

Improving a Compressively Strained $\text{Ga}_x\text{In}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$ Multiple Quantum Well Lasers for Emitting around 1300 Nm

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Abstract: The objective of this work is to study the effect of Nitrogen incorporation on the structural and optical properties of $\text{Ga}_x\text{In}_{1-x}\text{N}_y\text{As}_{1-y}$ semiconductor alloy in order to obtain quantum well $\text{Ga}_x\text{In}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$ structures emitting at wavelengths around 1.3 μm . We also investigated their effect on the band gap energy, the electron effective mass, the optical gain, and the optical confinement. The incorporation of Nitrogen in the $\text{Ga}_x\text{In}_{1-x}\text{As}$ alloy gave very particular and attractive properties, the most important being the reduction of the band-gap energy and a significant increase in effective mass, which results in an increase in the emission wavelength. The anticrossing band model describes these properties. It is also found that the optical gain and confinement factor were found to be strongly increased when the Nitrogen content was reduced. In order to achieve a wavelength of 1.3 μm and maintain a high-quality structure, we found that decreasing the Gallium composition (x) and increasing the Nitrogen composition (y) simultaneously gave accurate results.

1 INTRODUCTION

The GaInNAs/GaAs quantum-well system has attracted much interest over the past 10 years due to its advantages over conventional III-V alloys. The reduction of the band gap of GaInNAs and its lattice matching to GaAs allow for optoelectronic devices based on a GaAs substrate, which emits in the optical fibre windows of 1.3 and 1.55 μm (Qiu, 2008). Long-wavelength 1.3 and 1.55 μm optoelectronic devices such as lasers, detectors, filters, and optical amplifiers are key components of present optical fibre communications because of the minimum loss in this wavelength region (Fang, 2006). So far, many high-efficiency GaInNAs-based lasers have been reported. However, the physics of GaInNAs is still not fully understood and has been under intensive study for the last few years. Different approaches, such as the band-anticrossing model, empirical pseudo-potential super cell method, first principles pseudo-potential method, and tight-binding method, were proposed in order to explain the GaInNAs band structure and its optical properties (Kudrawiec, 2004). A major breakthrough was achieved for dilute nitride alloys with the demonstration by Walukiewicz and co-workers that the reduction in energy gap in $\text{Ga}(\text{In})\text{N}_x\text{As}_{1-x}$ is due to a band-anticrossing interaction between the

conduction band edge and higher-lying localised nitrogen resonant states (Shan, 1999).. Given the significant differences in the conduction band structure of GaInNAs compared to conventional III-V semiconductors, it is important to elucidate the influence of N not only on the electronic structure but also on the gain characteristics of ideal dilute nitride lasers (Broderick, 2012). In the present paper, our study has focused on the improvement of $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{N}_{1-y}/\text{GaAs}$ multiple quantum well lasers operating continuously for longer wavelengths with the incorporation of Nitrogen, and this by optimising the important parameters of the laser, which are the optical gain and the confinement factor. To this purpose, we carried out a detailed study of all the properties of the quantum well system based on $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{N}_{1-y}/\text{GaAs}$. We began with band gap energy and electron effective mass using the band-anticrossing (BAC) model, then determined the optical gain and confinement of the $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{N}_{1-y}/\text{GaAs}$ heterostructure.

2 THEORY AND MATERIAL PARAMETERS

The lasers used in this study are multiple quantum well lasers. Our suggested structure comprises a QW

layer of $\text{Ga}_{0.7}\text{In}_{0.3}\text{N}_y\text{As}_{1-y}$ material having a thickness of 7 nm placed between two wide band gap barrier layers of GaAs material having a thickness of 10 nm, followed by cladding layers of $\text{Al}_{0.4}\text{Ga}_{0.6}\text{As}$ material of 2 μm thickness. Clearly, the quantum well layer band gap is narrower as compared to that of the barrier region, and the barrier layer band gap is narrower as compared to that of the cladding region. Our structure has the same thickness and the same Gallium composition; the composition of Nitrogen is the only parameter that can be varied, as its value changes from 0 to 4%. The compositions of $\text{Ga}_{0.7}\text{In}_{0.3}\text{N}_y\text{As}_{1-y}$ alloys (well) suitable for long-wavelength lasers grown on GaAs alloy (barrier) are selected arbitrary, taking into account the built-in strain in the well material and a desired emission wavelength. We assumed that for 7 nm-wide QW grown on GaAs, the compressive strain should be $\leq 2\%$. The content of Gallium (x) is kept constant; only the Nitrogen content (y) is added to the well material. We found that it leads to a small reduction of the compressive strain in the QW. We also found that the lattice mismatch defined by the parameter (ϵ) is negative, whatever the value of the N concentrations. This means that our $\text{Ga}_{0.7}\text{In}_{0.3}\text{N}_y\text{As}_{1-y}/\text{GaAs}$ heterostructure is under compression. The choice of the alloy composition adopted in our study (y from 0 to 4%) is due to the low mesh mismatch ($\epsilon \leq 2\%$) between the well and the barrier for these compositions and the wavelength to be obtained. Our $\text{Ga}_{0.7}\text{In}_{0.3}\text{N}_{0.01}\text{As}_{0.99}/\text{GaAs}$ hetero-structure is characterised by a weak bi-axial compressive strain of the order $\epsilon = \Delta a/a = -1.9\%$, while the $\text{Ga}_{0.7}\text{In}_{0.2}\text{N}_{0.02}\text{As}_{0.98}/\text{GaAs}$ hetero-structure has a bi-axial compressive strain of the order $\epsilon = -1.7\%$ (Hadjaj, 2021). In order to improve the performance of $\text{Ga}_{0.7}\text{In}_{0.3}\text{N}_y\text{As}_{1-y}/\text{GaAs}$ quantum well lasers, the Nitrogen composition of the $\text{Ga}_{0.7}\text{In}_{0.3}\text{N}_y\text{As}_{1-y}$ well should be reduced, although this leads to increased strain in the quantum wells. The $\text{Ga}_x\text{In}_{1-x}\text{N}_y\text{As}_{1-y}$ alloy is a material that combines binary compounds such as GaAs, InAs, GaN, and InAs to crystallise in the zinc-blend structure. The parameters of the four binaries are as illustrated in Table 1.

Table 1: Basic properties of the binary semiconductors GaAs, InAs, GaN, and InN in the zinc-blende structure used for the computations: E_g , energy gap; a_0 , lattice constant; m_e/m_0 , electron effective mass; α and β , Varshni's parameters; and n, refractive index calculated by Herve and Vandamme relation (H.V.). Our calculated results were compared with the available theoretical and published values and showed excellent agreement (Ioffe, 2013).

Parameter	GaAs	InAs	GaN	InN
$E_g^T(0 \text{ K})$ (eV)	1.519 ^{a,b}	0.417 ^{a,b}	3.299 ^b	1.94 ^b
$E_g^T(300 \text{ K})$ (eV)	1.422 ^d	0.354 ^d	3.24 ^d	1.916 ^d
$\alpha(\Gamma)$ (10^{-4}eV/K)	5.405 ^b	2.76 ^b	5.93 ^b	2.45 ^b
$\beta(\Gamma)$ (K)	204 ^b	93 ^b	600 ^b	624 ^b
a_0 (\AA)	5.6533 ^b	6.0584 ^b	4.50 ^b	4.98 ^b
m_e/m_0	0.067 ^b	0.023 ^c	0.15 ^b	0.12 ^b
n (theoretical)	3.3 ^c	3.51 ^c	2.3 ^c	2.9 ^c
n (calculated by H.V)	2.99 ^d	3.758 ^d	2.208 ^d	3.404 ^d

^aRef. (Fox, 2010), ^bRef. (Vurgaftman, 2003), ^c Ref. (Ioffe, 2013), ^d Ref. calculated.

The refractive indices for the ternaries and for the quaternaries are then calculated from the indices of the binaries according to Vegard's laws (Takagi, 1982). The refractive index of ternary alloys $A_xB_{1-x}C$ and $AB_{1-x}C_x$ are usually given as:

$$n_{(AB_{1-x}C_x)}^2 = xn_{AB}^2 + (1-x)n_{AC}^2 \quad (1)$$

$$n_{(A_xB_{1-x}C)}^2 = xn_{AC}^2 + (1-x)n_{BC}^2 \quad (2)$$

And its expression for quaternary $A_xB_{1-x}C_yD_{1-y}$ is given by the following relation:

$$n_{ABCD}^2 = y(1-x)n_{AC}^2 + (1-x)(1-y)n_{AD}^2 + xyn_{BC}^2 + x(1-y)n_{BD}^2 \quad (3)$$

The variation of refractive index is also calculated using empirical Herve and Vandamme's formula, which is a function of band gap energy:

$$n = \sqrt{1 + \left(\frac{A}{B+E_g}\right)^2} \quad (4)$$

Where A and B have the values 6.13 and 3.4 eV, respectively. In fact, the semiconductor refractive index is a fundamental physical parameter that characterises optical and electrical properties (Koezuka, 1987).

3 BAND ANTI-CROSSING MODEL

Many models were proposed for the calculation of the band gap energy of GaInNAs alloys, and the most accepted theory is that of the band-anticrossing (BAC) model. Low concentrations of N introduce a highly localised acceptor-like level in conventional III-V semiconductors. This narrow resonant band interacts strongly with the conduction band, ultimately leading to the splitting of the conduction band and a reduction of the fundamental energy band gap. The two resulting coupled bands are identified as E⁻ and E⁺, and a simple model of two interacting energy levels can be used to find their dispersion relationship.

$$E_{\pm}(k) = 1/2 \{ [E_M(k) + E_N] \pm \sqrt{[E_M(k) - E_N]^2 + 4yV_{MN}^2} \} \quad (5)$$

Where $E_M(k)$ is the conduction band energy of InGaAs, E_N is the energy of the N level relative to the top of the valence band, and V_{MN} is the matrix element describing the interaction between E⁺ and E⁻ (Shan, 1999, Skierbiszewski, 2002). The functional form for V_{MN} and E_N parameters reads :

$$V_{MN} = C_{MN}\sqrt{y} \quad (6)$$

with $C_{MN} = 2.7$ for $x \leq 0.93$

In the above, y is the Nitrogen concentration, and C_{MN} is the parameter that depends on the matrix semiconductor, hence the In composition (Erol, 2008, Sze, 1981). Based on this BAC model, the shifting-down energy gap is given by (Yu, 2001):

$$\Delta E_g = \sqrt{[E_M - E_N]^2 + 4yV_{MN}^2} - [E_M + E_N]/2 \quad (7)$$

In semiconductors, the effective mass approximation only works for the parabolic energy dispersion at small wave vectors k and for small electron energies close to the minimal Γ point. However, due to N incorporation, the conduction band energy saturates at relatively low k magnitude, resulting in a heavy effective electron mass at higher energy levels in the GaInNAs alloys. To include the non-parabolic conduction band, the approach developed by Zawadzki is used. It calculates non-parabolic dispersion in small-band gap semiconductors (Zawadzki, 1974). Energy affects the electron effective mass m_e , and its inverse is as follows:

$$\frac{1}{m_e(k)} = \frac{1}{\hbar^2 k} \cdot \left| \frac{dE(k)}{dk} \right| \quad (8)$$

Replacing $E(k)$ by equation 5, the analytic expression for k -dependent inverse electron effective masses of Nitrogen-containing alloys is:

$$\frac{1}{m_{e\pm}(k)} = \frac{1}{2m_e^0(k)} \cdot \left\{ 1 \pm \frac{[E_M - E_N]}{[E_M - E_N]^2 + 4(C_{MN})^2 y} \right\} \quad (9)$$

Where $m_e^0(k)$ is the electron effective mass of the host material, such as Ga_xIn_{1-x}As in the case of Ga_xIn_{1-x}N_yAs_{1-y} (Skierbiszewski, 2000).

4 RESULTS AND DISCUSSION

First, we study the band properties of the Ga_xIn_{1-x}N_yAs_{1-y} alloy. We start by determining the variation of the band gap energy as a function of the Nitrogen composition ($y \leq 4\%$) for different Gallium compositions.

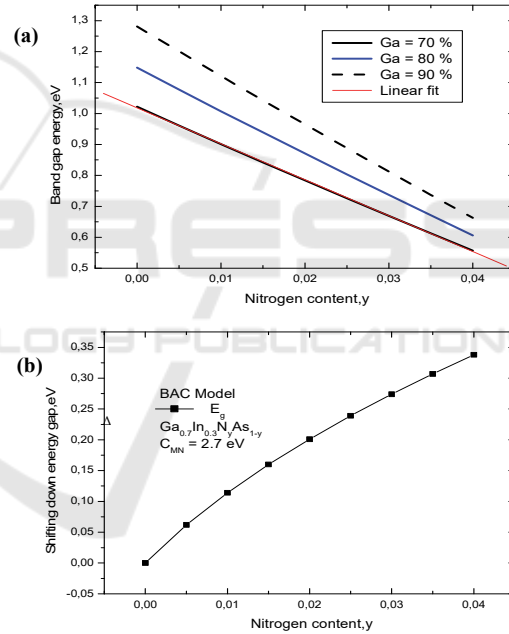


Figure 1: (a) The band gap energy and (b) the shifting down energy gap as a function of Nitrogen composition (y), for different compositions of Gallium (x) in Ga_xIn_{1-x}N_yAs_{1-y} alloys, the band gap is calculated using Vegard's law.

It can be seen that if the concentration of Nitrogen increases, the energy of the band gap decreases, if we set the concentration of Ga (x) at 0.7, the band gap of the Ga_{0.7}In_{0.3}N_yAs_{1-y} alloys as a function of the Nitrogen concentration y decreases with the increase in the proportion of Nitrogen y and it increases with increase in the proportion of Gallium x , Furthermore, the addition of N decreases

the band gap energy of $Ga_xIn_{1-x}As_{1-y}N_y$ material system, thus rapidly reaching the long wavelength emission region. Figure 1 shows also the variation of the shifting down energy gap as a function of Nitrogen composition (y) in $Ga_{0.7}In_{0.3}As_{1-y}N_y$ alloys. We found that when the Nitrogen concentration becomes important (4%), ΔE_g reaches 0.338 eV. From this we conclude that the shifting down energy gap is increased with an increase in Nitrogen content in $Ga_{0.7}In_{0.3}As_{1-y}N_y$ alloys.

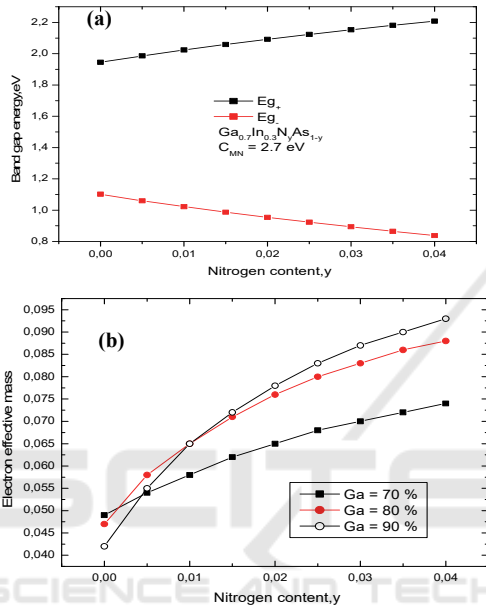


Figure 2: (a) The band gap energy and (b) the electron effective mass as a function of Nitrogen composition (y), the curves are calculated using the band-anticrossing model.

We see that at a certain percentage of Nitrogen, the band gap splits into two bands, and the more the Nitrogen concentration increases, the more this split becomes important. These results are very close to the theoretical results of Refs (Aissat, 2007, Spruytte, 2001, Yasar, 2015). The band anti-crossing (BAC) model can explain this significant reduction of the band gap with Nitrogen incorporation. Nitrogen atoms are smaller and have a higher electronegativity than as atoms, which leads to the formation of defect states near the edge of the conduction band. These Nitrogen-related defects are highly localised and form a narrow band that resonates with the extended states of the GaInAs conduction band. This coupling through anticrossing interaction results in the splitting of the conduction band into two subbands. Figure 2 shows also the variation of the electron effective mass m_e^* for

$Ga_xIn_{1-x}As_{1-y}N_y$ alloy with different Gallium and nitrogen contents. As can be seen, a very large increase of the effective mass is found with higher N composition, the reduced band gap energy by adding N increases the electron effective mass, which it is in good qualitative agreement with the predictions of the BAC model.

The optical gain in a semiconductor laser is an essential parameter to characterise fabricated lasers and to simulate their behavior. Figure 3 represents the variations of the optical gain as a function of the wavelength for different values of the Nitrogen composition. In order to obtain a structure with an emission wavelength of 1.3 μm , we decreased the Gallium composition, fixed it at 0.7, and increased the Nitrogen composition from 1% to 4% to reduce strain, as we had previously found that increasing Nitrogen decreases strain. Then we determined the best structure that gave us the desired emission wavelength.

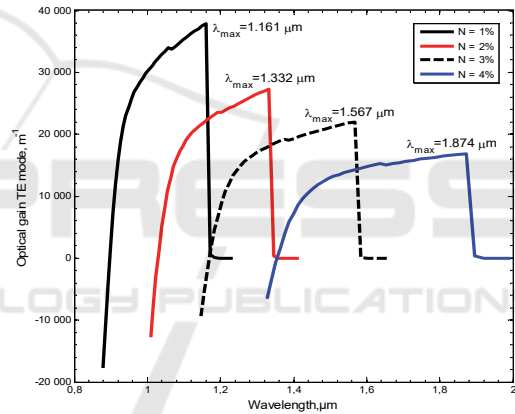


Figure 3: TE mode of the optical gain as function of wavelength for $Ga_{0.7}In_{0.3}N_yAs_{1-y}/GaAs$ SQWs for different compositions of Nitrogen (y) obtained for the well with 7 nm, a barrier of 10 nm, an intraband relaxation time of 0.5 ps, and an ambient temperature of 300 k.

It is noted that increasing the carrier density in the active region causes an increase in the maximum optical gain. This phenomenon is linked to the filling of the high states of the conduction and valence bands with an increase in the number of carriers. We easily observed that varying the N composition shifts the optical gain spectrum towards longer wavelengths and reduces the maximum optical gain, as shown in figure 3. The shift in the gain spectrum is due to the decrease in the gap of $Ga_{0.7}In_{0.3}N_yAs_{1-y}$ while the decrease in the maximum optical gain is particularly due to the reduction in optical confinement since the refractive index is higher in

the active layer than in the adjacent layers for a high concentration of Nitrogen. We conclude that the gain spectrum shifts by varying the Nitrogen and Gallium compositions. To reach high wavelengths, we must decrease the Gallium composition and increase the Nitrogen composition.

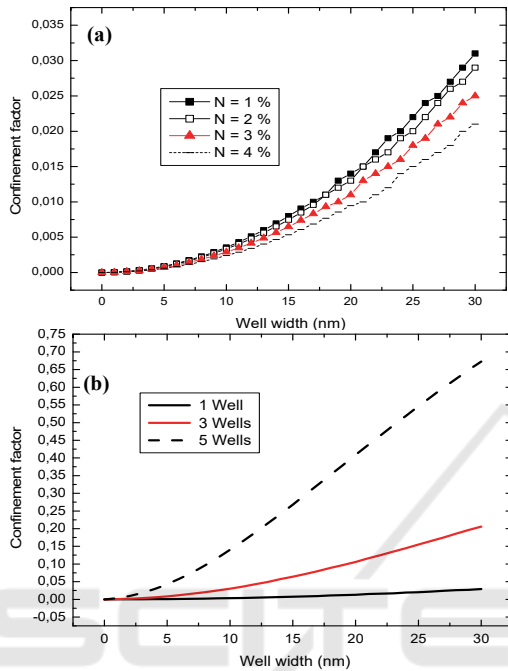


Figure 4: The confinement factor as a function of well width (a) for different Nitrogen composition (y) (b) for different well number.

Figure 4 displays how the confinement factor changes with well width for a $\text{Ga}_{0.7}\text{In}_{0.3}\text{N}_{0.02}\text{As}_{0.98}/\text{GaAs}$ structure with different numbers of wells. The number of wells multiplied by the well width is a crucial component of the structure that improves confinement factor. This figure also represents the variation of the confinement factor as a function of the well width for different N compositions. It is observed that the confinement factor increases with the increase in the well width and decreases with the increase in the N composition. We also see that the wavelength increases by increasing the Nitrogen composition; this increase is due to the decrease in the energy of the band gap with the Nitrogen composition. To reach a wavelength of 1.3 μm , we reduce the composition of Gallium and increase the concentration of Nitrogen from 1% to 4%, as well as the width of the quantum well. To achieve the desired wavelength, we must choose the right compositions of the Material used for the wells to

obtain the corresponding band gap energies. We must also choose the right compositions of the material used for the barrier to have a good mesh agreement or a mesh disagreement less than 2%. To avoid carrier leakage, we must have good confinement of electrons and holes. From this we conclude that the incorporation of Nitrogen has led to degradation in the structure's properties, as we noticed that adding a small percentage of Nitrogen reduces both gain and confinement. It also reduces the band gap, which increases the emission wavelength, in addition to increasing the strain.

5 CONCLUSIONS

In conclusion, the effect of the incorporation of Nitrogen on the properties of $\text{Ga}_x\text{In}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$ MQWs has been carried out. The band-anticrossing model (BAC) is used to describe the band gap energy and the effective mass when Nitrogen is incorporated into the quaternary $\text{Ga}_x\text{In}_{1-x}\text{N}_y\text{As}_{1-y}$. These properties are mostly degraded because a small amount of Nitrogen (usually less than 5%) is added to GaInAs to make GaInNAs alloys that emit at 1.3 μm . We come to the conclusion that increasing the Nitrogen ratio increases the emission wavelength while also significantly increasing the electron effective mass and decreasing the band gap energy. The decrease in energy is due to the interaction of the energy of the conduction band with the level of Nitrogen, and moreover, as the concentration of Nitrogen increases, the energy gap of the band decreases. The interaction splits the conduction band into two non-parabolic sub-bands with energy-dependent effective masses. The downward shift of the lower sub-band fully explains the N-induced reduction of the energy gap. Our results also show that increasing the proportion of Nitrogen makes it possible to reach wavelengths that can exceed 1.3 μm but causes a reduction in gain and confinement factor. Finally, to make $\text{Ga}_x\text{In}_{1-x}\text{N}_y\text{As}_{1-y}/\text{GaAs}$ quantum well lasers work better, this material needs to have an emission wavelength of 1.3 μm . To do this, it is important to look at how Gallium and Nitrogen are mixed. The composition of these two materials will give the appropriate energy band gap, hence the desired emission wavelength.

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