Simulation and analysis of 1300-nm In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$/GaAs$_{1-x}$N$_{x}$ quantum-well lasers with various GaAs$_{1-x}$N$_{x}$ strain compensated barriers

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ABSTRACT

In this article, the laser performance of the 1300-nm In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$/GaAs$_{1-x}$N$_{x}$ quantum well lasers with various GaAs$_{1-x}$N$_{x}$ strain compensated barriers (x=0%, 0.5%, 1%, and 2%) have been numerically investigated with a laser technology integrated simulation program. The simulation results suggest that with x=0% and 0.5% can have better optical gain properties and high characteristic temperature coefficient $T_0$ values of 110 K and 94 K at the temperature range of 300-370 K. As the nitrogen composition in GaAs$_{1-x}$N$_{x}$ barrier increases more than 1% the laser performance degrades rapidly and the $T_0$ value decreases to 87 K at temperature range of 300-340 K. This can be attributed to the decrease of conduction band carrier confinement potential between In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$ QW and GaAs$_{1-x}$N$_{x}$ barrier and the increase of electronic leakage current. Finally, the temperature dependent electronic leakage current in the InGaAsN/GaAs$_{1-x}$N$_{x}$ quantum-well lasers are also investigated.

Keywords: III-V semiconductor, InGaAsN, strain compensate, numerical simulation

1. INTRODUCTION

The InGaAsN quantum-well (QW) laser diodes (LDs) on GaAs substrate have demonstrated excellent lasing characteristics for 1300 nm semiconductor lasers, which are comparable to or superior to some of the best published results based on the conventional InP technology [1−11]. High-temperature operation has been anticipated in these material systems due to better electron and hole confinement as a result of increased band offsets and a more favorable band-offset ratio. Previous research showed that for pulse operation of InGaAsN QW LDs, the characteristic temperature coefficients $T_0$ value of exceeding 200 K were demonstrated [17−19] while for continue-wave (CW) operation, the $T_0$ of 70-110 K were also obtained [20−24]. Unfortunately, these high performance InGaAsN QW LDs showed only a slight improvement in $T_0$ values over those achievable by the conventional InP technology. Fehse et al. found that the unexpected low $T_0$ value of InGaAsN lasers is attributed to the existence of large Auger recombination [25]. The difficulty of nitrogen atoms incorporating into InGaAs alloys, which leads to poor crystal quality, and the hole leakage problem [26] might be the key issues that result in the unexpected low $T_0$ value of InGaAsN lasers. In addition, there have been several works investigating the InGaAsN QW LDs with strain-compensated GaAsN as direct barriers, which however, is a smaller band gap material system. Using GaAsN barrier instead of GaAs barrier could also reduce nitrogen outdiffusion from the well and balancing the highly compressive strain in InGaAsN QW [27]. The same phenomenon had also numerically obtained by Fan et al. [28]. However, adding more nitrogen atoms into barrier may decrease barrier potential and the carrier leakage problem follows at high device temperature, even though longer wavelength emission can be obtained.

In this article, the laser performance of In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$/GaAs$_{1-x}$N$_{x}$ QW lasers with various GaAs$_{1-x}$N$_{x}$ strain compensated barrier (x=0%, 0.5%, 1%, and 2%) are numerically investigated with a laser technology integrated program (LASTIP). It is shown that, in addition to the crystal quality of InGaAsN well layer during crystal growth, the nitrogen composition of GaAs$_{1-x}$N$_{x}$ strain compensated barrier also plays an important role in the characteristic temperature coefficient $T_0$ of lasers performance. Furthermore, the phenomenon of electronic leakage current with various nitrogen composition in GaAs$_{1-x}$N$_{x}$ barrier of InGaAsN QW lasers are also numerically investigated with the LASTIP simulation program.

2. METHOD AND STRUCTURE
Based on the $k \cdot p$ theory with valence band mixing effect, a 8×8 Hamiltonian of the Luttinger-Kohn type and an envelope function approximation are used to solve the InGaAsN/GaAsN QW subband structures. The method is followed by Chuang [29]. The optical gain of InGaAsN/GaAsN QW structures is calculated using the Coulomb enhanced gain spectral function:

$$
g(h_w) = \text{real} \left\{ \sum_{E_{cv}} \frac{1}{1 - q(E_{cv}, h_w)} \left[ 1 - \frac{E_{cv} - h_w}{\Gamma_{cv}} \right] I(h_w - E_{cv}, j)dE_{cv} \right\},$$  \hspace{1cm} (1)

in which

$$
q(E_{cv}, h_w) = -\frac{i\hbar}{\pi} |M_{\beta}(E_{cv})|^2 \int_0^k \frac{dk'k'}{E_{cv}'} \frac{f_+(E_{cv}')}{\Gamma_{cv}'} \times \left( \frac{1}{\Gamma_{cv}'} + i \frac{E_{cv}'}{h_w} \right) \Theta(k, k'),$$  \hspace{1cm} (2)

$$\Theta(k, k') = \left( \frac{2\pi}{k} \right) \frac{1 + C_{\beta\alpha} q_0^\delta / 32\pi N_{2D}}{1 + q/k + C_{\beta\alpha} q_0^\delta / 32\pi N_{2D}}, \quad q^2 = k^2 + k'^2 - 2kk' \cos \theta,$$  \hspace{1cm} (3), (4)

and $\theta$ is the angle between in-plane vectors $k$ and $k'$. $g(E_{cv})$ is the spectral wave function, which consists of a sum of $g_{ji}(E_{cv})$ contributions from transitions between $j$th-subband electrons and $i$th-subband holes. $\Gamma_{cv}$ represents the Lorentzian width and equals to $h_w / \tau_{cv}$, which is simplified without considering the dependence upon $h_w$ and $E_{cv}$ energies in our calculations. $a_0$ is exciton Bohr radius given by $\frac{4\pi^2\varepsilon_0\varepsilon_r E_0}{\varepsilon_r^2 m_e}$. $E_0$ is the corresponding Rydberg energy and $E_{cv}$ is specified by $E_{cv}(k) = E_{c,k} + \Delta E_{c,k} + E_{v,k}$, where $E_{c,k}$ and $E_{v,k}$ are electron and hole energies from $j$th-subband of conduction and $i$th-subband of valence band quantum well in the active region. $|M_{\beta\alpha}|^2$ is the transition matrix element and $C_{\beta\alpha}$ is a unitless constant typically in a range 1-4.

For this specific simulation, the ratio of conduction band to valence band offset is estimated to 0.7/0.3 [31]. The bandgap energy of In$_{1-x}$Ga$_x$As$_y$N$_{1-y}$ material at room temperature (RT, 300 K) is governed by the following bilinear terms with two bowing terms:

$$E_{x}(term1) = x \cdot y \cdot E_{x,GaAs} + x \cdot (1 - y) \cdot E_{x,GaN},$$  \hspace{1cm} (5)

$$E_{x}(term2) = (1 - x) \cdot y \cdot E_{x,InAs} + (1 - x) \cdot (1 - y) \cdot E_{x,InN},$$  \hspace{1cm} (6)

$$E_{x}(bowing) = x \cdot b_{GaAsN} \cdot y \cdot (1 - y) + y \cdot b_{InGaAs} \cdot x \cdot (1 - x),$$  \hspace{1cm} (7)

where $x$ and $y$ denote the gallium and arsenide compositions in InGaAsN alloy, and the bandgap energies of GaAs, InAs, GaN and InN are 1.424, 0.355, 3.42 and 0.77 [32] eV. The bowing parameters for GaAsN and InGaAs ternary alloys are -18 [33] and -0.6 eV. The temperature dependent bandgap energy is as follows:

$$E_{x}(T) = -5.5 \times 10^{-4} \cdot \left\{ \frac{T^2}{T + 225} - \frac{300^2}{300 + 225} \right\},$$  \hspace{1cm} (8)

where $E_{x}(T)$ is the bandgap energy of InGaAsN alloy at temperature $T$. Therefore, the temperature dependent bandgap energy of InGaAsN alloy is

$$E_{x}(InGaAsN) = E_{x}(term1) + E_{x}(term2) + E_{x}(bowing) + E_{x}(T).$$  \hspace{1cm} (9)

The effective mass of electrons used in simulation is as follow:

$$m_{e}(term1) = x \cdot y \cdot m_{e,GaAs} + x \cdot (1 - y) \cdot m_{e,GaN},$$  \hspace{1cm} (10)

$$m_{e}(term2) = (1 - x) \cdot y \cdot m_{e,InAs} + (1 - x) \cdot (1 - y) \cdot m_{e,InN},$$  \hspace{1cm} (11)

$$m_{e}(InGaAsN) = m_{e}(term1) + m_{e}(term2).$$  \hspace{1cm} (12)
where the effective mass of electrons in GaAs, InAs, GaN and InN are $0.064 \times m_0$, $0.023 \times m_0$, $0.2 \times m_0$ and $0.11 \times m_0$ respectively. The effective masses of light holes (LH) and heavy-holes (HH) are governed by the same form in Eq. (6), and the effective masses of light holes and heavy holes for GaAs are $0.09 \times m_0$ and $0.377 \times m_0$ and $0.263 \times m_0$ for InAs, $0.9767 \times m_0$ and $1.3758$ for GaN, and $0.5133 \times m_0$ and $1.5948 \times m_0$ for InN respectively. The Auger coefficients for InGaAsP and InGaAsN are $3.5 \times 10^{-42}$ and $1.5 \times 10^{-41}$ m²/s. Other material-dependent parameters are also taken from the default database values given in the LASTIP material macro file [30].

A schematic diagram of the preliminary InGaAsN / GaAsN ridge LD structure under this study is shown in Fig. 1. It is assumed that the InGaAsN ridge LD structure is grown on 100-µm-thick n-type GaAs substrate with doping concentration of $5 \times 10^{18}$ cm⁻³ and a GaAs layer with thickness of 100 nm and n-doping concentration of $5 \times 10^{18}$ cm⁻³. A 150-nm-thick lower AlGaAs cladding layer of aluminum grading from 0.3 to 0 and n-doping concentration of $2 \times 10^{18}$ cm⁻³ is grown on top of the GaAs layer, followed by a 100-nm-thick GaAs optical confinement layer with n-doping concentration of $2 \times 10^{18}$ cm⁻³. The undoped active region consists of single InGaAsN QW that is sandwiched between two GaAsN barriers. On top of the active region is a p-type GaAs optical confinement layer with doping concentration of $5 \times 10^{17}$ cm⁻³, and a 150-nm-thick upper AlGaAs cladding layer of aluminum grading from 0 to 0.3 with p-doping concentration of $5 \times 10^{17}$ cm⁻³. Finally, a 100-nm-thick GaAs layer with p-doping concentration of $1 \times 10^{19}$ cm⁻³ is capped to complete the structure.

Figure 1: Schematic diagram of the preliminary InGaAsN / GaAsN ridge LD structure under study.

The n-contact is assumed to locate on bottom of the n-type GaAs bottom layer and the p-contact is located on top of the p-type GaAs capping layer. The thickness of InGaAsN QW and GaAsN barrier are 6 and 12 nm, respectively. The ridge waveguide is 4 µm in width and 500 µm in length. Two end facets are assumed to anti-reflection and high-reflection coating that provide 20% and 98% reflectivity. Background loss of 30 cm⁻¹ and thermal conductivity of 40 Wm/K for InGaAsN material are assumed in the simulation.

3. TEMPERATURE DEPENDENT OPTICAL GAIN PROPERTIES

Temperature effects on the optical gain properties of In₀.₄Ga₀.₆As₀.₉₈₆N₀.₀₁₄ and In₀.₈Ga₀.₂As₀.₆₉P₀.₃₁ QW materials are studied in the first instance. For the purpose of obtaining an emission wavelength of 1.3 µm, the nitrogen composition in InGaAsN / GaAs active region is 1.4% when the indium composition in InGaAsN QW is 0.4. Figure 2 shows the material gains of RT In₀.₄Ga₀.₆As₀.₉₈₆N₀.₀₁₄ and In₀.₈Ga₀.₂As₀.₆₉P₀.₃₁ QW materials at an input carrier concentration of $2 \times 10^{18}$ cm⁻³. The barrier materials used under this study for In₀.₄Ga₀.₆As₀.₉₈₆N₀.₀₁₄ and In₀.₈Ga₀.₂As₀.₆₉P₀.₃₁ QW materials are GaAs₁₋ₓNₓ with x=0%, 0.5%, 1%, 2% and In₀.₉Ga₀.₁As₀.₂P₀.₇₆ [34]. It is clear

![Schematic diagram of the preliminary InGaAsN / GaAsN ridge LD structure under study.](http://proceedings.spiedigitallibrary.org/ on 04/27/2014 Terms of Use: http://spiedl.org/terms)
that In_{0.4}Ga_{0.6}As_{0.986}N_{0.014}/GaAs_{1-x}N_{x} (x=0%, 0.5%, 1%, 2%) materials have higher maximum material gains than that of InGaAsP material. The highest maximum material gain is obtained when x=0%, i.e. GaAs barrier, and the maximum material gain is found to be red shift from 1.3 to 1.34 µm by increasing x value from 0% to 2% in GaAs_{1-x}N_{x} barrier. In addition, the maximum material gain decreases rapidly with increasing x value in GaAs_{1-x}N_{x} barrier as a result of the decrease of conduction band carrier confinement potential. Nevertheless, the maximum material gain of In_{0.8}Ga_{0.2}As_{0.69}P_{0.31}/In_{0.9}Ga_{0.1}As_{0.24}P_{0.76} when the input carrier concentration is 2×10^{18} cm^{-3}.

![Figure 2: Material gains of RT In_{0.4}Ga_{0.6}As_{0.986}N_{0.014} and In_{0.8}Ga_{0.2}As_{0.69}P_{0.31} QW materials at an input carrier concentration of 2×10^{18} cm^{-3}.](image1)

The maximum material gain of using GaAs_{1-x}N_{x} barriers with x=0%, 0.5%, 1% and 2% as a function of temperature are shown in Fig. 3. The maximum material gain drops almost linearly with increasing temperature. A red shift of the maximum material gain with x=0% from 1.3 to 1.35 µm and the decrease of the maximum material gain value from 2443 to 1575 cm^{-1}, which is due to the wider spreading of the Fermi distribution of carriers and stronger Auger recombination losses, are numerically obtained when the temperature increases from 300 to 370 K. Manifestly, the severe decrease of the maximum material gain value caused by the linear increase of x value indicates that increasing nitrogen composition in GaAsN barrier may procure the poor laser performance as a result of the relatively low material gain.

![Figure 3: Maximum material gain of using GaAs_{1-x}N_{x} barriers with x=0%, 0.5%, 1% and 2% as a function of temperature.](image2)
Figure 4 shows the transparency carrier concentration as a function of temperature when using GaAs$_{1-x}$N$_x$ barriers with x=0%, 0.5%, 1% and 2%. The gain increases with input carrier concentration and the RT transparency carrier concentrations of In$_{0.5}$Ga$_{0.2}$As$_{0.6}$P$_{0.4}$/GaAs$_{1-x}$N$_x$ materials are noticeably lower than that of In$_{0.5}$Ga$_{0.2}$As$_{0.6}$P$_{0.4}$/In$_{0.9}$Ga$_{0.1}$As$_{0.2}$P$_{0.7}$ material, 1.35x10$^{18}$ cm$^{-3}$. The differential gains of In$_{0.5}$Ga$_{0.2}$As$_{0.6}$P$_{0.4}$/GaAs$_{1-x}$N$_x$ materials are also higher than that of In$_{0.5}$Ga$_{0.2}$As$_{0.6}$P$_{0.4}$/In$_{0.9}$Ga$_{0.1}$As$_{0.2}$P$_{0.7}$ material due to the fact that In$_{0.5}$Ga$_{0.2}$As$_{0.6}$N$_{0.014}$/GaAs$_{1-x}$N$_x$ based material has relatively high conduction band offset and more electrons can be confined in the active layer effectively. The transparency carrier concentrations at RT of using GaAs$_{1-x}$N$_x$ barriers with x=0% and x=2% are 9.8x10$^{17}$ and 1.06x10$^{18}$ cm$^{-3}$ respectively. For x=0%, the transparency carrier concentration increases almost linearly to 1.25x10$^{18}$ cm$^{-3}$ when the temperature is 370 K. The transparency carrier concentrations of using GaAs$_{1-x}$N$_x$ barriers with x=0.5% and 1% are slightly higher than that of GaAs barrier in a temperature range of 300-370 K. However, the transparency carrier concentration increases apparently when the x value is 2% and it increases rapidly when the temperature is higher than 350 K.

From the analysis of the optical gain properties of In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$ QW sandwiched between GaAs$_{1-x}$N$_x$ barriers with variant x values, we find that using GaAs$_{1-x}$N$_x$ barriers with x value ranging from zero to 1% can have better temperature dependent optical gain properties. When the x value increases to 2%, the maximum material gain and the transparency carrier concentration abate remarkably. It indicates that In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$ QW sandwiched between GaAs$_{1-x}$N$_x$ barriers may have better laser performance, i.e. lower threshold current density and higher slope efficiency, when the x value is zero or less than 2%. Especially, using high potential GaAs barrier provides better electron confinement and results in obtaining highest material gain and lowest transparency carrier concentration. A highest $T_0$ value may also be obtained as a result of reducing the probability of electronic leakage current if the LD structure is under high temperature operation. Besides, after the consideration of using GaAsN barrier instead of GaAs barrier has several advantages in experiment and longer wavelength can easier be obtained, we find in this study that using GaAs$_{1-x}$N$_x$ barriers with x=0.5% and 1% can also provide high material gain and low transparency carrier concentration.

4. L-I CHARACTERISTIC AND ELECTRONIC LEAKAGE CURRENT

The thermal heating effects are quite important and need to be incorporated for the discussion of L-I characteristic in a LD structure. For the preliminary LD structure under study, the heat sources, which are separated into Joule heat, optical recombination heat, Thomson and Peltier heating terms, are considered in our simulation. Figure 5 shows the L-I characteristics of In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$ QW sandwiched between GaAs$_{1-x}$N$_x$ barriers with x=0%, 0.5% and 1.0% in a device temperature range of 300-370 K. The threshold current of using GaAs$_{1-x}$N$_x$ barrier with x=0% increases from 37 to 70 mA and the slope efficiency decreases from 0.302 to 0.185 W/A when the device temperature increases.

![Figure 4: Transparency carrier concentration as a function of temperature when using GaAs$_{1-x}$N$_x$ barriers with x=0%, 0.5%, 1% and 2%.

![L-I Characteristic and Electronic Leakage Current](image-url)
from 300 to 370 K. However, we find in Figs. 5(b) and 5(c) that the laser performance becomes poorer when the \( x \) value increases to 0.5\% and 1.0\%, even though the optical gain properties of \( x=0.5\% \) and \( x=1.0\% \) are only slightly worse than GaAs barrier, as mentioned in Figs. 3 and 4. For \( x=0.5\% \), the threshold current increases from 52 to 89 mA when the device temperature increases from 300 to 350 K and no lasing is observed when the device temperature is higher than 360 K. For \( x=1\% \), the population inversion is more difficult to achieve and the threshold current increases rapidly from 58 to 91 mA when the device temperature increases from 300 to 340 K. No lasing is observed when the device temperature is higher than 340 K.

![Graphs showing L-I characteristics for different values of \( x \).](image)

Figure 5: \( L-I \) characteristics of In\(_{0.4}\)Ga\(_{0.6}\)As\(_{0.986}\)N\(_{0.014}\) QW sandwiched between GaAs\(_{1-x}\)N\(_{x}\) barriers with (a) \( x=0\% \), (b) 0.5\% and (c) \( x=1.0\% \) in a device temperature range of 300-370 K.

Figure 6 depicts the threshold currents of using GaAs\(_{1-x}\)N\(_{x}\) barriers with \( x=0\% \), 0.5\% and 1.0\% as a function of the device temperature. The \( T_0 \) value of using GaAs barrier obtained in this study in a device temperature range of 300-370 K is 110 K. When using GaAs\(_{1-x}\)N\(_{x}\) barriers with \( x=0.5\% \) and 1\%, the \( T_0 \) values are 94 and 87 K.
respectively. The simulation results indicate that the laser performance becomes poorer and the $T_0$ value decreases rapidly when the $x$ value in GaAs$_{1-x}$N$_x$ barrier increases from zero to 1%. This can be due to that adding more nitrogen composition in GaAs$_{1-x}$N$_x$ barrier results in the smaller conduction band carrier confinement potential and the electronic current leakages to the p-type layers effortlessly. Therefore the laser performance decreases rapidly when the device temperature increases.

![Image of Figure 6: Threshold currents of using GaAs$_{1-x}$N$_x$ barriers with $x=0\%$, $0.5\%$ and $1.0\%$ as a function of the device temperature.](image6)

**Figure 6:** Threshold currents of using GaAs$_{1-x}$N$_x$ barriers with $x=0\%$, $0.5\%$ and $1.0\%$ as a function of the device temperature.

![Image of Figure 7: Percentage of electronic leakage current as a function of the device temperature when the In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$ QW is sandwiched between GaAs$_{1-x}$N$_x$ barriers with $x=0\%$, $0.5\%$ and $1\%$ at an input current of 300 mA.](image7)

**Figure 7:** Percentage of electronic leakage current as a function of the device temperature when the In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$ QW is sandwiched between GaAs$_{1-x}$N$_x$ barriers with $x=0\%$, $0.5\%$ and $1\%$ at an input current of 300 mA.

Specifically, more and more electrons overflow to the p-type layers and do not contribute to the stimulated emission when the $x$ value in GaAs$_{1-x}$N$_x$ barriers increases. Using GaAs barrier provides relatively high conduction band carrier confinement potential and in turn reduces the probability of electronic current overflowing to the p-type layers in a device temperature range of 300-370 K. Most electronic current can be confined in active layer effectively when the device temperature is in a range of 300-340 K; however, when the device temperature is 350 K or higher the percentage of electronic leakage current increases and it reaches to $10.7\%$ when the device temperature raises to 370 K. For $x=0.5\%$ and $1.0\%$, the percentages of electronic leakage current are negligibly small when the device...
temperature is below 320 K. The percentage of electronic leakage current of x=0.5% increases from 1% to 19% with the temperature increases from 330 to 370 K. For x=1%, it already has 3% electronic leakage current when the device temperature is 330 K and more than 13% electronic current overflows to the p-type layers when the device temperature is higher than 340 K. It is noteworthy to mention that the In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$/GaAs$_{1-x}$N$_x$ LD does not lase when the percentage of electronic leakage current is higher than 13%.

5. CONCLUSION

In summary, the temperature dependent optical gain properties, laser performance and the electronic leakage current of In$_{0.4}$Ga$_{0.6}$As$_{0.986}$N$_{0.014}$/GaAs$_{1-x}$N$_x$ QW laser with various GaAs$_{1-x}$N$_x$ strain compensated barrier have been numerically analyzed for the first time. It is shown that, the nitrogen composition of GaAs$_{1-x}$N$_x$ strain compensated barriers play an important role in the characteristic temperature coefficient $T_0$ value. The simulation results also suggest that using GaAs$_{1-x}$N$_x$ strain-compensated barriers with x value less than 0.5% may provide better optical gain properties and higher $T_0$ value. No lasing is observed when the percentage of the electronic leakage current is higher than 13%.

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