. The calculation results show that the threshold current can be significantly reduced by p-type modulation doping around the wells but not by n-type doping, supposed that the layers are of a perfect quality and the impurity-induced defects are ignored. Also, the p-type modulation doping can make the threshold current more insensitive to the cavity loss compared with other cases. An optimized threshold current density can be achieved for single-quantum-well lasers by introducing p-type dopants. However, the dopant concentration is high and may be inaccessible. For double-quantum-well lasers an optimized low threshold current can be achieved with a slightly and practicable p-type doping level.

I. INTRODUCTION

In the last decades, the material preparation and device processing technologies in the nitride-based blue light source have made great progress.1–3 The short-wavelength light-emitting diodes and laser diodes (LDs) have recently been made up commercially by GaN and the related ternary (AlGaN and InGaN) and quaternary (AlGaInN) compounds due to their potential applications in full-color displays and high-density optical storage. However, the reliability is still a critical issue for the wide-gap nitride LDs because of the short lifetime resulting from the high threshold current. In order to reduce the threshold current, further improvements in material preparation and device processing technologies are still required to eliminate the undesired defects in the active region. In addition, the optimization on the LD structure is also required to diminish the leakage current resulting from the spillover of carriers, including the electron leakage from the active region to the p-type cladding layer, and the loss of high-energy electrons due to interband recombinations. The high-energy electrons generally occupy the continuous subband states and therefore give only a small contribution to the optical peak gain.

It has been found in recent works that inserting an AlGaN electron blocking layer (EBL) between the active region and the p-type cladding layer can reduce the electron leakage from the active region.4–7 Besides, more efforts can be made for further reducing the threshold current. For example, one can introduce dopants into the active region. Actually, n-type doping with Si in the InGaN/GaN quantum wells (QWs) has been performed in some experimental works.8–10 It is found that the Si doping can improve the crystalline quality of GaN layers and the InGaN/GaN interface.11 It is well known that the optimized temperature for the high crystalline quality of InGaN wells is lower than that suitable for the growth of GaN barriers. In order to get high quality of InGaN wells the GaN layers are generally compelled to be grown at low temperature. Hence, this forms the island-like spiral defects initiated by threading dislocations existing in the underlying GaN template. Fortunately, workers found that introducing Si impurities can dramatically suppress these island-like spiral structures of GaN layers. However, the n-type doping causes a large amount of electrons occupying high-energy states at threshold and leads to serious spillover of electrons. A high barrier of EBL is then needed to prevent the energetic electrons from leaking into the p-type cladding layer, but this gives rise to a reduction in optical confinement within the active region. From this point of view, the p-type doping should be a better choice than the n-type doping because it can reduce the number of spillover electrons at threshold. However, there are few experimental or theoretical works concerning the optical property of the p-type doped active region in InGaN/GaN QW LDs. In order to further improve the performance of the InGaN/GaN QW LDs, it is worthwhile to investigate the influence of p-type doping on the optical property of the active region.

In this paper, we investigate theoretically in detail the influence of different species (the n type and p type) and various levels of doping to the active region on the spontaneous emission rate and the threshold current density of InGaN/GaN LDs. Our results demonstrate that the amount of spillover electrons at threshold can indeed strongly depend on the species and the level of doping. Accordingly, we can obtain a low threshold current by optimizing the doping level with a preferred doping species. The paper is organized as follows. The calculation method is described briefly in the next section. Then, the results and discussions follow. Finally, the conclusion is drawn.

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4Electronic mail: styen@mail.nctu.edu.tw
of four components associated with the four kinds of optical transitions mentioned above; that is, $g = g_{bb} + g_{bc} + g_{cc} + g_{cb}$, $r_{sp} = r_{sp,bb} + r_{sp,bc} + r_{sp,cc} + r_{sp,cb}$, and $J = J_{bb} + J_{bc} + J_{cc} + J_{cb}$, where the subscripts indicate the kinds of optical transitions.

In most theoretical studies of QW lasers, the continuous subbands are generally neglected. However, it has been demonstrated in the studies of 630 nm band GaInP/AI Ga InP lasers \textsuperscript{15,17} and our previous work \textsuperscript{14} that the optical transitions involving spillover electrons play an important part in the threshold current. In this study the main interest is focused on the spillover effect on the laser threshold. So, we ignore the electron leakage to the $p$-type cladding and any indirect interband transitions.

The valence band structure is calculated based on the six-band $k \cdot p$ model which includes the coupling of the heavy-hole, the light-hole, and the spin-orbit split-off bands. \textsuperscript{18,19} The strain effect is also included. The formulas for calculating the valence bands can be found in our previous work. \textsuperscript{14} For conduction band states, we use the single-band effective-mass equation,

\begin{equation}
\frac{d}{dz} \left[ \frac{\hbar^2}{2m_e(z)} \frac{d}{dz} \phi(z) \right] = E \phi(z),
\end{equation}

\begin{equation}
V_{eff}(z) = \frac{\hbar^2 k_t^2}{2m_e(z)} + E_v(z) + P_{ex}(z),
\end{equation}

to solve the envelope functions $\phi$ and the energy $E$, where $m_e$ is the electron effective mass in the direction along (transverse to) the growth direction, $E_v(z)$ is the $z$-dependent conduction band edge of the undeformed materials composing the heterostructure, and $P_{ex}$ is the hydrostatic energy shift in the conduction band. Once the energy states of both the valence and the conduction subbands have been solved, the momentum matrix elements can be obtained using the formulas in Refs. 14 and 20.

The dopants are assumed to be introduced into the barriers around the QW. For convenience, we also assume that the carriers released from the dopants are all relaxed to the well region. The charge neutrality in the active region then allows us to write

\begin{equation}
p_s + N_{D,s} = n_s + N_{A,s},
\end{equation}

where $p_s$, $n_s$, $N_{D,s}$, and $N_{A,s}$ are the sheet concentrations of holes, electrons, ionized donors, and ionized acceptors, respectively. Here we use the sheet concentrations instead of the volume concentrations to avoid the complexity arising from the penetration of the bound wave functions into the barriers. For a given ionized acceptor (or donor) concentration, one can obtain the quasi-Fermi levels of the conduction bands $F_v$ and the valence bands $F_h$ as functions of the carrier concentrations. Consequently, the Fermi-Dirac distributions of carriers in energy can be determined. One can then further obtain the gain spectrum, the spontaneous emission spectrum, and the current density due to radiative recombinations. The related formulas can be found from our previous work. \textsuperscript{14}
thus take the valence band partition ratio values for the band offset of the nitride heterointerfaces. We assume the well is an important factor that influences the spillover of the emission rate at threshold. The EBL is an Al_{0.2}Ga_{0.8}N layer. The widths of various doping levels for 3.6 nm In_{0.2}Ga_{0.8}N/GaN single-QW LDs with the Fermi level for single-QW structures with various doping levels, as assumed in Ref. 21 for wurtzite GaN, InN, and AlN. For the ternary compounds InGaN and AlGaN, the parameters are obtained by the linear interpolation between the binary compounds, except those already given in Ref. 21. The depth of the well is an important factor that influences the spillover of carriers, but until now there have been no unambiguous values for the band offset of the nitride heterointerfaces. We thus take the valence band partition ratio $Q_v$ as a variable parameter, where $\Delta E_v = Q_v \Delta E_d$ ($\Delta E_d$ and $\Delta E_g$ being the valence band offset and the band gap difference, respectively). The confinement factor for the lasers is assumed to be $3 \times 10^{-3} \Phi_w$, where $\Phi_w$ is the active region width in units of nanometers. The total loss of the cavity $\alpha$ and the temperature $T$ are set at 60 cm$^{-1}$ and 300 K, respectively, except in the case where they are considered as variable parameters.

Figure 2 shows the spectra of the total spontaneous emission rate $r_{sp}$ and one of its components, $r_{sp,cb}$, at threshold for single-QW structures with various doping levels, assuming $Q_v = 0.33$ in panel (a) and $Q_v = 0.45$ in panel (b). The $N_{d,sp}$ and $N_{a,sp}$ are the sheet concentrations of ionized donors and acceptors, respectively.

### III. RESULTS AND DISCUSSION

In this section we present and discuss the calculated results of the spontaneous emission spectra and the current densities for modulation-doped In_{0.2}Ga_{0.8}N/GaN single-QW LDs at threshold. The EBL is an Al_{0.2}Ga_{0.8}N layer. The widths of the QW and the EBL are fixed at 3.6 and 20 nm, respectively, for all structures. For the double-QW structure, a 6 nm GaN barrier is inserted between the wells. All the values of material parameters used in our calculation can be found from Ref. 21 for wurtzite GaN, InN, and AlN. For the ternary compounds InGaN and AlGaN, the parameters are obtained by the linear interpolation between the binary compounds, except those already given in Ref. 21. The depth of the well is an important factor that influences the spillover of carriers, but until now there have been no unambiguous values for the band offset of the nitride heterointerfaces. We thus take the valence band partition ratio $Q_v$ as a variable parameter, where $\Delta E_v = Q_v \Delta E_d$ ($\Delta E_d$ and $\Delta E_g$ being the valence band offset and the band gap difference, respectively). The confinement factor for the lasers is assumed to be $3 \times 10^{-3} \Phi_w$, where $\Phi_w$ is the active region width in units of nanometers. The total loss of the cavity $\alpha$ and the temperature $T$ are set at 60 cm$^{-1}$ and 300 K, respectively, except in the case where they are considered as variable parameters.

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Figure 3 shows the spectra of the total spontaneous emission rate $r_{sp}$ and one of its components, $r_{sp,cb}$, at threshold for single-QW structures with various doping levels, assuming $Q_v = 0.33$ in panel (a) and $Q_v = 0.45$ in panel (b). The $N_{d,sp}$ and $N_{a,sp}$ are the sheet concentrations of ionized donors and acceptors, respectively.

It is noticed that the LDs with $p$-type doping have smaller $r_{sp,cb}$ at threshold than the undoped one, while the one with $n$-type doping has a larger $r_{sp,cb}$. This gives rise to the narrowing of $r_{sp}$ for $p$-type doping and the broadening of $r_{sp}$ for $n$-type doping, as shown in Figs. 2(a) and 2(b). As expected, the $p$-type doping alleviates the electron spillover while the $n$-type doping worsens it. To further understand the dependence of electron spillover on the doping level and species, we appeal to the diagram in Fig. 3, where there are schematically the conduction and valence bands together with the Fermi level $F_c$ and the quasi-Fermi levels $F_e$ and $F_v$ at threshold. The levels $F_c$, $F_e$, and $F_v$ lie at upper positions for $n$-type doping than for the undoped, while for $p$-type doping the levels lie at lower positions, as illustrated in Fig. 3. Furthermore, because of the large asymmetry in density of states between the conduction and valence bands, the quasi-Fermi level $F_v$ is much more sensitive to the doping level than $F_c$. For $n$-type doping, the high position of $F_c$ implies serious electron spillover at threshold which causes the broadening of $r_{sp}$, as has been shown in Fig. 2. On the contrary, the $p$-type doping has a lower $F_c$ and hence can diminish the electron spillover. This can also reduce the thermionic emission current leaking across the EBL. Besides, it is difficult for the $p$-type doping to cause the hole spillover because of the large density of states of the valence bands. As the spillover becomes negligibly small, further increasing the $p$-type doping level will not be a benefit, but causes an increase in the spontaneous emission rate at threshold. This is reflected by the increase of $r_{sp}$ at energy about the main peak with the $p$-type doping level, as shown in Fig. 2.
Figure 4 shows the current densities $J$, $J_{bb}$, and $J_0$ at threshold versus the ionized dopant concentration for single-QW structures, similarly assuming the partition ratio $Q_v=0.33$ in panel (a) and $Q_v=0.45$ in panel (b). The $J$ is the total threshold current density, the $J_{bb}$ is the current density due to the bound-to-bound process, and the $J_0$ is the threshold current density calculated without considering the carrier spillover.

It is noticed that the current density $J_0$ behaves quite differently from $J$ for $Q_v=0.45$, implying that it is important to consider the electron spillover in calculation of the threshold current for a shallow QW. Peculiarly, the $J_{bb}$ and $J_0$ decrease with the $n$-type doping level but increase with the $n$-type doping level. As the $p$-type doping level is very high (about $1.5 \times 10^{13}$ cm$^{-2}$ for $Q_v=0.33$ and about $2 \times 10^{13}$ cm$^{-2}$ for $Q_v=0.45$), the benefit from the $p$-type doping vanishes and the current density $J$ seems to approach an asymptotic value. In practice, such high $p$-type doping is difficult to achieve in the nitride compounds due to the large activation energy of acceptors.

Figure 5 shows the threshold current density $J$ as a function of the cavity loss $\alpha$ of single-QW LDs with different doping levels for (a) $Q_v=0.33$ and (b) $Q_v=0.45$. As expected, the $J$ increases with $\alpha$. The increase is particularly obvious for the case of $n$-type doping (as well as for the case of the undoped). Moreover, most of the curves are somewhat superlinear because the electron spillover plays a more and more important role with $\alpha$ increasing in the interband process.

Until now the calculated results have been for LDs with a cavity loss of 60 cm$^{-1}$. For a higher cavity loss, it requires a higher carrier density in the QW to reach threshold. In this case, the problem of electron spillover becomes more important. Figure 5 shows the threshold current density $J$ versus the cavity loss $\alpha$ for 3.6 nm In$_{0.2}$Ga$_{0.8}$N/GaN single-QW LDs with various doping levels for $Q_v=0.33$ in panel (a) and $Q_v=0.45$ in panel (b).
not negligible for the shallow well. This reflects the fact that with the p-type doping \( N_{d,s} = 2 \times 10^{13} \text{ cm}^{-2} \), the \( J-\alpha \) curve is almost linear for \( Q_v = 0.33 \) but obviously nonlinear for \( Q_v = 0.45 \).

The temperature characteristic is also an important issue for lasers. We plot the threshold current density \( J \) versus temperature \( T \) with various doping levels for single-QW LDs in Fig. 6, assuming \( Q_v = 0.33 \) in panel (a) and \( Q_v = 0.45 \) in panel (b). It can be seen that the \( J-T \) curves are linear and almost parallel to each other. It seems that introducing dopants to the active region does not significantly influence the temperature characteristic. However, the situation will not be the case if the electron leakage into the p-type cladding layer is considered. As has been pointed out, such leakage is serious for n-type doping and further deteriorates at high temperature. The p-type doping can be used to reduce the electron leakage into the p-type cladding layer as well as the electron spillover.

In Fig. 7, the current densities \( J, J_{bb} \), and \( J_0 \) at threshold of double-QW LDs are plotted as functions of the ionized dopant concentration for (a) \( Q_v = 0.33 \) and (b) \( Q_v = 0.45 \). Similar to the case in Fig. 4, the \( J_{bb} (= J - J_{bb}) \) and the amount of spillover electrons increase with the n-type doping level while decrease with the increase of p-type doping level. Compared with the case of single-QW LDs, the electron spillover is smaller for the double-QW LDs because of the smaller carrier density required for threshold. As a result, the \( J_{bb} \) has a minimum at a certain p-type doping level and increases as the p-type doping level further increases. In this situation, the drawback of increasing electron-hole recombination goes beyond the advantage of reducing electron spillover. The \( J_{bb} \) reaches the minimum at about 2.5 \( \times 10^{12} \text{ cm}^{-2} \) for \( Q_v = 0.33 \) and at about 5 \( \times 10^{12} \text{ cm}^{-2} \) for \( Q_v = 0.45 \), where the threshold current density \( J \) reaches or approaches the minimum value.

Comparing the threshold current densities in Fig. 4 and those in Fig. 7, one can see that the favorable structure for the lowest \( J \) is the single-QW one with heavily p-type doping for both \( Q_v = 0.33 \) and \( Q_v = 0.45 \). However, in reality, the high activation energy of acceptors in the wide-gap nitride compounds may make such optimization difficult to achieve. If the heavily p-type doping could not be achieved, the double-QW structure with a lower p-type dopant concentration is a good choice. The optimized p-type doping levels are about 2.5 \( \times 10^{12} \text{ cm}^{-2} \) (\( \sim 6.9 \times 10^{18} \text{ cm}^{-3} \)) for \( Q_v = 0.33 \) and about 7 \( \times 10^{12} \text{ cm}^{-2} \) (\( \sim 1.9 \times 10^{19} \text{ cm}^{-3} \)) for \( Q_v = 0.45 \). The ionization efficiency depends on the doping level and is still unclear for p-type modulation-doped InGaN/GaN QWs. From the experimental work with structures similar to those used here, a uniformly doped 4 nm In\(_{0.2}\)Ga\(_{0.8}\)N/4 nm GaN superlattice with a Mg concentration of 3 \( \times 10^{19} \text{ cm}^{-3} \) has a spatially averaged hole concentration of about 2.6 \( \times 10^{19} \text{ cm}^{-3} \). Since the main contribution of released holes is from the acceptors in the GaN barriers, the ionization efficiency of the modulation doping is about 100%. Thus, the optimized carrier concentrations mentioned above are possible to be achieved.

IV. CONCLUSION

The radiative current densities and the spontaneous emission spectra in modulation-doped InGaN/GaN QW LDs have been investigated with the electron spillover above the barriers considered. The calculated results indicate that the consideration of electron spillover is important in studying
the effects of modulation doping to the active region especially for shallow electron QW structures. When the influence of introducing impurities on crystal quality is ignored, the threshold current density can be significantly reduced by p-type doping, but increased by n-type doping which is conventionally used. The benefit from the p-type doping is particularly obvious for a large cavity loss. An optimized low threshold current can be achieved for single-QW LDs with heavily p-type doping. For double-QW LDs, more slightly p-type doping is required to obtain low threshold current.

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