INVESTIGATION OF WAVELENGTH GaInNAs 1300-1550 nm STRAINED QUANTUM WELLS ON GaAs SUBSTRATES

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Abstract

In this paper the band structures of $Ga_xIn_{1-x}N_yAs_{1-y}$/GaAs strained quantum wells are investigated using 4x4 **k.p** Hamiltonian including the heavy hole, light hole and spin-orbit splitting bands. The III–V-nitride semiconductor alloys, $Ga_xIn_{1-x}N_yAs_{1-y}$, operating at optical fibre telecommunications wavelengths around 1.3 μm, attract an increasing amount of attention in the last couple of years not only due to its promising application but also due to its unusual optical and physical properties. By changing the well width, x composition and nitrogen composition (y), the effects of quantum confinement and compressive strain are examined. We also studied the influence of the incorporation of nitrogen (y) and antimony (Sb) in our structure.

Key words: lasers diode -strained quantum wells s - GaInNAs/GaAs– GaInNAsSb/GaAs optoelectronics

1. INTRODUCTION

Ever since the GaInNAs/GaAs material was introduced as a possible candidate to replace GaInAsP/InP material as the conventional long-wavelength laser emitter and detector, it has continued to attract attention from the research community. Not only that samples were grown by both molecular beam epitaxy (MBE) to explore the possibility of achieving 1.3μm [1] and near 1.55μm [2] emission, but also various theories were proposed in an attempt to predict the compositional dependence of the $Ga_xIn_{1-x}N_yAs_{1-y}$ bulk material. The $Ga_xIn_{1-x}As$/GaAs quantum well has been shown to exhibit very low threshold current density due to the presence of compressive strain in the well layer under lattice mismatch [3]. However, the compressive strain will build up when more indium are being added to the well layer to increase the emission wavelength and thus imposed a limit to the thickness of the quantum well. By adding nitrogen atom into the matrix to form $Ga_xIn_{1-x}N_yAs_{1-y}$/GaAs, it was found to further reduce the band gap energy and simultaneously reduce the compressive strain present in the well layer. This special material exhibits very different behaviours, including the larger than normal band gap bowing factor and enhancement of electron effective mass m_e* by the addition of a nitrogen atom. The dependence of band gap energy on nitrogen composition has been predicted very well by the band anticrossing (BAC) model, which states that the large reduction of the fundamental band gap energy of $Ga_xIn_{1-x}N_yAs_{1-y}$ is due to the repulsion between a localized nitrogen-related energy level E_N and the extended conduction band of the $Ga_xIn_{1-x}As$ host matrix [4]. To date, the BAC model is used extensively and successfully in the prediction of the energy band gap of $Ga_xIn_{1-x}N_yAs_{1-y}$ with low gallium composition and GaN_yAs_{1-y} [5].

2. Strained Quantum Well

The energy of the band gap of a semi conducting material depends on its strained state, if the active lattice parameter is higher than that of the substrate the strain is a compression, in the contrary case the strain is extensive. In the case of two-dimensional and pseudo morphic deposit lattice on a substrate, the

strain is bi axial and the strains tensor can always break up into two components:

- a hydrostatic component, which decreases the band energy gap in the case of an increase in volume or which increases it in the contrary case
- a shearing component, which causes to take the heavy holes-light holes degeneration from the band of the valence band.

In a compressive strained quantum well the lattice parameter of the well is larger than that of the barrier fig.1.

$$\varepsilon(x,y)=\frac{a_{GaAs}-a_{GaAsNAs}(x,y)}{a_{GaAs}} \quad (1)$$

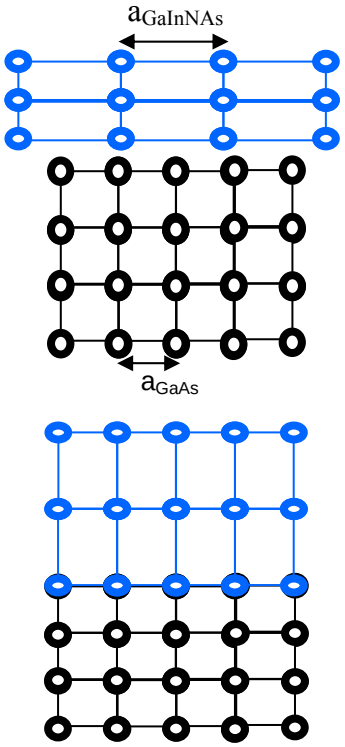

Fig.1: compressive strained quantum well
($a_{GaAs} < a_{GaInNAs}$)
$\Delta a/a \approx 3\%$

In order to calculate the band offsets of the conduction band and valence band we use the Model Solid Theory. The model-solid theory was first proposed by van de Walle and Martin to calculate strain effects on the band lineups. Conduction band position calculated by adding strained band gap energy to the valance band position fig.2.

$$P=2a_v\left(1-\frac{C_{12}}{C_{11}}\right)\varepsilon(x,y) \quad (2)$$

$$Q=b\left(1+\frac{C_{12}}{C_{11}}\right)\varepsilon(x,y) \quad (3)$$

$$E_v=E_{v,av}+\frac{\Delta}{3}+\Delta E_{hh} \quad (4)$$

$$\Delta E_{hh}=-P-Q \quad (5)$$

$$\Delta E_c=2a_c\left(1-\frac{C_{12}}{C_{11}}\right)\varepsilon(x,y) \quad (6)$$

$$E_{g-}^{st}=E_{g-}+\Delta E_c-\Delta E_{hh} \quad (7)$$

$$E_{g-}(Ga_xIn_{1-x}N_yAs_{1-y})= \\ =\frac{1}{2}\left[E_g(Ga_xIn_{1-x}As)+E_N \right. \\ \left. -\sqrt{[\,E_g(Ga_xIn_{1-x}As)-E_N\,]^2+4V_{MN}^2(y)}\,\right] \quad (8)$$

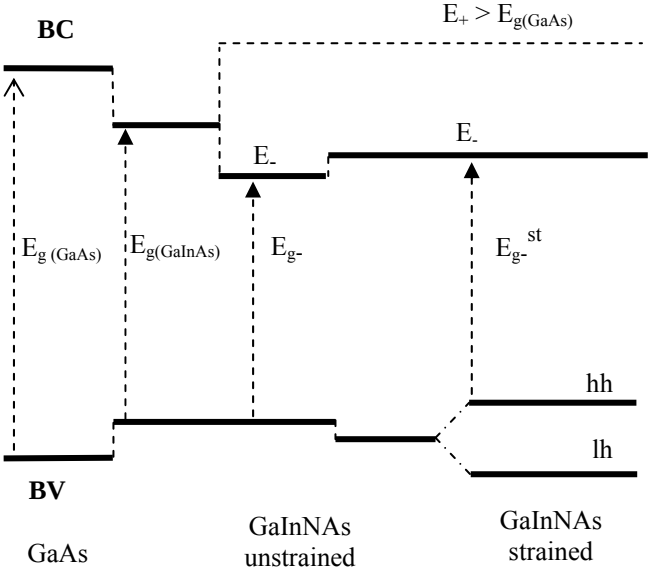

Fig.2: alignments of bands of GaInN compressive strained on GaAs

2. Band model

In order to take into account the influence of the band structure by the nitrogen-induced level, E_N, a 10-band **k·p** model was proposed which add two more spin-degenerated states to the 8-band Hamiltonian through the following matrix [6,7]:

$$H=\begin{pmatrix} N & 0 & C_{NC}\sqrt{y} & 0 \\ 0 & N & 0 & C_{NC}\sqrt{y} \\ C_{NC}\sqrt{y} & 0 & A & 0 \\ 0 & C_{NC}\sqrt{y} & 0 & A \end{pmatrix} \quad (9)$$

where

$$A = E_{g-} + \varepsilon_1(z) + \frac{\hbar^2}{2m_0} \times \times \left(\frac{1}{m_e} - \frac{2m_0 P}{3\hbar^2}\left(\frac{2}{E_{g-}} + \frac{1}{\Delta + E_{g-}} \right) \right)\left(k_x^2 + k_y^2 + {}_z^2\right) \quad (10)$$

$$N = E_N + \varepsilon_2(z) \quad (11)$$

$$\varepsilon_1(z) = 2(a_c + a_v)\left(\frac{C_{11} - 2C_{12}}{C_{11}} \right)\varepsilon_{XX} \quad (12)$$

$$\varepsilon_1(z) = b\left(\frac{C_{11} + 2C_{12}}{C_{11}} \right)\varepsilon_{XX} \quad (13)$$

There are two sets of E_N and V_{NC} available. The first set has been proven to agree very well with experimental E_g in GaN_yAs_{1-y} [8].

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$$E_N = 1.65(1-x) + 1.44x - 0.38x(1-x) \quad (14)$$

$$C_{NC} = 2.7(1-x) + 2.0x - 3.5x(1-x) \quad (15)$$

E_{g-} *is* the unstrained band gap of the material Δ is the spinorbit splitting energy, a_c and a_v are the hydrostatic deformation potential for conduction and valence band, respectively. b is the shear deformation potential. C_{11} and C_{12} are the elastic stiffness constants $\varepsilon_{xx}=(a_0-a)/a$ is the in-plane strain, a_0 and a are the lattice constants for the substrate and well layer, respectively, $\varepsilon_{zz} = -2C_{12}/C_{11}\varepsilon_{xx}$ is the strain in the perpendicular direction. P is the Kane matrix element and is normally expressed in terms of energy units as [9].

We have shifted E_N by the amount of energy caused by the shear strain, $\varepsilon_2(z)$ since the origin of our calculation is at the middle of the heavy-hole and light-hole band edge after splitting. For compressive strain, the heavy-hole band edge is taken as the valence band maximum. We have neglected the interaction between E_N and the valence subbands [10] which is consistent with assumption of the band anticrossing model that the influence of E_N on valance band energy is minimal and negligible.

3. Determination of Wavelength

For the determination of the quantification energy in the finished potential quantum well of a structure based on $Ga_xIn_{1-x}N_yAs_{1-y}/GaAs$ the simplest formalism is the use of the approximation of the function envelope. The theory of the function envelope applies well to the structures such as the quantum wells. The function envelope is given to a good approximation with the Schrödinger equation:

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(z)}{dz^2} + (V(z) - E_n)\psi(z) = 0 \quad (16)$$

where ψ is an envelope wave function, E_n the level n quantification energy and V(z) the potential barrier. The connecting conditions are given by continuities of the envelope function and the current density at the interfaces.

The energy of transition is given by the following equation:

$$E_{tre-hh} = E_{g-}^{st} + E_n + E_{hh} \quad (17)$$

The potential V(z) is a fraction of the variation of energy of the band gap ΔE_g on both sides of the heterojunction well/barrier, given by $V=Q\Delta E_g$, with Q=72% [11]. The wavelength of emission is given by the following relation:

$$\lambda_{e-hh} = \frac{1.24}{E_{tre-hh}} \quad (18)$$

Fig.3 shows the behavior of the quantification energy of the electrons and heavy holes under the effect of the width well for level n=1. When L_P becomes significant "higher than 120Å" the quantification energy tends towards the energy conduction band (not of quantification). Fig.4 illustrates the evolution wavelength according to the width well. From the structure $Ga_{0.70}$ $In_{0.30}$ $N_{0.005}$ $As_{0.995}/GaAs$ we can determine a range wavelength which varies from 0.850-1µm table. I.

x(%)	y(%)	L_p(Å)	λ_e(µm)
70	0.05	30	0.920
70	0.05	50	0.960
70	0.05	95	1.000

Table. I: parameters for changed the emission wavelength

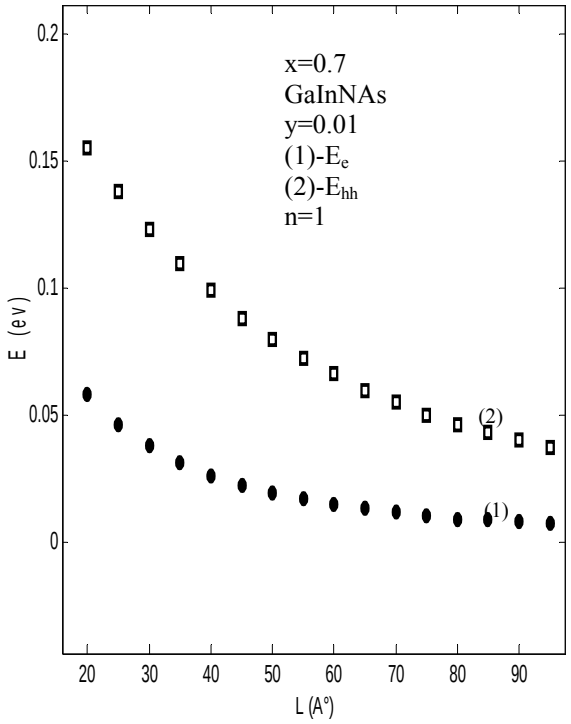

Fig.3: variation of the energy of quantification of the carriers in the conduction and valence bands according to the quantum well width

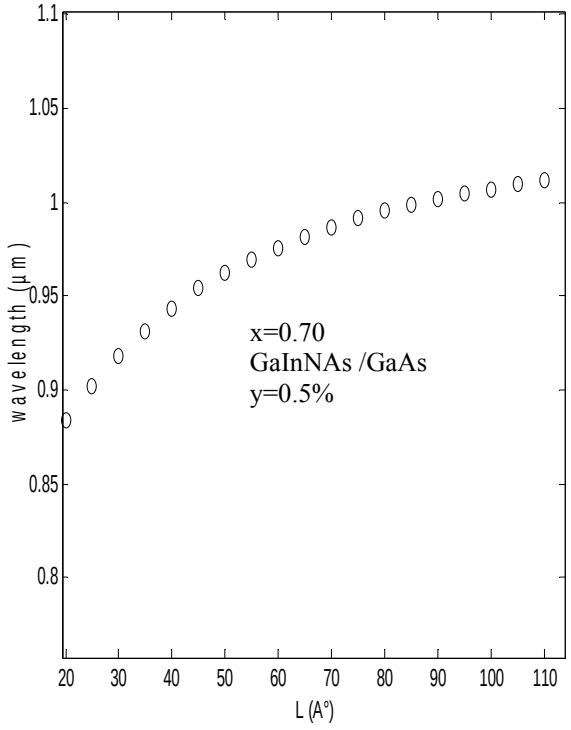

Fig.4: Variation in the length of wave of emission according to the quantum well width

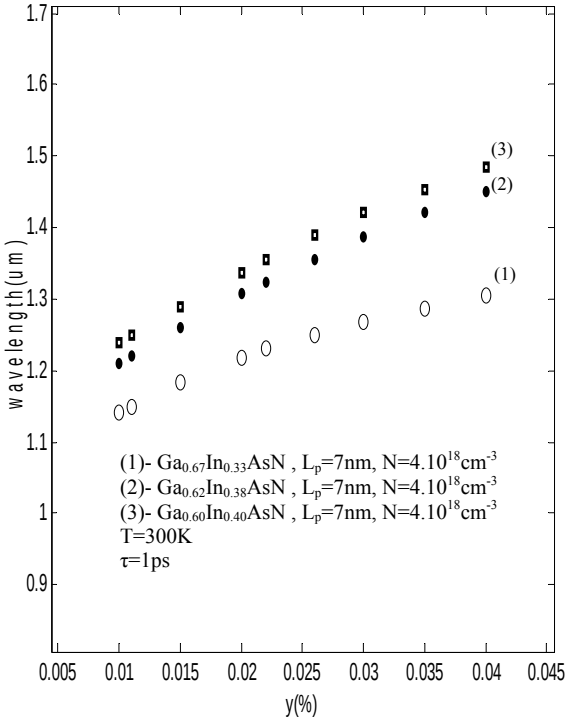

Fig.5: Evolution wavelength of emission according to the nitrogen concentration for various structures

If we change the parameters (composition of gallium, nitrogen concentration, width well, concentration of injection) the emission wavelength varies. Then starting from these structures we can reach the range 1.3-1.55µm fig.5.

4. Conclusion

The effect of the strain on the of conduction and valence bands causes a shift of the revolved gravity centre of the two bands and changes the energy of the band gap of the structure. The incorporation of nitrogen on these GaInAs, GaInAsSb structures induced a split of the conduction band in two bands E_- and E_+ for a composition of nitrogen ranging between 0.05% and 4%. The optical and electronic properties of nitride alloys with weak band gap are very particular, because the nitrogen atom is very different from the arsenide atom for which it is substituted. These differences are at the origin of the rigorous reduction in the band gap non strain and strain compressive with the composition of nitrogen, which in particular makes it possible to acquire the emission at 1.3 to 1.55µm. The BAC model makes it possible quantitatively to show the evolution of the energy of the band gap with the nitrogen concentration. One may study the evolution of the optical gain as a function of the wavelength and starting from these results one

calculates the current of threshold of the laser diode with strained quantum well of the proposed structure. It can be deduced that the increase in nitrogen introduction decreases the threshold current of the laser diode with strained quantum well. From these structures we can build lasers diode with reliable strained quantum well for the applications such as safety, telecommunications and space communications.

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