Electronic bandstructure and optical gain of lattice matched III-V dilute nitride bismide quantum wells for 1.55 μm optical communication systems

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Dilute nitride bismide GaN_xBi_yAs_{1-x-y}/GaAs is a potential semiconductor alloy for near- and mid-infrared applications, particularly in 1.55 μm optical communication systems. Incorporating dilute amounts of bismuth (Bi) into GaAs reduces the effective bandgap rapidly, while significantly increasing the spin-orbit-splitting energy. Additional incorporation of dilute amounts of nitrogen (N) helps to attain lattice matching with GaAs, while providing a route for flexible bandgap tuning. Here we present a study of the electronic bandstructure and optical gain of the lattice matched GaN_xBi_yAs_{1-x-y}/GaAs quaternary alloy quantum well (QW) based on the 16-band $k\cdot p$ model. We have taken into consideration the interactions between the N and Bi impurity states with the host material based on the band anticrossing and valence band anticrossing model. The optical gain calculation is based on the density matrix theory. We have considered different lattice matched GaN_xBi_yAs_{1-x-y}/GaAs QW cases and studied their energy dispersion curves, optical gain spectrum, maximum optical gain, and differential gain and compared their performances based on these factors. The thickness and composition of these QWs were varied in order to keep the emission peak fixed at 1.55 μm . The well thickness has an effect on the spectral width of the gain curves. On the other hand, a variation in the injection carrier density has different effects on the maximum gain and differential gain of QWs of varying thicknesses. Among the cases studied, we found that the 6.3 nm thick GaN₃Bi_{5.17}As_{91.83} lattice matched QW was most suited for 1.55 μm (0.8 eV) GaAs-based photonic applications. *Published by AIP Publishing.* [<http://dx.doi.org/10.1063/1.4962214>]

I. INTRODUCTION

The dilute nitride bismide semiconductor, GaN_xBi_yAs, has attracted much attention recently due to its potential applications in the near- and mid-infrared photonic devices, particularly in the 1.55 μm GaAs-based laser diodes for fiber optical communication systems.^{1,2} Per % of bismuth (Bi) incorporation reduces the effective bandgap by $\sim 60\text{--}80\text{ meV}$,³ while nitrogen (N) helps to achieve lattice matching. The dilute-N-Bi quantum wells (QWs) are therefore expected to have better electron and hole quantum confinement. This fundamental property of the electronic structure makes this material more suitable for the telecom laser applications compared to the conventional III-V materials such as InP based InGaAsP devices, particularly at high temperature.⁴

However, to achieve this, a significant count of As atoms must be replaced with Bi atoms. This leads to lattice mismatching and other interface defects. This effect can be compensated for by an appropriate incorporation of N into the alloy. It has been found that in GaN_xBi_yAs semiconductor alloy, when the N:Bi composition ratio is 0.58 we can obtain lattice matching with GaAs.⁵ Co-alloying N and Bi opens up avenues for bandstructure engineering and precise strain control in the GaN_xBi_yAs quaternary alloy.⁶ In dilute-Bi alloys, the bandgap reduction is caused due to coupling between

Bi-resonant state and the valence band (VB) state; while on the other hand, in dilute-N alloys, this effect is induced due to N-resonant state coupling with conduction band (CB) state.⁷ In the GaN_xBi_yAs alloy, both these effects work independently and simultaneously. The origins of such behavior in dilute-N-Bi alloys can be described using a band anti-crossing (BAC) model. Since dilute-N alloys predominantly affect the CB, we use the conduction BAC model. By contrast, for dilute-Bi alloys we use the valence BAC (VBAC) model in which the VB is most affected.³

In this work, we will study various cases of the lattice matched GaN_xBi_yAs QWs grown on the GaAs barrier, aiming for applications in the 1.55 μm GaAs-based laser for fiber optical communication systems. A recent work⁸ by the O'Reilly group has reported GaBiAs/GaAs QWs, while our work focuses on the GaN_xBi_yAs QWs, which has better electron confinement due to repulsion between N and the host material's band edge. The larger CB and VB offsets of GaN_xBi_yAs/GaAs benefit the QW laser performance, such as rendering a larger characteristic temperature. Nasr *et al.*⁹ have worked on the GaN_xBi_yAs QWs, but limited their investigation only up to optical absorption. Here we shall study the optical gain essential for device design and performance, plus report the modeling and optimization of lattice matched GaN_xBi_yAs QW lasers. Gladysiewicz *et al.*¹⁰ have reported GaInAsBi QWs, which differs from GaN_xBi_yAs. To study the electronic structure and the optical properties of our GaN_xBi_yAs QWs and comment on

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the performances, we have laid down a $k \cdot p$ 16-band Hamiltonian capable of incorporating the effects of N and Bi doping, as we shall explain now.

II. THEORETICAL FRAMEWORK

Broderick *et al.* had proposed a 12- and 14-band $k \cdot p$ Hamiltonian for GaN_{1-x}Bi_x.¹¹ Here, we propose a 16-band Hamiltonian including the so_{Bi} energy level ($E_{Bi,so}^0$), which was not accounted for in their model. The 16-band model is more accurate, especially for the higher excited states of hole, which can be closer to $E_{Bi,so}^0$, and thus the interaction between them cannot be ignored. We have extended the Kane's 8-band Hamiltonian and used the BAC and VBAC

models to form a 16-band Hamiltonian. In addition to Kane's 8-bands, the incorporation of N needs two additional bands to address the local N resonant s -like states. On the other hand, Bi introduces p -like states, for which six additional bands must be considered with the freedom of spin, including so coupling. The 16-band Hamiltonian for GaN_xBi_yAs_{1-x-y} epilayer can be written in the form

$$H_{16 \times 16} = \begin{bmatrix} H_{2 \times 2} & H_{2 \times 8} & 0 \\ H_{8 \times 2} & H_{8 \times 8} & H_{8 \times 6} \\ 0 & H_{6 \times 8} & H_{6 \times 6} \end{bmatrix}, \quad (1)$$

where $H_{8 \times 8}$ is the 8-band Hamiltonian and is given by²

$$H_{8 \times 8} = \begin{bmatrix} E^c & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. \\ 0 & E^c & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. \\ \frac{1}{\sqrt{2}}P_- & 0 & P+Q & c.c. & c.c. & c.c. & c.c. & c.c. \\ -\sqrt{\frac{2}{3}}P_z & \frac{1}{\sqrt{6}}P_- & S^* & P-Q & c.c. & c.c. & c.c. & c.c. \\ -\frac{1}{\sqrt{6}}P_+ & -\sqrt{\frac{2}{3}}P_z & -R^* & 0 & P-Q & c.c. & c.c. & c.c. \\ 0 & -\frac{1}{\sqrt{2}}P_+ & 0 & -R^* & -S^* & P+Q & c.c. & c.c. \\ -\frac{1}{\sqrt{3}}P_z & -\frac{1}{\sqrt{3}}P_- & \frac{S^*}{\sqrt{2}} & -D & -\sqrt{\frac{3}{2}}S & \sqrt{2}R & P-\Delta & c.c. \\ -\frac{1}{\sqrt{3}}P_+ & \frac{1}{\sqrt{3}}P_z & -\sqrt{2}R^* & -\sqrt{\frac{3}{2}}S^* & D & \frac{S}{\sqrt{2}} & 0 & P-\Delta \end{bmatrix}. \quad (2)$$

The Hamiltonian contains of both kinetic terms H_k and strain terms H_ϵ . Detailed expressions of the $H_{8 \times 8}$ Hamiltonian terms are given in our previous work.² The $H_{2 \times 2}$ is the s_N -like localized N impurity Hamiltonian and is given by^{2,12}

$$H_{2 \times 2} = \begin{bmatrix} E_N^0 & 0 \\ 0 & E_N^0 \end{bmatrix}. \quad (3)$$

In a strained III-V-N material, the nitrogen level parameter, E_N , is with respect to the valence band maximum (VBM) with strain consideration, such that E_N weakly shifts with applied pressure.¹³ However, for the unstrained VBM, the nitrogen level, E_N^0 , is given by

$$E_N^0 = E_N + VBM^S, \quad (4)$$

where VBM^S is the top of strained valence band at Γ -point ($k=0$). This can be calculated by utilizing the strain induced 8-band H at $k=0$ point.²

Similar to N, in order to include the Bi band broadening effect, a modified $H_{6 \times 6}$ is proposed for the p -like localized Bi impurity Hamiltonian³ and is given by

$$H_{6 \times 6} = \begin{bmatrix} E_{Bi}^0 & 0 & 0 & 0 & 0 & 0 \\ 0 & E_{Bi}^0 & 0 & 0 & 0 & 0 \\ 0 & 0 & E_{Bi}^0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_{Bi}^0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{Bi,so}^0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{Bi,so}^0 \end{bmatrix}. \quad (5)$$

Similar to N, the Bi levels with respect to the unstrained VBM, E_{Bi}^0 and $E_{Bi,so}^0$, are given by

$$E_{Bi}^0 = E_{Bi} + VBM^S, \quad (6a)$$

$$E_{Bi,so}^0 = E_{Bi,so} + VBM^S. \quad (6b)$$

The $H_{8 \times 8}$ Hamiltonian is for the interaction between the s_N -like localized N impurity state (with N composition x) and the host material state and is given by

$$H_{8 \times 2} = \sqrt{x} V_N \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}. \quad (7)$$

Similarly, the $H_{6 \times 8}$ Hamiltonian is for the interaction between the p -like localized Bi impurity state (with Bi composition y) and the host material state and is given by³

$$H_{6 \times 8} = \sqrt{y} V_{Bi} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \quad (8)$$

V_N and V_{Bi} are the coupling coefficients in the BAC model for N and Bi, respectively. $H_{8 \times 6}$ and $H_{2 \times 8}$ are the transpose of the $H_{6 \times 8}$ and $H_{8 \times 2}$, respectively.

We can expand the sixteen dimensional hole envelope wave function for the QWs as

$$\Phi_m = \{\Phi_m^j\} (j = 1, 2, \dots, 16), \quad (9)$$

where

$$\Phi_m^j = \exp[i(k_x x + k_y y)] \sum_m a_{n,m}^j \frac{1}{\sqrt{L}} \exp\left[i\left(k_z + m \frac{2\pi}{L}\right)z\right]. \quad (10)$$

The QW period is $L = l + d$, where the width of the well is l while the barrier width is d . k_i ($i = x, y, z$) are the wave-vectors, $a_{n,m}^j$ is the expansion coefficient while n is the energy subband index.¹⁴

For the calculation of the optical gain, the squared optical transition matrix element (TME) is important. It is a measure of the momentum of transition strength between the hole and the electron subbands, and is given by¹⁵

$$\mathcal{P}_{cv,i} = \langle \Psi_{c,\mathbf{k}} | \mathbf{e}_i \cdot \mathbf{p} | \Psi_{v,\mathbf{k}} \rangle, \quad i = x, y, z, \quad (11)$$

where $\Psi_{c,\mathbf{k}}$ and $\Psi_{v,\mathbf{k}}$ are the real electron and hole wavefunctions, respectively, and $\mathbf{p}$ is the momentum operator.¹⁶ Detailed expressions for the TMEs along the x , y , and z directions are furnished in our previous work.¹⁶

A higher average of the TMEs along the x and y directions would result in a higher transverse electric (TE) mode optical gain, while a higher TME along the z direction would lead to a higher transverse magnetic (TM) mode optical gain. The TE mode gain polarized in the x - y plane is usually higher for QWs compared to the TM mode gain polarized in the z direction.

The linear optical gain spectra are calculated based on the density-matrix theory using the following equations:^{14,17}

$$G(E) = \left[1 - \exp\left(\frac{E - \Delta F}{k_B T}\right) \right] \frac{\pi^2 c^2 \hbar^3}{n^2 E^2} R_{sp}(E), \quad (12)$$

$$R_{sp}(E) = \frac{ne^2 E}{\pi m_0^2 \epsilon_0 \hbar^2 c^3} \sum_c \sum_v \iint \frac{|\mathcal{P}_{cv}|^2}{4\pi^2 l} f_c f_v \times \frac{1}{\pi} \frac{\hbar/\tau}{(E_{eh} - E)^2 + (\hbar/\tau)^2} dk_x dk_y, \quad (13)$$

where $R_{sp}(E)$ is the spontaneous emission rate. f_c and f_v are the Fermi-Dirac distributions for the electrons and holes in the CB and VB, respectively, and are given by¹⁴

$$f_c = \frac{1}{1 + \exp[(E_{enc} - E_{fc})/k_B T]}, \quad (14a)$$

$$f_v = \frac{1}{1 + \exp[(E_{hnc} - E_{fv})/k_B T]}, \quad (14b)$$

where E_{fc} and E_{fv} are the electron and hole quasi-Fermi levels, respectively, and $\Delta F = E_{fc} - E_{fv}$ is the quasi-Fermi energy separation, both of which depend on the injection carrier density. k_B is the Boltzmann constant and T is the absolute temperature. The results reported in this paper correspond to 300 K. e is electron charge, E is photon energy, n is refractive index, ϵ_0 is free-space dielectric constant, and c is speed of light. $\mathcal{P}_{cv}$ is the TME, E_{eh} is the transition energy, and τ is the intraband relaxation time. Band parameter of GaAs at 300 K are tabulated in Table I, while the BAC and VBAC parameters to study the effect of N and Bi alloying are tabulated in Table II. The references from where these values have been taken are cited alongside. The parameters for the alloy semiconductor are obtained by linear interpolation method.

III. RESULTS AND DISCUSSION

The bandgap (E_g) for $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}$ semiconductor alloy pseudomorphically grown on GaAs depends on the compositions of N (x) and Bi (y) replacing the As from GaAs. Both GaN and GaBi have lower bandgap compared to

TABLE I. Band parameters of GaAs at 300 K.

Parameter (unit)	Value
a (Å)	5.65325 ^a
m_e^* (m_0)	0.067 ^b
γ_1	6.8 ^b
γ_2	1.9 ^b
γ_3	2.73 ^b
E_p (eV)	25.5 ^a
$E_{g\Gamma}$ (eV)	1.424 ^b
Δ_{so} (eV)	0.341 ^a
a_c (eV)	-7.17 ^c
a_v (eV)	1.16 ^c
b (eV)	-1.7 ^c
d (eV)	-4.55 ^c
C_{11} (10^{11} dyn/cm ²)	11.879 ^b
C_{12} (10^{11} dyn/cm ²)	5.376 ^b

^aReference 7.

^bReference 18.

^cReference 19.

TABLE II. BAC and VBAC parameters for N and Bi.

Parameter (unit)	Value
E_N (eV)	1.65 ^a
V_N (eV)	2.7 ^a
E_{Bi} (eV)	-0.4 ^b
$E_{Bi,so}$ (eV)	-1.9 ^b
V_{Bi} (eV)	1.55 ^c
ΔE_{CBM}	-2.1 ^c
ΔE_{VBM}	-0.8 ^c
ΔE_{so}	-1.1 ^c

^aReference 13.^bReference 3.^cReference 20.

GaAs, and the combined addition of N and Bi reduces the E_g of GaNBiAs alloy as shown in Fig. 1 contour (this result is at 300 K). The lattice constant of GaN is smaller than GaAs, while that of GaBi is larger. Therefore, a sufficiently large N fraction induces a tensile strain ($\epsilon_{xx} > 0$), while a sufficiently large Bi fraction induces a compressive strain ($\epsilon_{xx} < 0$). In this work, we focus on the lattice matched GaNBiAs/GaAs QW structures, for which it is essential to maintain a ratio of N:Bi = 0.58 for zero strain, as shown by the red line, which is the line of lattice matching.

From the viewpoint of device physics, strain in the QW material may be beneficial, for example, compressive strain reduces the hole effective mass to improve the laser performance. But, from the viewpoint of material growth, strain has the potentially deleterious effects on the performance of laser.²¹ Furthermore, the critical thickness of the strained quantum well limits thicker material growth. So, lately there have been many works reporting strain compensated structure to minimize the strain to achieve the high-performance lasers.^{22,23} Here, we adhere to the condition of lattice matching, and we have studied the photon emission energy of GaNBiAs/GaAs QWs for varying well widths as shown in Fig. 2. Focusing on the 1.55 μm emission wavelength optical

FIG. 1. Variations in the bandgap (E_g) of GaNBiAs pseudomorphically grown on GaAs at 300 K vs. N and Bi composition (%). The red line is the line of lattice matching (ratio of N:Bi = 0.58).

FIG. 2. Photon emission energy/wavelength vs. well width of lattice matched GaNBiAs QWs with varying N and Bi concentration. Cases A to D are labeled.

fiber telecom communication applications, we have chosen 4 cases labeled A to D, with varying well widths of 4, 4.8, 6.3, and 9.6 nm, respectively. These cases correspond to varying N compositions of 3.5%, 3.25%, 3%, and 2.75% and corresponding Bi compositions for lattice matching with GaAs. The well width increases from Cases A to D, and therefore, the extent of quantum confinement decreases. Ideally, this should lead to a fall in the photon emission energy. But since the composition of N and Bi also reduces simultaneously, this effect is compensated for. A lower fraction of N and Bi is less capable of reducing the effective bandgap of GaNBiAs. Therefore, these two contrasting phenomenon suitably counterbalance and all the four cases exhibit emission around the 0.8 eV (1.55 μm) mark targeted towards telecom devices, as shown.

The energy dispersion curves for the first 3 electrons and the first 5 holes subband states along the [100] and [110] wavevector direction for Cases A to D GaNBiAs/GaAs QWs are shown in Fig. 3. The well width of each case is mentioned in the figure. The electron states are labeled E1 to E3, while for the holes states we have specified heavy hole (HH) and light hole (LH) states distinctly. We can see that the energy dispersion curves clearly depend on the well width and the (N, Bi) composition. As the well width increases from Cases A to D, the (N, Bi) composition falls, and the two counteracting effects balance to ensure the 1.55 μm emission. We see that the conduction subband energy dispersion curves are isotropic-like due to the isotropy of electron effective mass. On the other hand, the valence subband energy dispersion curves are more affected by varying well width and composition. There is an anisotropy effect in all cases, and they are more spread along the [110] wavevector direction compared to [100] direction. Also, from Cases A to D, their $\mathbf{k}$ span decreases. But in all four cases, the hole type sequence is same: HH1, LH1, HH2, HH3, LH2. We also notice that as the well width increases from Cases A to D, the gap between the adjacent E states and adjacent H states reduces. On the whole, Δ_{E1-E3} reduces from 403 meV in Case A to 222 meV in Case D. Similarly, $\Delta_{HH1-LH2}$ reduces from 234 meV in Case A to 96 meV in Case D. This can be attributed to the loosening confinement effect. For instance

FIG. 3. First 3 electron and first 5 hole energy dispersion curves of lattice matched GaNBiAs QWs of ((a): *Top Left*) Case A (well width = 4 nm); ((b): *Top Right*) Case B (well width = 4.8 nm); ((c): *Bottom Left*) Case C (well width = 6.3 nm); ((d): *Bottom Right*) Case D (well width = 9.6 nm). k is the wavevector along the [100] and [110] directions. E stands for electron, HH for heavy hole levels, and LH for light hole levels. The photon emission energy for all cases is ~ 0.8 eV ($1.55 \mu\text{m}$).

in Case D, due to these effects, E1 and E2 have come very close, and so have HH1 and LH1. This affects the optical performance as we shall subsequently examine.

The TE mode optical gain spectra of GaNBiAs QWs of Cases A to D are shown in Fig. 4. The injection carrier density was varied from 2 to $8 \times 10^{18} \text{ cm}^{-3}$. The temperature considered is 300 K. The intraband relaxation time τ was taken to be 0.1 ps. For any particular GaNBiAs QW case, there is a marginal blue shift in the emission peak position as the injection carrier density increases. With more and more carriers being injected, they begin to occupy the electronic states further away from the bottom of the conduction band and top of the valence band. Now, the excited state recombinations that incur from such transitions will have their

emission energy larger than the E1–HH1 separation, thus resulting in a blue shift. This effect is also generally known as band filling effect in QWs. Comparing Cases A to D, we can observe that the band filling effect is more profound in thicker QWs compared to thinner QWs. In thicker QWs, the quantum confinement effect is weaker and therefore the permissible energy levels are much closely packed. With the injection of more and more carriers, there is a higher probability of them occupying the next nearest electronic state and contributing to the emission. Comparing the gain curves, we see that the spectral width increases from Cases A to D. There are several factors dictating this trend, the primary being band filling effect as just discussed. Additionally, as seen for Fig. 3, the adjacent E and adjacent H states come

FIG. 4. TE mode optical gain spectra of lattice matched GaNBiAs QWs at 300 K for ((a): *Top Left*) Case A (well width = 4 nm); ((b): *Top Right*) Case B (well width = 4.8 nm); ((c): *Bottom Left*) Case C (well width = 6.3 nm); and ((d): *Bottom Right*) Case D (well width = 9.6 nm), for varying injection carrier density (n) = 2, 4, 6, and $8 \times 10^{18} \text{ cm}^{-3}$. The peak emission position of all cases is ~ 0.8 eV ($1.55 \mu\text{m}$).

closer. Under such circumstances if we increase the injection carrier density, there is a high probability that electrons exceed E1 and start to occupy E2 and so on. Similarly, holes can exceed HH1 and occupy LH1, HH2, etc. Considering Case D for instance, it has a fairly large gain spectral width—because it results from electron-hole recombinations not only from E1-HH1, but also from E1-LH1, E2-HH2, etc. However, smaller gain spectral width is better for stable single mode operation.

The maximum optical gain of the 4 GaNBiAs QW cases studied in Fig. 4 is presented in Fig. 5(a), with some additional data points. We have ignored $2 \times 10^{18} \text{ cm}^{-3}$ because at such low density, there is no positive gain. There are several factors affecting the maximum gain, such as TME, quasi-Fermi levels, temperature, and thickness of the QW among others [see factors in Eqs. (12) and (13)]. Usually, thicker QWs have higher TMEs due to the higher absolute overlap of the electron and hole wavefunction. Also, the difference between the quasi-Fermi level separation (ΔF) and photon energy (E) is important and for positive (maximum) gain, ΔF must be larger than the fundamental transition energy E1-HH1. Finally, from Eqs. (12) and (13), we can also see that the gain (thus maximum gain) is inversely proportional to the well width (L). Therefore, combining the effects of these and other parameters involved, we get the final result as shown in Fig. 5(a). The overall observation is that as the injection carrier density increases, so does the maximum optical gain. This is because a higher carrier density results in more and more electronic states getting filled and greater number of recombinations occur around the near-E1-HH1 energy gap. Now comparing the 4 QW cases, we found that their transparency carrier density²⁴ is around the $1.9\text{--}3.3 \times 10^{18} \text{ cm}^{-3}$ mark. This is the carrier density that gives us neither gain nor absorption around the emission peak position (we get zero gain). But on a closer inspection, we found that thinner GaNBiAs QWs have higher transparency carrier density requirement compared to thicker QWs. It was found to be $3.3, 2.5, 2.1, 1.9 \times 10^{18} \text{ cm}^{-3}$ for QW Cases A to D, respectively, by interpolation method. Just after the onset of gain, say, at $4 \times 10^{18} \text{ cm}^{-3}$, the maximum gain pattern is Case D > C > B > A, in accordance with their thicknesses. But with further increase in carrier density, the maximum gain is affected by other factors such as band filling effect and reduced confinement. The overall effect on the 4 QW cases can be seen in Fig. 5(a). While in Cases C and D, QWs have steadily increasing maximum gain, Case C

exceeds D at $8 \times 10^{18} \text{ cm}^{-3}$ density, as D approaches saturation. We shall further discuss this effect in the detailed context of Fig. 5(b), which shows the differential gain of the 4 GaNBiAs QW cases being studied. A higher differential gain translates to a greater modulation speed and narrower width of emission spectra.^{25,26} Thus, differential gain is a performance index of how effectively injected carriers produce the photon emissions. The thinner QWs (Cases A and B) have a steadily increasing differential gain initially, before dipping at sufficiently high densities. On the other hand, the thicker QWs (Cases C and D) have a relatively more stable differential gain, but they decrease with the increasing carrier densities. Among these, Case D has a lower differential gain and also it is monotonically decreasing from density 2 to $8 \times 10^{18} \text{ cm}^{-3}$. Case C has a higher and more stable differential gain across varying carrier densities.

Now we are in a situation to compare the 4 GaNBiAs QW cases studied, on the basis of their optical gain spectral width [Fig. 4], transparency carrier density, maximum optical gain [Fig. 5(a)], and differential gain [Fig. 5(b)]. The gain spectral width increases from Cases A to D. While Cases A, B, and C have a steady form function, for Case D it gets very wide with the increasing carrier density. This is because at such a large thickness, the confinement effect drops and the gap between adjacent E and H states shrinks. Other excited electron-hole transition routes open broadening the spectra. This has an adverse effect on the optical performance, as smaller gain spectral width is better for stable single mode operation. When it comes to the maximum optical gain, Cases C and D have a steady increment. Also at sufficiently high carrier density, the maximum gain of Case C exceeds that of Case D. The maximum gain of Case B also increases rapidly, but it is much less at lower densities. Moreover, the transparency carrier density of Cases C and D are relatively lower than that for A and B. Finally, the study of differential gain shows us that Case C has the best suitable characteristics to deliver high and steady optical performance over a wide range of injection carrier density. The other cases exhibit diminishing differential gain at either low density or high density. These observations are symbolically summarized in Table III.

Fig. 6 shows the squared wavefunction of the first 3 electron and the first 5 hole energy levels at $\mathbf{k}=0$ point for Cases A to D GaNBiAs/GaAs QWs. We can see that as the thickness increases, the E and H wavefunctions spread out, as expected due to larger well width. In all the cases, the

FIG. 5. ((a): Left) Maximum optical gain and ((b): Right) Differential gain of lattice matched GaNBiAs QWs at 300 K for Case A (well width = 4 nm), Case B (well width = 4.8 nm), Case C (well width = 6.3 nm), and Case D (well width = 9.6 nm) vs. varying injection carrier density. Each case is labeled.

TABLE III. Comparative analysis of the 4 GaN_{0.5}Bi_{0.5}As QW cases studied.

GaN _{0.5} Bi _{0.5} As QW case	N:Bi:As	Gain spectral width	Maximum gain	Transparency carrier density	Differential gain
Case A (4.0 nm)	3.50:6.03:90.47	✓	×	×	×
Case B (4.8 nm)	3.25:5.60:91.15	✓	×	×	×
Case C (6.3 nm)	3.00:5.17:91.83	✓	✓	✓	✓
Case D (9.6 nm)	2.75:4.74:92.51	×	✓	✓	×

wavefunctions of E1 have a reasonable overlap with that of HH1, which causes the E1-HH1 fundamental transition. Transitions among higher E and H states follow the optical transition rule and depend on the extent of probability of wavefunction overlap.

On the whole, as summarized in Table III, we find that for our intended 1.55 μm (0.8 eV) GaAs-based fiber optic laser diode applications, the 6.3 nm thick GaN_{0.5}Bi_{0.5}As_{91.83} lattice matched quantum well (Case C) gives the best optical performance. This is in comparison with the other three cases. Further fine tuning may lead us to better design parameters. GaN_{0.5}Bi_{0.5}As QWs are excellent candidates for 1.55 μm optical applications. But it is important to carefully consider the design parameters which determine the final optical performances.

Having concluded our findings above, we would now like to highlight a couple of important research aspects relating to the dilute-N-Bi QW lasers. First, it is well known that for the bulk material, the conduction-heavy hole-split off hole-heavy hole (CHSH) Auger recombination is significant. However, there exist contradictory viewpoints in the QW domain. For example, Hausser *et al.* have experimentally shown that the Auger recombination in QWs is about 3 times smaller than that in bulk.²⁷ Other works have reported a reduction in Auger recombination by two orders of magnitude in QWs compared to bulk.²⁸ These works show that the Auger recombination in QWs is of very minor significance,

owing to which we have chosen to simplify our calculations. However, there are some counterarguments in existing literature, which state that Auger recombination is a significant problem for long wavelength QW semiconductor lasers.^{29,30}

In this context, more conclusive work is elicited to obtain a comprehensive understanding of the Auger effects in GaN_{0.5}Bi_{0.5}As QWs. In order to fully understand the nonradiative recombination, we would also like to trigger the investigation of the other two types of Auger recombination in GaN_{0.5}Bi_{0.5}As QWs: conduction-heavy hole-conduction-conduction (CHCC) and conduction-heavy hole-light hole-heavy hole (CHLH). We know that the CHSH Auger recombination can be suppressed by controlling the Bi composition (ensuring that the spin-orbit splitting energy exceeds the effective bandgap¹) and more readily so in the presence of N. But this does not continue to hold in case of CHCC or CHLH Auger recombination, for which there is no significant evidence in the literature. Second, the major challenge with GaN_{0.5}Bi_{0.5}As QW laser is that it is difficult to grow high quality material even with advanced molecular beam epitaxy or metal organic chemical vapor deposition. Incorporating both N and Bi requires different growth optimizations. One issue is that adding N into GaAs degrades the material quality.³¹ On the other hand, Bi as surfactant may increase the efficiency of N incorporation in GaNAs by up to 60%.³² However, too high a Bi % can also be detrimental to the material quality. The Volz group has demonstrated GaBiAs

FIG. 6. First 3 electrons and first 5 holes squared wavefunctions at $\mathbf{k} = 0$ point for GaN_{0.5}Bi_{0.5}As QWs of ((a): *Top Left*) Case A (well width = 4 nm); ((b): *Top Right*) Case B (well width = 4.8 nm); ((c): *Bottom Left*) Case C (well width = 6.3 nm); and ((d): *Bottom Right*) Case D (well width = 9.6 nm) vs. distance from the center plane of QW along the [001] direction. E stands for electron, HH for heavy hole levels, and LH for light hole levels.

QW lasers³³ with 2.2% Bi having a threshold current density of 1.56 kA/cm².

IV. SUMMARY AND CONCLUSION

We have studied the electronic bandstructure and optical properties of lattice matched GaN_{1-x}Bi_xAs/GaAs quaternary alloy quantum well (QW) based on the 16-band *k*-*p* model. The different QW cases studied have their thicknesses and N:Bi:As composition tuned in such a way to have their emission peak at 1.55 μ m, aiming towards optical communication systems. We have obtained insights on how the well thickness and (N, Bi) compositions affect the energy dispersion curves and closeness of electron and hole energy levels. An increase in the injection carrier density increases the maximum gain and also the gain spectral width. In our study, we see that while thinner wells have decreasing differential gain at lower density, thicker wells show the same at higher density. It is, thus, of significant importance to determine the critical well thickness for a steady optical performance. Among our cases studied, we have identified the 6.3 nm thick GaN₃Bi_{5.17}As_{91.83} lattice matched QW to exhibit optimized optical performance for our intended 1.55 μ m (0.8 eV) optoelectronic device/system applications. Therefore, it is recommended that the design parameters such as material composition and well width must be carefully considered from the device application point-of-view for an accurate optimization of the optoelectronic performance characteristics.

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