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Effects of tensile strain in barrier on optical gain spectra of GaInNAs/GaAsN quantum wells

W. J. Fan,^{a)} S. T. Ng, and S. F. Yoon

School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798

M. F. Li and T. C. Chong

Department of Electrical and Computer Engineering, National University of Singapore, Singapore 117567

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The band structures, optical gain spectra, and transparency radiative current densities of compressive-strained GaInNAs quantum wells (QWs) with different tensile-strained GaAsN (N composition from 0 to 3%) barriers are systematically investigated using a modified 6×6 $k \cdot p$ Hamiltonian including the heavy hole, light hole, and spin-orbit splitting bands. We found that the transition energy decreases when increasing the N composition in the barrier. The optical gain spectra and maximum optical gain as a function of carrier density and radiative current density are obtained for the GaInNAs/GaAsN QWs with well width of 5 nm, $\text{In}_W=28\%$, and $\text{N}_W=2.66\%$ emitting around $1.55 \mu\text{m}$. The transparency carrier density increases with the nitrogen composition in the GaAsN barrier. The transparency radiative current density decreases with more nitrogen being added into the barrier, which is in agreement with the recent experimental observation. © 2003 American Institute of Physics. [DOI: 10.1063/1.1566469]

Diluted nitride GaInNAs/GaAs quantum well (QW) lasers have been attracting great interest due to their potential applications of laser diodes emitting at 1.3 and $1.55 \mu\text{m}$ for optical fiber communication.^{1–5} Increasing N composition in the GaInNAs well is often used to achieve longer emitting wavelength. However, this results in higher threshold current density due to the formation of N-related nonradiative recombination centers during the crystal growth. Recently, the conventional GaAs barrier was replaced by the tensile-strained GaAsN in order to achieve emission at longer wavelength and lower threshold current density.^{4,5} However, the related theoretical investigation of such a compressive-strained GaInNAs quantum well with a tensile-strained GaAsN barrier is scarce in the literature.

We report a comparison study of GaInNAs/GaAsN (N composition in barrier, N_B , from 0% to 3%) QWs grown on the (001)-oriented GaAs substrates with well width of 5 nm, $\text{In}_W=28\%$, and $\text{N}_W=2.66\%$ emitting around $1.55 \mu\text{m}$. The conduction band structures of the compressive-strained GaInAsN quantum wells with tensile-strained GaAsN barriers are calculated using the one-band parabolic model. The 6×6 Hamiltonian in Ref. 6 is modified to investigate the valence band structures. Taking into account the tensile strain effect in the GaAsN barrier, the matrix elements of strain term are written as

$$\langle n | \varepsilon | n \rangle = (l\varepsilon^w + d\varepsilon^b)/L, \quad (1)$$

$$\langle m | \varepsilon | n \rangle = \frac{\varepsilon^w - \varepsilon^b}{\pi(n-m)} \sin[(n-m)\pi l/L], \quad m \neq n, \quad (2)$$

where superscripts w and b represent the well and barrier, ε is the strain, $L=l+d$, and l and d are the well width and

barrier width, respectively. The strains in the well and barrier are given by $\varepsilon^w = b^w(1 + 2c_{12}^w/c_{11}^w)e_{xx}^w$ and $\varepsilon^b = b^b(1 + 2c_{12}^b/c_{11}^b)e_{xx}^b$, respectively. b represents the valence-band shear strain deformation potential. c_{11} and c_{12} are the elastic stiffness constants. e_{xx} is the in-plane strain.

The band structure parameters used in this work are from Ref. 7. The band gap and electron effective mass of GaInNAs are calculated using Chow *et al.*'s phenomenological relationships.⁸ Due to the lack of the band offset parameter of GaInNAs/GaAsN, we have to extract it using the following assumptions. The experimental results show that the band offset ratio of GaInNAs/GaAs quantum wells, Q_c , increases when increasing the indium and nitrogen compositions in the quantum well.^{9–12} Therefore it is possible to formulate a phenomenological relationship for Q_c , similar to the one proposed by Chow *et al.* for the band gap energy after fitting the data reported in Refs. 8 and 13.

$$Q_c(\text{Ga}_{1-x}\text{In}_x\text{N}_y\text{As}_{1-y}/\text{GaAs}) = Q_c(\text{Ga}_{1-x}\text{In}_x\text{As}/\text{GaAs}) + 17.705 \times \Delta e(x, y), \quad (3)$$

$\Delta e(x, y)$ is the difference between the strain in GaInNAs and GaInAs. For a GaInNAs/GaAsN QW, the edge of the light hole in the tensile-strained GaAsN is assumed to be aligned with the top of the valence band of GaAs, so that the valence band discontinuity $\Delta E_v(\text{GaInNAs/GaAsN})$ is assumed the same as $\Delta E_v(\text{GaInNAs/GaAs})$. This assumption is reasonable since the valence band discontinuity for GaNAs/GaAs is believed to be very small so that the reported band line-up for GaNAs/GaAs is type I or type II confusion.^{14–16}

The optical gain spectra are calculated by

$$g(E) = \left[1 - \exp\left(\frac{E - \Delta F}{k_B T}\right) \right] \frac{\pi^2 c^2 \hbar^2}{n^2 E^2} r_{\text{sp}}(E), \quad (4)$$

^{a)}Electronic mail: ewjfan@ntu.edu.sg

FIG. 1. The in-plane energy dispersion curves of the bound states in the valence band of the GaInNAs/GaAsN QWs with a well width of 5 nm, $\text{In}_W = 28\%$ and $N_W = 2.66\%$ at the different N compositions in the barrier, $N_B = 0, 1\%, 2\%$, and 3% .

$$r_{\text{sp}}(E) = \frac{ne^2E}{\pi m_0^2 \epsilon_0 \hbar^2 c^3} \sum_{n_c, n_v} \int \int \frac{Q^{n_c n_v}}{4\pi^2 l} \times f_c f_v \frac{1}{\pi} \frac{\hbar/\tau}{(E_{eh} - E)^2 + (\hbar/\tau)^2} dk_x dk_y, \quad (5)$$

where $r_{\text{sp}}(E)$ is the spontaneous emission rate, ΔF is the quasi-Fermi level separation and dependent on carrier density, E is the photon energy, k_B is the Boltzmann's constant, T is the temperature, m_0 is the electron effective mass in the free space, e is the electronic charge, ϵ_0 is the free-space dielectric constant, n is the refractive index, c is the light velocity, $Q^{n_c n_v}$ is the squared optical transition matrix elements of momentum for transitions between the valence hole subband (n_v) and the conduction electron subband (n_c), l is the QW well width, and f_c and f_v are the Fermi–Dirac distributions for electrons in the conduction bands and holes (not electrons) in the valence bands, respectively. τ is the intraband relaxation time, we use $\tau = 0.1$ ps in our calculations. E_{eh} is the transition energy.

The radiative current density J_{rad} can be calculated from the spontaneous emission spectrum⁶

$$J_{\text{rad}} = el \int r_{\text{sp}}(E) dE. \quad (6)$$

In this work, the GaInNAs/GaAs QW well width and barrier width are fixed at 5 and 20 nm, respectively. The In composition in the well, In_W is 28%, and the N composition in the well, N_W is 2.66%. Figure 1 shows the in-plane energy dispersion curves of the bound states in the valence band of the GaInNAs/GaAsN QWs at the different N compositions in barrier, $N_B = 0$ (GaAs barrier case), 1%, 2%, and 3%. When increasing N_B from 0 to 3%, lh2 shifts into the well and becomes a bound state from a continue state due to the deduction of the barrier height and the number of the bound state in the well becomes 4. The effective mass calculations show that the hhl effective mass increases with N_B .

Figure 2 shows the TE mode optical gain spectra of the GaInNAs/GaAsN QWs at the different $N_B = 0, 1\%, 2\%$, and

FIG. 2. The TE mode optical gain spectra of the GaInNAs/GaAsN QWs at the different N_B and carrier density $n = 6 \times 10^{18} \text{ cm}^{-3}$.

3%, and carrier density $n = 6 \times 10^{18} \text{ cm}^{-3}$. The TM mode optical gain spectra are strongly depressed because of the compressive strain in the well and are not plotted in the graph. It is observed that the transition energy decreases with the N composition in the barrier. This is attributed to the deduction of energy band gap of GaAsN due to its larger negative bowing factor and the tensile strain effect in the barrier.

Figure 3 shows the maximum optical gain of the TE mode as a function of (a) carrier density and (b) radiative current density for the GaInNAs/GaAsN QWs at $N_B = 0, 1\%, 2\%$, and 3% . When N_B increases, the transparency carrier density increases. The transparency carrier density depends primarily on the band curvatures and thus is sensitive to the effective mass.⁸ Our calculations show that the heavy hole (hhl) effective mass and the density of state increase with the tensile strain in the barrier. So, the tensile strain in the barrier increases the transparency carrier density by increasing the heavy hole effective mass; and, the increment in transparency carrier density is more significant with the larger $N_B = 3\%$. This is attributed to that the more bound states in QW enhance the density of state at larger $N_B = 3\%$. The transparency radiative current density decreases with more nitrogen being added into the barrier, which is in good agreement with the experimental observation.⁵ The radiative current density is calculated from the integrated spontaneous emission rate, and is proportional to the QW band gap.¹⁷ Our calculations show that the transition matrix elements are almost the same at $k=0$ for the different N_B . So, the deduction of the QW band gap due to more nitrogen in the barrier results in the transparency radiative current density decreasing.

The advantages of the tensile-strained GaAsN barrier include the longer wavelength of emission due to the deduction of the barrier height; the lower transparency radiative current density; and reducing the nitrogen out-diffusion from the well (this effect is not considered in our calculation), which leads to the undesired blueshift of laser wavelength. On the other hand, we would like to note that the tensile-strained GaAsN barrier may reduce the characteristic temperature T_0

FIG. 3. Maximum optical gain of the TE mode as a function of (a) carrier density and (b) radiative current density for the GaInNAs/GaAsN QWs at the different N_B .

due to the poor electron confinement compared with GaAs barrier.

In summary, the band structures, optical gain spectra, and transparency radiative current densities of GaInNAs

QWs with different GaAsN (N composition from 0 to 3%) barriers are systematically investigated using the modified $6 \times 6 k \cdot p$ Hamiltonian including the tensile strain effect in the barrier. The band offset parameters for GaInNAs/GaAsN are proposed. The calculations show that number of bound states in QW may increase and the transition energy decreases when increasing the N composition in the barrier. The tensile strain in the barrier increases the transparency carrier density by increasing the heavy hole effective mass and density of state. The deduction of the QW band gap due to more nitrogen in the barrier results in the transparency radiative current density decreasing.

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