Effect of strain on $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y/\text{GaAs}$ to extract the electronic band structure and optical gain by using 16-band kp Hamiltonian

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Abstract. $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ is a suitable candidate for $1.06\ \mu\text{m}$ solid state lasers and high-efficiency solar cells. Mathematical models such as 16-band kp model is used to study the band structure, strain generated effect, band offset and variation of their parameters with Bi and N concentrations. Lattice constants of alloy $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ with $x/y = 0.58$ can match those of GaAs with the incorporation of Bi and N into GaAsN. Arsenic atom substitution due to the incorporation of N and Bi impurity atoms causes a significant band gap reduction of $\sim 200\ \text{meV}$ for $\text{GaAs}_{0.937}\text{N}_{0.023}\text{Bi}_{0.04}$ alloys under lattice-matched conditions and in addition, by tuning the concentrations of N and Bi, the electrical and optical properties of GaAsN can be controlled. Optical gain of $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ quantum well (QW) and GaAs as a barrier are calculated in generalized mode and observed the effect of the energy level of GaAs barrier on the GaAsN QW.

Keywords. $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$; kp method; strain; optical gain.

1. Introduction

During the last few decades, III–V–Bi/N alloys have attracted attention towards research because of good physical properties. The co-alloying of Bi and N in GaAs provides application in optoelectronics and makes them attractive candidates for the design of highly capable mid- and far-infrared optical and spintronics devices, providing large and resilient parameter space for band structure engineering [1]. $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ is proposed as quaternary alloys to fabricate new devices in optoelectronic fields, such as $1.06\ \mu\text{m}$ solid-state lasers and high-efficiency multi-junction solar cells, and became important to study optical and electronic properties [2]. GaAsN has been studied in the past few decades because of the large bowing parameter and nitrogen is known to be responsible for structural and electronic defects that effect on optoelectronic efficiency, but it decreases the band gap and lattice constants; obtaining high-quality GaAs GaAsN/GaAs is difficult where as co-alloying with Bi effectively matched the lattice constant of GaAs [3]. A lower value of energy band gap is attainable with GaAsN/Bi with lattice constant matched with GaAs by changing the concentrations of N and Bi. The corresponding band gap reductions are due to resonant interactions rather than alloying. In the case of N, an isolated state resonant with the conduction band of GaAs is imported, while Bi imported a state resonant with the valence band which leads to increase in the carrier concentration without change in mobility [4]. In addition, incorporation of N and Bi into GaAs introduced the compressive and tensile strains. Strong perturbation for Bi concentration for low value of strain auger-suppressing

band structure condition satisfied $E_g < \Delta_{\text{SO}}$ [5]. Tight banding model (TB), semi-empirical methods, band anti-crossing (BAC) theory and density functional theory (DFT) are effective to focus on theoretical simulations of structural and electronic properties of III–V dilute Bi and N containing structure including surfaces, thin films, nanostructures and clusters. Among those reliable computational methods, the most popular one is the kp model. The kp model provides simple and accurate descriptions of the band structure of dilute Bi and N alloys of GaAs in the vicinity of the band edges and hence, will be of importance for the modelling and design of future III–V dilute N- and Bi-based optoelectronic devices. Here, we have studied the 16-band kp model to obtain the band structure and to observe the effect on energy with different mole fractions of N and Bi in $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ for a strained layer. In addition, the kp method is widely used to describe band structure of bulk and nanostructures of semiconductors near the Γ point and the band parameters, such as the band gap, band offsets, spin-orbit (SO) splitting energy and strain of GaAsBiN alloys on GaAs have been reported [5,6]. For the first time Yoshimoto *et al* [7] experimentally have grown successfully GaAsBi by molecular beam epitaxy with a Bi content of 4% and an N content of 8% in 2004. The highest Bi content of 4.7% in the GaAsBi epilayer lattice matched with the GaAs substrate was achieved by Wei *et al* [8] in 2005. The reduction of band gap is well explained using a double BAC model by Lin *et al* [9]. This paper is organized as follows: section 2 provides the theoretical model and physical parameters for calculation of the electronic band structure, optical properties and the corresponding band parameters. Results

Table 1. Material parameters.

E_g^{GaAs} [1]	E_g^{GaN} [1]	E_g^{GaBi} [1]	C_{GaAsN} [1]	C_{GaAsBi} [1]	C_{GaAsNBi} [1]	a_{GaAs} [17]	a_{GaN} [17]	a_{GaBi} [18]
1.43 eV	3.26 eV	−1.45 eV	20 eV	6.1 eV	16.2 eV	5.653 Å	4.50 Å	6.324 Å

of 16-band kp model for the bulk alloy GaAsNBi/GaAs are expressed in section 3. The effects of strain on the band structure have also been discussed in this section and we have also discussed the deviation in band gap energy as a function of Bi concentration in this section. Section 4 contains the essence of our work contribution related to the relevant area.

2. Mathematical modelling

16-band kp Hamiltonian is used to calculate the band structure of bulk $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ alloy. Hamiltonian is a combination of valence BAC (VBAC) and conduction BAC (CBAC) [10]. Material parameters used for calculation are provided in table 1. Here, we used 8- and 16-band kp Hamiltonian required for the calculation of the band structure of GaAsNBi/GaAs quantum wells (QWs). This section is organized as follows. In subsection 2.1, theoretical models and material parameters used to determine electronic band structure with different Bi mole fractions are introduced. The variations of energy and band structure under strain are presented in subsection 2.2. Then, we have calculated the band offset with and without strain in subsection 2.3. In subsection 2.4, the optical gain of $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y/\text{GaAs}$ is presented and unstrained energy for GaAsNBi/GaAs QWs [11] is derived from equation (1):

$$E^{\text{unstrained}}(x, y) = (1 - x - y) \cdot E_g^{\text{GaAs}} + x \cdot E_g^{\text{GaN}} + y \cdot E_g^{\text{GaBi}} - C_{\text{GaAsN}}x(1 - x) - C_{\text{GaAsNBi}}xy, \quad (1)$$

where C is a bowing coefficient.

2.1 VBAC and CBAC models

Bi and N incorporation into GaAs perturbed the valence and conduction bands as Bi generates a resonant impurity state in the valence band as a strongly perturbed host state, while N produces a resonant impurity state additional to the host states in the conduction band. We are taking into account the effect of VBAC and CBAC perturbations using a 16-band Hamiltonian, by the inclusion of 6Bi and 2N related impurity states to the 8-band Hamiltonian of the host semiconductor matrix [10–15]. This approach has been used to study the BAC interaction of Bi and N impurity model predicting the conduction band minima, as there is a N-related impurity state because of quantum anticrossing interaction due to the upward shift of the heavy hole (HH)/light hole (LH) and SO split off due to modification in the valence band structure and

SO-related level bands is well-explained by the VBAC model [13]. The 16-band Hamiltonian reduces to a 6×6 Hamiltonian at the Γ point ($k = 0$) which is as given below [10]:

$$H_{6 \times 6} = \begin{bmatrix} C' & 0 & 0 & V_N(x) & 0 & 0 \\ 0 & H'/L' & 0 & 0 & V_{\text{Bi}}(y) & 0 \\ 0 & 0 & S & 0 & 0 & V_{\text{Bi}}(y) \\ V_N(x) & 0 & 0 & E_N & 0 & 0 \\ 0 & V_{\text{Bi}}(x) & 0 & 0 & E_{\text{Bi}} & 0 \\ 0 & 0 & V_{\text{Bi}}(x) & 0 & 0 & E_{\text{Bi-SO}} \end{bmatrix}, \quad (2)$$

where $C' = E_g^{\text{GaAs}} + \Delta E_{\text{CBM}}(x, y)$, $H'/L' = \Delta E_{\text{VBM}}(x, y)$; and $S = (1/2)(H' + L') - \Delta_0^{\text{GaAs}} = \Delta E_{\text{SO}}(x, y)$, E_g^{GaAs} is unstrained band gap of GaAs and $\Delta E_{\text{CBM}}(x, y)$, $\Delta E_{\text{VBM}}(x, y)$ and $\Delta E_{\text{SO}}(x, y)$ are conduction band offset (CBO), valence band offset (VBO) and SO split off band between the end-point ternary compounds GaAsN and GaAsBi with the following equations:

$$\begin{aligned} \Delta E_{\text{CBM}}(x, y) &= x \Delta E_{\text{CBM}}^{\text{GaAsN}}(x, y) + y \Delta E_{\text{CBM}}^{\text{GaAsBi}}(x, y), \\ \Delta E_{\text{VBM}}(x, y) &= x \Delta E_{\text{VBM}}^{\text{GaAsN}}(x, y) + y \Delta E_{\text{VBM}}^{\text{GaAsBi}}(x, y). \end{aligned} \quad (3)$$

In the same way, we can define $\Delta E_{\text{SO}}(x, y)$, the coupling parameters take care $V_{\text{Bi}}(y) = C_{\text{Bi}}\sqrt{y}$ and $V_N(x) = C_N\sqrt{x}$ of the coupling between the Bi impurity states and the valence band extended states with the host conduction band matrix of the N resonant states. E_N and E_{Bi} give the energy of the N- and Bi-related resonant states and $E_{\text{Bi-SO}}$ is the atomic SO splitting energy for Bi. 6-band Hamiltonian of equation (2) yields six different eigen states corresponding to the splitting of the CB, HH/LH and SO split-off bands into E_+ and E_- sub-bands given by the following set of equations:

$$E_{\text{CB}\pm} = \frac{1}{2} \left(C' + E_N \pm \sqrt{(C'^2 - 2C'E_N + E_N^2 + 4V_N(x)^2)} \right), \quad (4a)$$

$$E_{\text{HH/LH}\pm} = \frac{1}{2} \left(H' + E_{\text{Bi}} \pm \sqrt{(H'^2 - 2H'E_{\text{Bi}} + E_{\text{Bi}}^2 + 4V_{\text{Bi}}(y)^2)} \right), \quad (4b)$$

$$E_{\text{SO}\pm} = \frac{1}{2} \left(S' + E_{\text{BiNSO}} \pm \sqrt{(S'^2 - 2S'E_{\text{BiNSO}} + E_{\text{BiNSO}}^2 + 4V_{\text{Bi}}(y)^2)} \right). \quad (4c)$$

The band gap energy of the quaternary alloy $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ that is a combination of VBAC and CBAC models is given as

$$E_g(x, y) = \frac{1}{2} \left[E_g^{\text{GaAs}} + \Delta E_{\text{CBM}}(x, y) + E_N - \sqrt{(C' - E_N)^2 + 4C_N^2 y} \right] - \frac{1}{2} \left[\Delta E_{\text{VBM}}(x, y) + E_{\text{Bi}} - \sqrt{(H' - E_{\text{Bi}}^2) + 4C_{\text{Bi}}^2 x} \right]. \quad (5)$$

Using Vegard's law, the lattice constant of $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ can be obtained by linear interpolation of endpoint compound of lattice constant [16,17]:

$$a_{\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y} = (1-x-y)a_{\text{GaAs}} + ya_{\text{GaBi}} + xa_{\text{GaN}}, \quad (6)$$

the value of lattice constant is given in table 1. The band parameters required for the calculation of VBAC and CBAC band gap and SO splitting energy for the $\text{GaAsN}_x\text{Bi}_y$ are listed in table 2.

As kp models have some advantages compared with other models like DFT, etc. and also have some limitation: firstly, we are only able to see the energy variation with respect to wave vector in the first Brillouin zone (BZ). Secondly, only certain values of doping atom concentration are feasible in this model if large concentration of doping atom shifts to another model like DFT. In our model, we used 16-band kp Hamiltonian which is the mixture of impurity and potential matrix, and these matrices depend upon end-point ternary compound and coupling parameter, which in turn depends upon the incorporation of Bi concentration into GaAs. Substituting a small percentage of As by Bi in GaAs produces a huge reduction of band gap energy from 60 to 90 meV/Bi% of incorporation described by the VBAC model. The band gap reduction in bismide alloys is mainly due to the movement of HH and LH

bands. However, the position of the split off SO band is found unchanged significantly, resulting in a huge increase in the SO splitting energy (Δ_o). This makes $\text{GaAs}_{1-x}\text{Bi}_x$ a unique material for possible applications in spintronics. Following this model, incorporation of Bi in GaAsBi alloys grown over GaAs substrates leads to perturbation in the valence band which then leads to the formation of six sub-valence bands which can be grouped in levels $E_{+, (\text{HH}, \text{LH}, \text{SO})}$ and $E_{-, (\text{HH}, \text{LH}, \text{SO})}$. The energy level related to the six above-mentioned sub-bands depends on the Bi Concentration. At $x > 10\%$ Bi, the energy splitting of the split off band exceeds the band gap ($\Delta_o \geq E_g$). This feature in the band structure could suppress an important Auger recombination channel and improve the performance of semiconductor lasers having Bi-containing active layers [5,11,12,22].

2.2 16-band kp model

Substitution of arsenic atoms in GaAs by Bi and N leads to the formation of localized defect states near the valence sub-bands HH/LH, SO and CB of the host semiconductor in which the energy levels E_{Bi} , $E_{\text{Bi-SO}}$ and E_N , respectively, were included in the 16-band Hamiltonian. The electronic band structure of $\text{GaAs}_{1-x-y}\text{N}_x\text{Bi}_y$ can be determined using this Hamiltonian which is the modified form of the 8-band kp Hamiltonian based on the eight band second-order Kane model applied to the zinc blended structure and Löwdin perturbation theory [16]. The resultant (16×16) matrix of the Hamiltonian can be written as [9,14]:

$$H_{16 \times 16} = \begin{bmatrix} H_{8 \times 8}^{\text{mod}} & V_{8 \times 8}^{\text{N,Bi}}(y, x) \\ V_{8 \times 8}^{\text{N,Bi}}(y, x) & E_{8 \times 8}^{\text{mod}} \end{bmatrix}, \quad (7)$$

where $H_{8 \times 8}$ is modified with strain effect include 8×8 matrix given below:

$$H_{8 \times 8} = \begin{bmatrix} C & 0 & -\frac{1}{\sqrt{2}}P_+ & \sqrt{\frac{2}{3}}P_Z & \frac{1}{\sqrt{6}}P_- & 0 & \frac{1}{\sqrt{3}}P_Z & \frac{1}{\sqrt{3}}P_- \\ 0 & C & 0 & \frac{1}{\sqrt{6}}P_+ & \sqrt{\frac{2}{3}}P_Z & \frac{1}{\sqrt{2}}P_- & \frac{1}{\sqrt{3}}P_+ & -\frac{1}{\sqrt{3}}P_Z \\ -\frac{1}{\sqrt{2}}P_+^* & 0 & H & \alpha & \beta & 0 & \frac{i\alpha}{\sqrt{2}} & -i\sqrt{2}\beta \\ \sqrt{\frac{2}{3}}P_Z & \frac{1}{\sqrt{6}}P_+^* & \alpha^* & L & 0 & \beta & i\left(\sqrt{2}\varepsilon - \frac{D}{\sqrt{2}}\right) & i\alpha\sqrt{\frac{3}{2}} \\ \frac{1}{\sqrt{6}}P_-^* & \sqrt{\frac{2}{3}}P_Z & \beta^* & 0 & L & -\alpha & -i\alpha^*\sqrt{\frac{3}{2}} & i\left(\sqrt{2}\varepsilon - \frac{D}{\sqrt{2}}\right) \\ 0 & -\frac{1}{\sqrt{2}}P_-^* & 0 & \beta^* & -\alpha^* & H & -i\sqrt{2}\beta^* & -\frac{i\alpha^*}{\sqrt{2}} \\ \frac{1}{\sqrt{3}}P_Z & -\frac{1}{\sqrt{2}}P_+^* & \frac{i\alpha^*}{\sqrt{2}} & i\left(-\sqrt{2}\varepsilon + \frac{D}{\sqrt{2}}\right) & i\alpha\sqrt{\frac{3}{2}} & i\sqrt{2}\beta & S & 0 \\ \frac{1}{\sqrt{3}}P_-^* & -\frac{1}{\sqrt{3}}P_Z & i\sqrt{2}\beta^* & -i\alpha\sqrt{\frac{3}{2}} & i\left(\sqrt{2}\varepsilon - \frac{D}{\sqrt{2}}\right) & \frac{i\alpha}{\sqrt{2}} & 0 & S \end{bmatrix}, \quad (8)$$

Table 2. Band parameters of GaAsN and GaAsBi alloys for VBAC and BAC calculations.

Parameter	Considered value (eV)
E_N	0.89 [22]
C_N	2.83 [22]
E_{Bi}	-1.25 [19]
E_{Bi-SO}	-2.7 [19]
C_{Bi}	1.01 [19]
E^{GaAs}	1.43 [20]
Δ^{GaAs}	0.341 [20]
E_P^{GaAs}	28.8 [20]
ΔE_{CBM}^{GaAsN}	0.07 [17]
ΔE_{VBM}^{GaAsN}	1.84 [17]
ΔE_{SO}^{GaAsN}	1.52 [17]
ΔE_{CBM}^{GaAsBi}	-2.30 [21]
ΔE_{VBM}^{GaAsBi}	0.6 [21]
ΔE_{SO}^{GaAsBi}	-1.3 [21]

where

$$C = E_g + \frac{\hbar^2}{2m_0} \left[\frac{1}{m_e^*} - \frac{E_P}{3} \left(\frac{2}{E_g} - \frac{1}{E_g + \Delta_{SO}} \right) \right] \times (K_x^2 + K_y^2 + K_z^2) + \Delta E_{CBM}(x, y) + \varepsilon_1(z), \quad (9a)$$

$$H = \frac{-\hbar^2}{2m_0} [(K_x^2 + K_y^2)(\gamma_1 + \gamma_2) + K_z^2(\gamma_1 - 2\gamma_2)] + \Delta E_{VBM}(x, y) + \varepsilon_2(z), \quad (9b)$$

$$L = \frac{-\hbar^2}{2m_0} [(K_x^2 + K_y^2)(\gamma_1 - \gamma_2) + K_z^2(\gamma_1 + 2\gamma_2)] + \Delta E_{VBM}(x, y) - \varepsilon_2(z), \quad (9c)$$

$$S = 1/2(L + H) - \Delta_{SO} - \Delta E_{SO}(x, y) - \varepsilon_2(z), \quad (9d)$$

$$D = L - H, \quad (9e)$$

$$P_{\pm} = P(K_x \pm iK_y) - P(e_{xx}K_x \pm ie_{yy}K_y), \quad (9f)$$

$$P_z = PK_z - P(e_{zz}K_z), \quad (9g)$$

$$\alpha = \frac{\hbar^2}{2m_0} 2\sqrt{3} [K_z(K_x - iK_y)\gamma_3], \quad (9h)$$

$$\beta = \frac{\hbar^2}{2m_0} \sqrt{3} [(K_x^2 + K_y^2)\gamma_2 - 2iK_xK_y\gamma_3], \quad (9i)$$

$$\varepsilon_1(z) = \begin{cases} 2(a_c + a_v)(1 - C_{12}/C_{11})e_{xx} & \text{in the well,} \\ 0 & \text{in the barrier,} \end{cases}$$

$$\varepsilon_2(z) = \begin{cases} b(1 + 2C_{12}/C_{11})e_{xx} & \text{in the well,} \\ 0 & \text{in the barrier.} \end{cases} \quad (10)$$

Here C , H , L and S are modified with band offsets and related to strain parameters $\Delta E(x, y)$ and $\varepsilon(z)$, respectively. In equation (10), a_c and a_v are the hydrostatic deformation potential for conduction and valence band, respectively, b is the shear deformation potential and C_{11} and C_{12} are the elastic stiffness constants:

$$e_{xx} = \frac{a' - aM}{aM}, \quad (11a)$$

e_{xx} is in plane strain where a' and aM are the lattice constants for the substrate and well layer, respectively. P is the Kane matrix element and is normally expressed in terms of electron volt (eV) as below [19–22]:

$$E_P = \frac{2m_0}{\hbar^2} P^2. \quad (11b)$$

In the 8×8 Hamiltonian, valence band parameters related to the Luttinger parameters are used in the 6×6 valence band Hamiltonian due to inclusion of the conduction band states in the 8×8 Hamiltonian [22]. The relation between the modified Luttinger parameters and the Luttinger parameters related to VBAC is given below [23,24]:

$$\gamma_1 = \gamma_1^{VB} - \frac{E_P}{3E_g},$$

$$\gamma_2 = \gamma_2^{VB} - \frac{E_P}{6E_g},$$

$$\gamma_3 = \gamma_3^{VB} - \frac{E_P}{6E_g}. \quad (12)$$

2.3 Strain-related VB and CB shifts for GaAsNBi/GaAs QWs

The conduction band and valence band edges shifted due to the effect of hydrostatic and shear strain in GaAsNBi/GaAs QWs. Strain-induced ones shift the conduction band minimum and the valence band maxima calculated using the Bir-Pikus Hamiltonian [25], and are responsible for the quantum confinement of electrons and holes in QW structures. The shear component of strain that causes the separation between the valence sub-bands E_{VB-HH} and E_{VB-LH} by removing the valence band degeneracy is given as [26]:

$$E_{CB}(\varepsilon) = E_{CB}(\varepsilon = 0) + \Delta E_{CB}^{hy},$$

$$E_{VB-HH}(\varepsilon) = E_{VB}(\varepsilon = 0) + \Delta E_{VB}^{hy} - 1/2\Delta E_s,$$

$$E_{VB-LH}(\varepsilon) = E_{VB}(\varepsilon = 0) + \Delta E_{VB}^{hy} + 1/2\Delta E_s, \quad (13)$$

where $\Delta E_{CB}^{hy} = 2a_c \left(1 - \frac{c_{12}}{c_{11}}\right) e_{xx}$ and $\Delta E_{VB}^{hy} = 2a_v \times \left(1 - \frac{c_{12}}{c_{11}}\right) e_{xx}$ influence of hydrostatic components of strain on the conduction and valence bands, respectively and $\Delta E_s = 2b \left(1 + \frac{c_{12}}{c_{11}}\right) e_{xx}$ contribute shearing of strain to the band structure.

Figure 1. Energy level positions of $E_{\pm}$ with respect to CB, HH, LH and SO bands as a function of Bi and N mole fractions for (a) compressive-strained and (b) tensile-strained GaAsNBi/GaAs QWs at room temperature ($T = 300$ K). Dashed lines represent the lattice-matched conditions.

2.4 Optical gain

Optical gain $g(\hbar\omega)$ for GaAsNBi/GaAs QWs is calculated by taking into account all the transitions between respective sub-bands as per density matrix theory [27,28]. A conformist method [29] based on the intraband relaxation time (τ_{in}) approximation convoluted with a Lorentzian function with suitable broadening time (1×10^{-14} s) is used to evaluate optical gain spectra [30] given as:

$$g(\hbar\omega) = \frac{\pi q^2}{n_r c \omega L_w \epsilon_0 m_0^2} \sum_{n,m} \int_0^\infty \frac{k_p dk_p}{2\pi} |M_{nm}(k_p)|^2 \times L(E_{n,m}^{c,v}(k_p)) \{f_n^c(E_n^c(k_p)) - f_m^v(E_m^v(k_p))\}, \quad (14)$$

where c and ϵ_0 are the velocity of light and relative permittivity in free space, n_r is the refractive index of the QW, L_w is the thickness of the QW, k_p is the in-plane wave vector, $M_{nm}(k_p)$ is the momentum matrix element between the m th valence sub-band and n th conduction band sub-band. f_n^c and f_m^v are the Fermi-Dirac distribution for electrons and holes, given as

$$f_n^c(k_p) = \left[1 + \exp \left\{ \frac{E_n^c(k_p) - E_f^c}{k_B T} \right\} \right]^{-1},$$

$$f_m^v(k_p) = \left[1 + \exp \left\{ \frac{E_m^v(k_p) - E_f^v}{k_B T} \right\} \right]^{-1}. \quad (15)$$

The Lorentzian function defined in [26] is as follows:

$$L(E_{n,m}^{c,v}(k_p)) = \frac{1}{\pi} \frac{\hbar/\tau_{in}}{[E_n^c(k_p) - E_m^v(k_p) - \hbar\omega]^2 + \left(\frac{\hbar}{\tau_{in}}\right)^2}. \quad (16)$$

where E_n^c and E_m^v are the energy dispersion curves of the n th and the m th sub-bands, respectively, consider the barrier effecting [30–32], E_f^c and E_f^v are the quasi-Fermi levels of corresponding bands.

3. Results and discussion

Figure 1 shows the variation of E_+ and E_- energy levels related to the CB and VB in strained GaAsNBi/GaAs QWs. Figure 1a shows the variation of energy level which is linear in compressive strain and figure 1b shows the deviation under tensile strained with respect to the dashed line under lattice matched conditions is more considerable, showing the effect of N on band structure is more than Bi impurity and non-linear variation of E_{CB+} and E_{CB-} in tensile-strained. For unstrained conditions in figure 1a (lattice-matched conditions as shown by the dashed line), addition of Bi and N into GaAs, pushes the energy level E_{CB-} in the downward direction nearly about 100 meV/%Bi and E_{HH}/L_{H+} in the upward direction by 47 meV/%Bi. The SO split off energy level E_{SO+} moves upward by nearly 6 meV/%Bi which shows that there is a slight increase of the SO splitting energy.

Figure 2 presents the difference in the band structure of tensile- and compressive-strained GaAsNBi/GaAs QW structures. These strains of band structure are plotted for N and Bi concentration ratios of 5 and 0.2, respectively, which is greater than or less than the matched lattice N to Bi concentration ratio of 0.58. The band gap is calculated to be lower as 0.47 eV under the tensile-strained GaAs_{0.94}N_{0.05}Bi_{0.01}/GaAs QWs; however, in the case of compressive-strained GaAs_{0.94}N_{0.01}Bi_{0.05}/GaAs QWs where such considerable splitting is not observed and band gap with a

Figure 3. Variation of (a) CBO, (b) VBO, (c) CBO ratio and (d) VBO ratio for GaAsNBi with Bi mole fraction (y) for different values of N concentration in the material. Dashed lines are used to represent the lattice-matched conditions ($x/y = 0.58$).

Figure 4. (a) The band offset of conduction band (BOCB), (b) heavy hole (BOHH) and light hole (BOLH) under strain conditions as a function of Bi mole fraction under different nitrogen concentrations.

wavelength; for fixed value of carrier density, this occurs because energy of sub-band is inversely proportional to the well width. Stronger carrier confinement occurs as the overlap

of the exciton wave function increases, and transition energy of the carrier that shift the peak gain towards lower wavelength as shown in figure 7.

Figure 5. Comparison between calculated and experimental [34] and from the literature [11,35] value of band gap for GaAsNBi as a function of bismuth concentration at $T = 300$ K.

Figure 6. Optical gain plot against photon energy for different values of carrier concentrations exhibiting the interband transitions in GaAs_{0.937}N_{0.023}Bi_{0.040}/GaAs QWs with the barrier effect of GaAs.

Figure 7. Optical gain considered barrier effect of GaAs in the GaAs_{0.937}N_{0.023}Bi_{0.040}/GaAs QWs for different values of width for the fixed value of carrier concentration of $3 \times 10^{16} \text{ m}^{-2}$.

Figure 8. Optical gain spectra having 10 nm width of the GaAs_{0.937}N_{0.023}Bi_{0.040}/GaAs QWs considered barrier effect of GaAs, for different values of carrier concentrations.

Figure 9. Quantum confinement potential and energy levels for electrons and holes for 10 nm wide GaAsNBi/GaAs QWs under lattice-matched conditions.

Optical gain variation with different values of carrier density of the GaAs_{0.937}N_{0.023}Bi_{0.040}/GaAs QWs with a 10 nm active layer is shown in figure 8. As we see from the graph, increasing the rate of carrier density leads to improvement in the difference of the Fermi function in the mid-infrared region. For optoelectronic devices like sub-band energy, it will act as a tuning parameter. We also observed from the graph that with fixed width of QWs and varying carrier density causes the shift in peak towards lower wavelength.

The quantum confinement potential and the positions of CB and VB energy levels for lattice matched 10 nm-wide GaAsNBi/GaAs QWs and the dispersion of the corresponding telecommunication window ($1.55 \mu\text{m}$) are shown in figure 9.

4. Conclusions

Band structure of GaAsNBi alloy lattice matched with GaAs substrates and band structure was calculated using 16-band *kp* Hamiltonian. VBO and CBO as well their ratios are calculated as a function of both Bi and N mole fractions. CBO as high as 470 meV and VBO of 220 meV are obtained which can improve the device characteristics by providing strong carrier confinement. Band gap values of 0.47 and 0.78 eV are obtained for tensile-strained GaAs_{0.94}N_{0.05}Bi_{0.01}/GaAs QWs and compressive-strained GaAs_{0.94}N_{0.01}Bi_{0.05}/GaAs QWs, respectively. Injected charge carrier density increases with an increase in the optical gain of QWs, but for constant value of injected charge carrier density with increase in the dimension of QWs, optical gain decreases because of reduction in the density of state in the sub-band. Hence, the reduction in width of quantum well and peak of optical gain shows the blueshift. Bi and N in GaAs will perturb the valence band without affecting mobility. This leads to improvement in speed response. Inter sub-band transition occurred in GaAsNBi/GaAs between HH and LH sub-bands. Inter sub-band transitions occurring between the VB and CB sub-bands could make possible the fabrication of solar cells and lasers operating in the 1.5 μm wavelength region.

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