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Modeling of Quinary Structures $Ga_xIn_{1-x}N_yAs_{1-y-z}Sb_z$ based on Strained Quantum Well

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ABSTRACT

This work deals with the modeling of a quinary structure, based on a strained quantum well $Ga_xIn_{1-x}N_yAs_{1-y-z}Sb_z$. We studied the effect of the incorporation of nitrogen N(y%) and antimony Sb(z%) in ternary alloys $GaInAs$. Indeed, the incorporation of a weak composition of nitrogen causes a split of the conduction band into two sub bands while antimony causes the split of the valence band. Under the effect of this split, there is reduction of the bandgap, which is very interesting to obtain the emission wavelength of 1.55µm. We also studied the effect of the strained on the band structure. The energy of carriers confinement and the emission wavelength depending on the thickness of the active layer have been determined for different alloy compositions In%, N% et Sb% taking into consideration the influence of strained, temperature and well width. This study allows us to choose structures to improve VCSEL's diodes for fiber optic communications.

Key words : quantum well, strained, laser, optoelectronics.

1. INTRODUCTION

quaternary GaInNAs was discovered in 1996 by Kondow [1] it is now the alloy III-NV best known. During the last decade, the need for low-cost and non-cooled optical sources led to the rapid development of this quaternary. Strained quantum wells based on GaInNAs / GaAs become prime candidates to replace the GaInPAs/InP based systems for transmitting at the wavelength 1.3µm, edge-emitting lasers and VCSELs based on this alloy have quickly emerged [2]. The GaInNAs is also being studied for the realization of multi-spectral high-performance solar cells [3], and heterojunction bipolar transistors (HBT), low offset voltage [4] and working at higher modulation frequencies than with the conventional transistors based on AlGaAs or GaInP. Taking advantages of these characteristics, HBT based on GaInNAs have become components of choice for high-performance amplifiers used in devices requiring very good linearity and reduced consumption [5].The combination of the five elements that constitute the two quaternaries that is to say (ie) that the GaInNAsSb quinary alloy is particularly interesting. To have a good compromise between electronic containment and emission wavelength. This material has been the subject of relatively few studies. The first published studies have focused on the improvement of optical and electronic properties of the GaInNAs with the incorporation of antimony, the degradation of these properties is mainly due to the incorporation of a high percentage of nitrogen (5%) to have an emission at 1.55µm, but at such percentage the material loses its optical qualities. Thus the incorporation of antimony becomes necessary to have an emission beyond 1.3µm while maintaining good optical properties.

2. THEORETICAL MODEL

The incorporation of nitrogen into GaInAs matrix introduces a level located at 1.65eVabove the top of the valence band it is called: iso-electronic level because the valence of the nitrogen atom is identical to the level of arsenic atom, this level of impurity is resonant with the conduction band. According to the bands anticrossing model proposed by Shan et al [6], localized states due to the nitrogen atoms isolated in the GaInAs matrix are coupled with the States of the minimum Γ of the conduction band of this same matrix. To determine the configuration of the valence band after the incorporation of antimony we use the anticrossing model of valence bands 'VBAC'. This model is based on the famous *kp* method [7] by considering six valence states of coupled semiconductor with six valence states of atoms introduced 'impurities', the Hamiltonian diagonalization leads to six doubles eigenvalues and degenerate corresponding to two bands: ahigher band $E_{hh\pm}$ and alower band $E_{lh\pm}$ which are the result of the bands anticrossing of heavy holes HH light holes LH. The determination of the eigenvalues of the energy states leads to two solutions:

$$E_{\pm hh} = \frac{1}{2}\left[E_{Sb} + E_{hh}(\kappa) \pm \sqrt{(E_{Sb} - E_{hh}(\kappa))^2 + 4V_{PQ}{}^2}\right] \quad (1)$$

$$E_{\pm lh} = \frac{1}{2}\left[E_{Sb} + E_{lh}(\kappa) \pm \sqrt{(E_{Sb} - E_{lh}(\kappa))^2 + 4V_{PQ}{}^2}\right] \quad (2)$$

where

$$V_{PQ} = C_{Sb}\sqrt{z} \quad (3)$$

C_{Sb}=1.05 and E_{Sb}=-1eV. And z is the incorporated antimony fraction [6].

The calculation of electronic transitions that occur in a semiconductor is a key parameter for the study of the optical properties such as gain or absorption, but this requires knowledge of the band structure of the material, that is to say (ie) energy bands and their corresponding wave functions. In optoelectronics this calculation is often done by solving the Schrödinger equation according to the formalism of Ben-Daniel-Duke [8]:

$$\left(-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m_e}\frac{\partial}{\partial z}\right)+\frac{\hbar^2 k^2}{2.m_e}+V_c(z)\right)\varphi(z)=E\varphi(z) \quad (4)$$

There are several methods that allow solving this equation. To calculate the band structure of a quantum well under strained, there are those that are purely numerical, such as finite differences and finite elements, or semi-analytical, like the famous *kp* method, Method called LCAO (linear combination of Atomic orbitals) [9] The transfer matrix [10] and the Galerkin method. The number of States confined in the well will then be:

$$n_{states}=\frac{1}{2}+\frac{2.L_w}{\hbar}.\sqrt{2.m_w^*.V_{inf}}+\frac{1}{\pi}\arctan\left(\sqrt{\frac{m_{sup}^*.V_{inf}}{m_w^*.|V_g-V_d|}}\right) \quad (5)$$

We can know the number of States confined in the well by considering that the last state (of the higher energy) is located below the lowest potential barrier. $E \le V_{inf}=\min(V_g, V_d)$. To determine the number of states, we consider m_{inf}^*, m_{sup}^* the masses in the lower potential barrier and the highest potential barrier respectively. For our structure, we have a balanced well, therefore:

$V_g = V_d = V_b$ (V_b potential in the barrier).

Equation (5) becomes:

$$\kappa_w L_w + 2.\arctan\left(\frac{m_b^*}{m_w^*}\frac{\kappa_w}{\kappa_b}\right)+n\pi=0 \quad (6)$$

with m_b^* : effective mass of the electron in the barrier. κ_b, κ_w : wave vectors in the barrier and in the wells respectively, the number of states will be then :

$$n_{states}=1+\frac{2.L_w}{\hbar}.\sqrt{2.m_w^*.V_b} \quad (7)$$

Solving the equation to the eigenvalues gives us quantum levels in the well.

3. RESULTS AND DISCUSSION

We simulated the effect of indium, nitrogen and antimony on the strained. We found that indium accentuates the strained (Figure.1) and decreases the critical thickness and that antimony act in the same way but its effect is less intense, while nitrogen reduces the strained and slows the dislocation (Figure. 2).

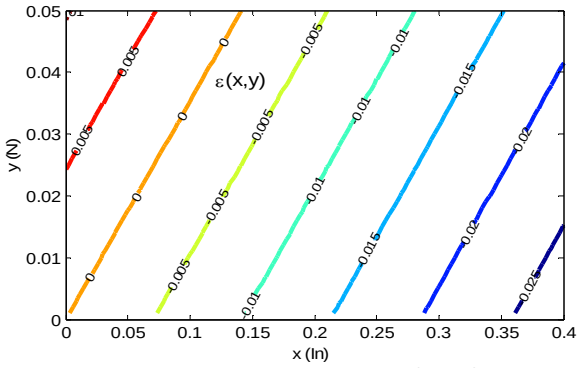

Figure 1: Iso-strained curves in terms of x, y for z = 0.06 : concentrations of indium, antimony and nitrogen respectively. . The surface of positive values represents the couplets zone (x, y) of voltage, and the couplets negative values (x, y) of compression and the '0' line represents the agreement of mesh.

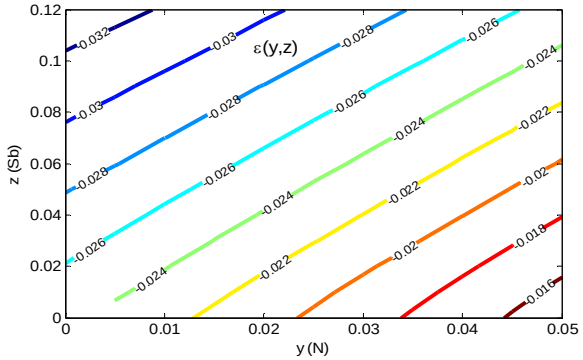

Figure 2: Iso-strained curves in terms of y, z for x = 0.30: concentrations of nitrogen, indium and antimony respectively.

To determine the energy of the bandgap, we use the VBAC model (Valence Band Anti-crossing) to calculate the conduction band and the valence band, and then we introduce the effect of the strained, and in the end the gap. Simulation results that we have obtained are shown in Figure 3 and Figure 4 which describe the evolution of the gap energy as a function of indium and nitrogen fractions, and as a function of nitrogen and antimony fractions respectively.

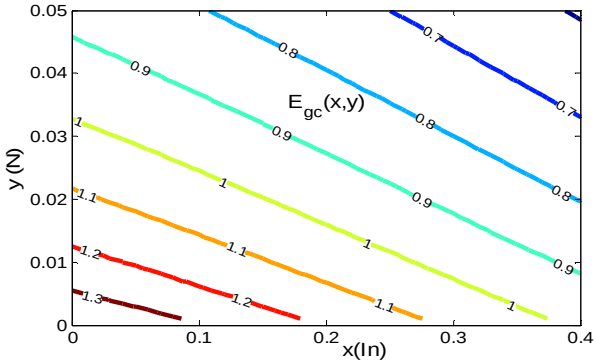

Figure 3: Iso-gap curves (eV) as a function of x, y for z = 0.04: nitrogen of indium and antimony concentrations respectively.

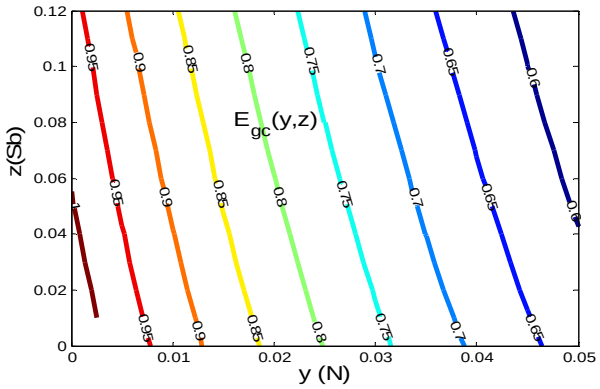

Figure 4: Iso-gap curves (eV) as a function of y,z for x=0.30: nitrogen , antimony and indium concentrations respectively.

Solving the eigenvalues equation gives us the energy levels of the electrons in the quantum wells. Figures 5 and 6 show the evolution of these levels in the well in terms of their thickness for different fractions of indium, antimony and nitrogen. These results are valid for isolated quantum wells that is to say (ie) for barrier thicknesses much higher than that of wells. We note that the number of energy levels increases with increasing thickness of the active zone, and the spacing between these levels decreases. These results also show that increasing fractions of indium and nitrogen increases energy quantization in the well while antimony decreases it.

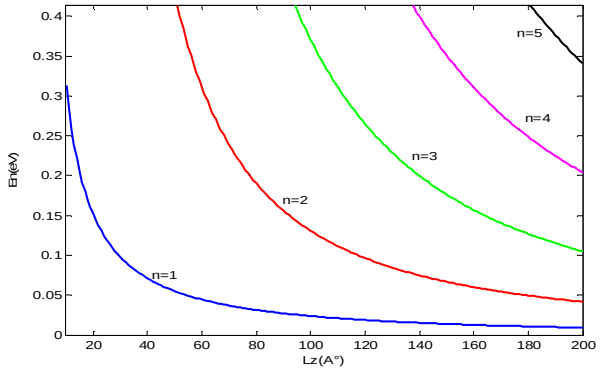

Figure 5: Energy Evolution of electrons in the quantum well based on $Ga_{0.70}$ $In_{0.30}$ $N_{0.025}$ $As_{0.955}$ $Sb_{0.02}$ at T=300°K.

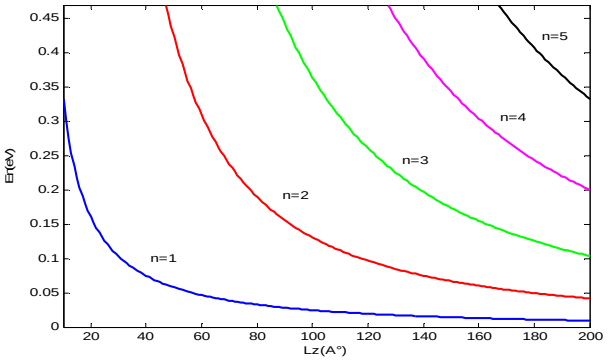

Figure 6: Energy Evolution of electrons in the quantum well based on $Ga_{0.70}$ $In_{0.30}$ N0.025 As_0.855 Sb_0.12 at T=300°K.

Figure 7 gives the evolution of the wave length as function of the thickness of the active layer and fractions of composition x (In), y (n), z (Sb). This figure allows us to see that the three compounds increase the emission wavelength, and that with this structure we reach more easily the privileged wavelength of optical telecommunications 1.55µm.

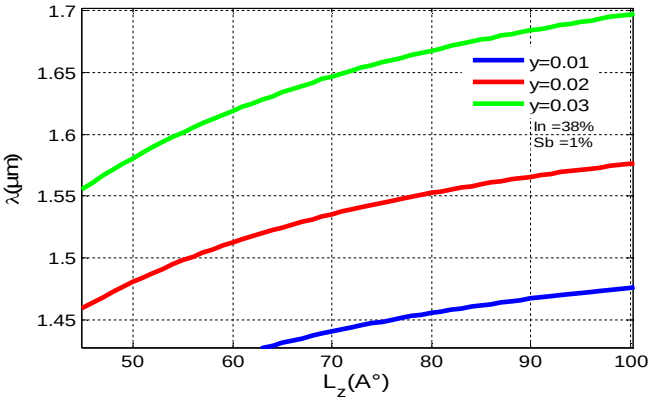

Figure 7: Wavelength Evolution depending on the width of the well, at T = 300 °K for different concentrations of In, N and Sb.

4. CONCLUSION

In this paper we highlight the fact that this structure is a good compromise that allows us to take advantage of the qualities of both quaternaries GaInNAs and GaNAsSb, including good containment, reduction of the gap energy and reducing strained which adds additional flexibility to the realization of structures with different methods of growth, all that with reducing the disadvantages presented by the two quaternaries, thanks to a very attractive property in GaInNAsSb and which adds another degree of freedom in the design of devices based of this alloy, It's the fact of being able to change several settings independently, and then, playing on the composition of fractions x, y, z indium, antimony and nitrogen respectively. Subsequently we have studied the influence (x (In), y (N), z (Sb)) and thickness L_z on the emission wavelength. We can achieve the wavelength 1.55µm, with the GaInNAsSb structure which is preferred for fiber optic communications.

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