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Optical gain analysis of strain-compensated InGaN–AlGaN quantum well active regions for lasers emitting at 420–500 nm

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Abstract Strain-compensated InGaN quantum wells with tensile AlGaN barriers are analyzed as improved gain media for laser diodes emitting at 420–500 nm. The band structure is calculated using the 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism, taking into account valence band mixing, strain effect, and spontaneous and piezoelectric polarizations. The optical gain analysis exhibits significant improvement in the peak optical gain and differential gain for the strain-compensated structures. The calculation also shows a significant reduction of threshold carrier density and current density for diode lasers employing the strain-compensated InGaN–AlGaN QW active regions.

Keywords Strain-compensated QW · InGaN QW gain media · Diode lasers

1 Introduction

III-Nitride diode lasers and light emitting diodes (LEDs) emitting in the 420–500 nm region play important roles for medical, optical storage, DVD, and solid state lighting. Conventional III-nitride gain media emitting in the visible regime is based on type-I InGaN QWs with GaN barriers (Nakamura et al. 1995; Zhang et al. 2000; Guo et al. 2001). Major challenges preventing high performance conventional InGaN QWs are (1) high strain misfit dislocation density from the large strain-mismatch of the InGaN/GaN, (2) large phase separation in high-In content InGaN QW, and (3) the existence of electrostatic field in III-nitrides. The high strain misfit dislocation density leads to low radiative efficiency, while spontaneous and piezoelectric polarizations induce a built-in electrostatic field resulting in significant reduction of electron–hole wavefunctions overlap. Recently, polarization engineering via

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staggered InGaN QWs had also been demonstrated to enhance the radiative efficiency of the LEDs emitting at 420–510 nm (Arif et al. 2007).

In this paper, we analyze the optical gain properties of strain-compensated InGaN quantum well employing tensile barriers of AlGaN material, emitting in the 420–500 nm regimes. The utilization of strain-compensated QW structure allows a strain-balanced structure, which in turn leads to the reduction in the strain energy and strain-misfit dislocation density inside the QW. The use of larger bandgap barriers of AlGaN also leads to improved carrier confinement in the InGaN QW, which is important for achieving high performance LEDs and lasers operating at high temperature. Our analysis indicates a reduction of the threshold carrier density and threshold current density for diode lasers employing the strain-compensated QW active region.

2 Numerical model

Energy dispersion relations, wavefunctions, and optical matrix elements were calculated using a 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism for wurtzite semiconductor (Chuang 1996; Piprek 2003) taking into account the valence-band mixing, strain effects, spontaneous and piezoelectric polarization fields (Bernardini and Fiorentini 1999). The band parameters for the III-nitride alloys were obtained from references (Vurgaftman and Meyer 2007, 2003), and these parameters are presented in Table 1. The strain effect from the difference of lattice constants for the QW and barrier layers is taken into account, as follow:

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_0 - a}{a}, \tag{1a}$$

$$\varepsilon_{zz} = -\frac{2C_{13}}{C_{33}}\varepsilon_{xx}, \tag{1b}$$

$$\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0, \tag{1c}$$

where a_0 and a are the lattice constants of the GaN barrier and InGaN QW, respectively. The C_{13} and C_{33} are the stiffness constants of the InGaN layer.

The analytical expression for the QW band structure, the interband optical matrix element, and the optical gain spectra were computed using the treatment in Chuang (1996). The effects of the built-in spontaneous and strain-induced piezoelectric fields in semiconductors were taken into account, which led to the energy band bending. As a result of the polarization fields inside the nitride materials, the electrostatic fields in each layer (jth) can be expressed as:

$$E_j = \frac{\sum_k l_k P_k/\varepsilon_k - P_j \sum_k l_k/\varepsilon_k}{\varepsilon_j \sum_k l_k/\varepsilon_k}, \tag{2}$$

where P is the total macroscopic polarization, ε is the static dielectric constant, and l is the thickness of the layers. The subscripts k and j corresponds to the kth and jth layers. The Eq. 2 satisfies the boundary conditions for the electric fields as follow

$$\sum_k l_k E_k = 0, \tag{3}$$

where the summation include all layers including the QW and barrier regions.

Table 1 Material parameters for GaN, AlN, and InN used in QW band structure calculations

Parameters	GaN	AlN	InN
$m^*_{//}/m_0$ at 300 K	0.21	0.32	0.07
$m^*_{\perp}/m_0$ at 300 K	0.20	0.30	0.07
A_1	−7.21	−3.86	−8.21
A_2	−0.44	−0.25	−0.68
A_3	6.68	3.58	7.57
A_4	−3.46	−1.32	−5.23
A_5	−3.40	−1.47	−5.11
A_6	−4.90	−1.64	−5.96
E_g (eV) at 300 K	3.437	6.00	0.6405
Δ_{cr} (eV)	0.010	−0.227	0.024
Δ_{so} (eV)	0.017	0.036	0.005
a_{cz} (eV)	−7.1	−3.4	−4.2
a_{ct} (eV)	−9.9	−11.8	−4.2
D_1 (eV)	−3.6	−2.9	−3.6
D_2 (eV)	1.7	4.9	1.7
D_3 (eV)	5.2	9.4	5.2
D_4 (eV)	−2.7	−4.0	−2.7
C_{13} (GPa)	106	108	92
C_{33} (GPa)	398	373	224
d_{13} (pmV^{-1})	−1.0	−2.1	−3.5
d_{33} (pmV^{-1})	1.9	5.4	7.6
P_{sp} (C/m^2)	−0.034	−0.090	−0.042

The values are taken from Vurgaftman and Meyer (2003, 2007)

3 Simulation results and discussions

The optical gain calculations were carried out for both conventional InGaN–GaN QW and strain-compensated InGaN–AlGaN–GaN QW structures. Figure 1a, b show schematics of the energy band diagram for the conventional InGaN–GaN QW and strain-compensated InGaN–AlGaN QW structures, respectively, utilizing 25 Å $In_{0.27}Ga_{0.73}N$ QW ($\Delta a/a = +2.93\%$) as the active region emitting in the 500 nm regimes. In the strain-compensated structure, we employed thin 1 nm $Al_{0.1}Ga_{0.9}N$ barriers ($\Delta a/a = -0.25\%$) surrounding the InGaN QW. The use of low Al-content AlGaN layers serves as the strain-compensating layers, which also provides increase in the electron and hole confinement energy. Both conventional and strain-compensated QW structures should be feasible to grow by metal-organic chemical vapor deposition.

The optical gain spectra were calculated for both structures emitting in the 500 nm regime with carrier density (n) ranging from 2×10^{19} up to 10×10^{19} cm^{-3} at $T = 300$ K, as shown in Fig. 2. The linewidth broadenings with Lorentzian shape of $\tau_S = 0.1$ ps were used throughout the calculations. Figure 2 indicates that the gain spectra for the strain-compensated InGaN–AlGaN QW exhibit improved optical gain for all carrier densities, in comparison to that of the conventional InGaN QW.

In the optical gain analysis for polar III-nitride semiconductor, we took into account all the quantized states transitions (both of same and different quantum numbers) between the conduction bands and valence bands. At low carrier density, the dominant transitions occur for the transitions between $n = 1$ (electron) to $n = 1$ (HH) and $n = 1$ (electron) to $n = 1$ (LH). At higher carrier density, band filling occurs as a result of the transitions between the $n = 1$ (electrons) and $n = 2$ (HH and LH). In the conventional QW systems without

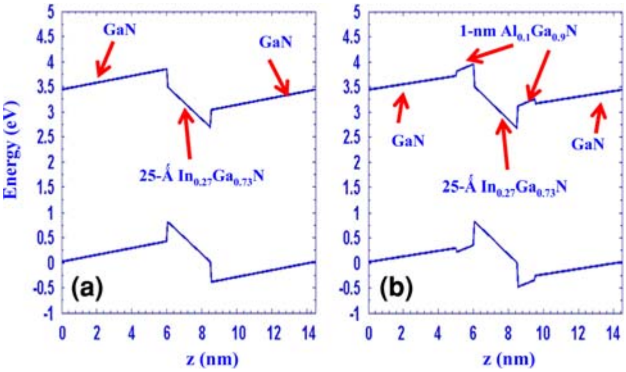

Fig. 1 Band lineup and wavefunction of (**a**) conventional 25 Å In$_{0.27}$Ga$_{073}$N–GaN QW and (**b**) strain-compensated 25 Å In$_{0.27}$Ga$_{0.73}$N-Al$_{0.1}$Ga$_{0.9}$N QW

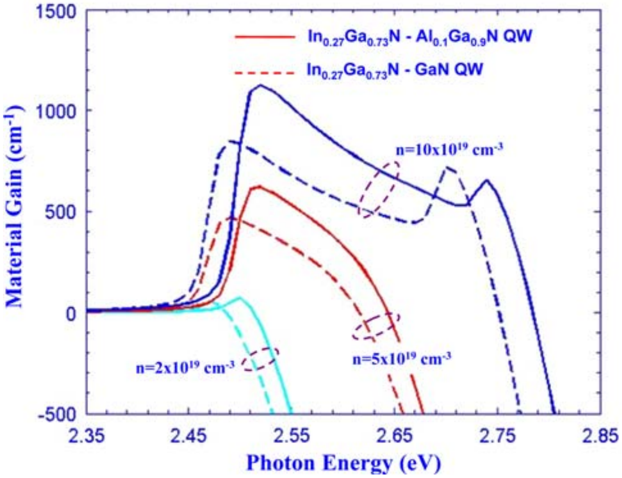

Fig. 2 TE-polarized optical gain spectra of strain-compensated 25 Å In$_{0.27}$Ga$_{0.73}$N–Al$_{0.1}$Ga$_{0.9}$N QW and conventional 25 Å In$_{0.27}$Ga$_{0.73}$N-GaN QW for carrier density (n) from 2×10^{19} cm^{-3} up to 10×10^{19} cm^{-3}

polarization fields, only transitions with similar quantum numbers are allowed. In the QW systems with polarization fields, it is important to note that the transitions between states with different quantum numbers could have significant non-zero transition matrix elements. The band filling due to the transitions with states with dissimilar quantum numbers results in the saturation of the peak gain, in particular for 500 nm emitting InGaN QW systems.

The calculated peak material gains (g_p) and differential gains (dg/dn) as a function of carrier density are shown in Figs. 3 and 4, respectively, for both the conventional and strain-compensated structures at room temperature. The transparency carrier densities (n_{tr}) for both structures are relatively similar, in the range of 1.99–2 × 10^{19} cm^{-3}. The peak optical gain of the strain-compensated InGaN–AlGaN QW structures exhibit improvement of 30–35% ($g_p = 1123.4\,\text{cm}^{-1}$, for $n = 10 \times 10^{19}\,\text{cm}^{-3}$), in comparison to those of conventional InGaN–GaN QW structure ($g_p = 844.3\,\text{cm}^{-1}$, for $n = 10 \times 10^{19}\,\text{cm}^{-3}$). The differential gains near transparency for the conventional and strain-compensated structures were calculated as

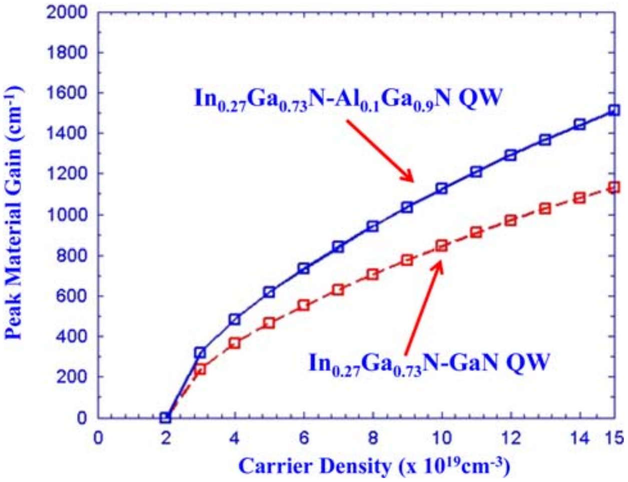

Fig. 3 Material gain as a function of carrier density at 300 K for 25 Å $In_{0.27}Ga_{073}N$–GaN QW and strain-compensated 25 Å $In_{0.27}Ga_{0.73}N$–$Al_{0.1}Ga_{0.9}N$ QW

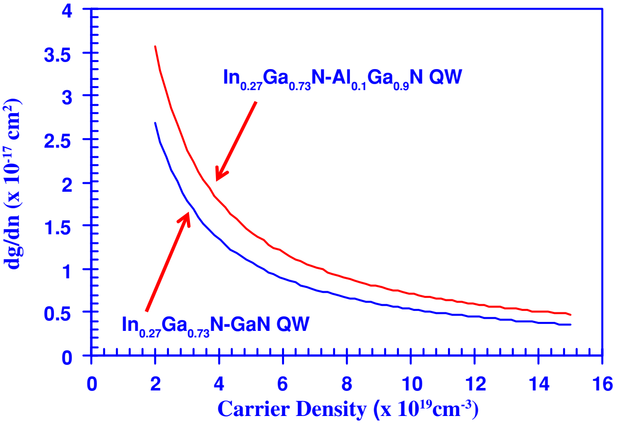

Fig. 4 Differential gain as a function of carrier density at 300 K for conventional 25 Å $In_{0.27}Ga_{073}N$–GaN QW and strain-compensated 25 Å $In_{0.27}Ga_{0.73}N$–$Al_{0.1}Ga_{0.9}N$ QW

2.68×10^{-17} and $3.57 \times 10^{-17}\,cm^2$, respectively. The improvement in the material gain and differential gain in the strain-compensated InGaN–AlGaN QW structures can be attributed to the improved carrier confinement in the QW and electron–hole wave function overlap.

Optical gain analysis was also carried out for the strain-compensated 25 Å $In_{0.15}Ga_{0.85}N$ QW with $Al_{0.1}Ga_{0.9}N$ barriers, emitting in the 420 nm wavelength regimes. The utilization of the strain-compensation approach on the 420 nm emitting InGaN–AlGaN QW also leads to improvement of +50% of peak optical gain ($g_p = 1459.2\,cm^{-1}$, for $n = 5 \times 10^{19}\,cm^{-3}$), in comparison to that of conventional InGaN–GaN QW ($g_p = 979\,cm^{-1}$, for $n = 5 \times 10^{19}\,cm^{-3}$).

To evaluate the feasibility of strain-compensated $In_{0.27}Ga_{0.73}N$–$Al_{0.1}Ga_{0.9}N$ QW active region for diode lasers emitting at 500 nm regimes, we employed a typical nitride-based laser structure using 4-stage quantum wells with optical confinement factor (Γ) of 0.04 and internal loss (α_{i}) of $26\,\mathrm{cm}^{-1}$. For as-cleaved nitride laser structures with cavity length of $700\,\mu\mathrm{m}$ ($\alpha_{\mathrm{m}} = 25.5\,\mathrm{cm}^{-1}$), the threshold gain ($\mathrm{g}_{\mathrm{th}}$) of each quantum well is $1287.5\,\mathrm{cm}^{-1}$ (per QW). The calculated threshold carrier density (n_{th}) for the strain-compensated InGaN–AlGaN QW is $12 \times 10^{19}\,\mathrm{cm}^{-3}$, which corresponds to a reduction of the threshold carrier density by 42% of that for conventional QW. Reduction in the threshold carrier density in the strain-compensated QW structure is crucial in minimizing the non-radiative threshold current density. The total radiative threshold current density ($\mathrm{J}_{\mathrm{th\_Rad}}$, for four QWs) for the strain-compensated QW structure is also found as reduced by 56% than that of the conventional QW.

4 Summary

In summary, strain-compensated InGaN quantum wells employing tensile AlGaN barriers have been analyzed as active regions for LEDs and diode lasers emitting in the 420–500 nm range. Optical gain analysis showed that the use of tensile AlGaN barriers provides improvement in the material gain and differential gain of the strain-compensated InGaN QW active region for emission wavelengths of 420–500 nm. Significant reduction in the threshold carrier density and radiative current density ($\mathrm{J}_{\mathrm{th\_Rad}}$) is predicted for diode lasers employing the strain-compensated InGaN–AlGaN QW active regions.

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