Effect of antimony on structure strained quantum well laser

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This work consists of highly strained quantum well $Ga_xIn_{1-x}N_yAs_{1-y-z}Sb_z$ quaternary structure modeling. We have studied the effect nitrogen and antimony incorporation into ternary semiconductor III-V alloys. We found that incorporating nitrogen in the structure leads to a splitting of the conduction band into two sub bands while adding antimony will split the valence band. This separation will give a reduced a band gap energy which is interesting for getting a 1.55µm wavelength optical fiber window. We have also studied the effect of strain on the band structure and particularly on the conduction band. We have calculated the x(Ga), y(N) and z(Sb) concentrations taking into account the effects of the strain, the temperature and the quantum well width.

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1. Introduction

III-V semiconductors group such as (Al, Ga, In) - (As, P) on InP and GaAs substrates have been the basis of a wide range of electronic and optoelectronic components [1, 2]. Entire range of possible compositions was explored in order to obtain new properties, including new wavelengths. This can be achieved by varying the dimensions of the systems (for example quantum dots indium gallium arsenide/gallium arsenide, InGaAs/GaAs [2]. However, it is tempting to explore other elements of columns III-V to have more compositions choice. Given the band gap energy of GaN, adding III-V elements, in principle, allow the resulting materials to cover the entire visible spectrum. However, studies on the incorporation of nitrogen were previously limited to typical concentrations of impurities such ($N < 10^{19}$cm-3). Early studies of this new material were initially concentrated on the evolution of the band gap energy as a function of nitrogen concentration that gives the highest concentration without phase separation [3-5]. Only a small addition of Sb is necessary to shift the band gap to much longer wavelengths. It is suggested that Indium pushes the conduction band away from the N related level and thus minimizing the effect of N on bandgap reduction. However, a small addition of Sb (group V) can shift the conduction band towards the N resonant level and thus increase further the N effect on bandgap energy. Furthermore, even though GaInNAsSb wavelength has been increased. When we add In and Sb, the uniformity on the micron scale has improved, as it can be seen with cathodoluminescence (CL).

2. Solid model theory

Typically, the lattice parameters of semiconductor materials constituting the wells and barriers are different depending on their relaxed form. If a thin layer constituting the well is grown over a thick layer forming the barrier of the semiconductor, the latter imposes its lattice parameter in the well (x–y) plane. It is thus possible to grow elastically strained quantum wells by either compression or tension. The epilayer is under a biaxial stress in such a way that its in-plane lattice constant $a_e(x,y,z)$ equals the substrate lattice constant. The net strain in the layer plane ε_{xx} is given by

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_s - a_e(x,y,z)}{a_s} \quad (1)$$

$$\varepsilon_{zz} = -\left(\frac{2.C_{12}(x,y,z)}{C_{11}(x,y,z)}\right).\varepsilon_{xx} \quad (2)$$

where C_{ij} are elastic stiffness constants.

The hydrostatic component ε is given by

$$\varepsilon = 2\varepsilon_{xx} + \varepsilon_{zz} \quad (3)$$

The conduction band position can be calculated by simply adding the strained band gap energy to the valence band position. The unstrained valence band edge of the well material is set as the zero energy reference [6].

The compressive strain band gaps can then be expressed as

$$E_G^{st} = E_G(x,y,z) + \delta E_c(x,y,z) - \delta E_{hh}(x,y,z) \quad (4)$$

where $\delta E_{hh}(x,y,z)$ is heavy hole valence band offset energy and $\delta E_c(x,y,z)$ the conduction band offset energy [6]

The band offsets ratios of the band-edge discontinuities for conduction and valance bands are given by

$$Q_c(x,y,z) = \frac{\Delta E_c(x,y,z)}{\Delta E_G(x,y,z)} \quad (5)$$

$$Q_v^{hh}(x,y,z) = 1 - Q_c(x,y,z) \quad (6)$$

For more precise calculation of the band structure, it is necessary to solve the Hamiltonien by the **k.p** 8.8 method. The **k.p** method is considered more appropriate. It is about a distributive calculation aiming at developing the structure of bands around an extremum Γ (k=0) which is abundantly used for the III-V materials with direct band gap [7-10]. Conduction-valence interactions are to be ignored. This approximation is common in the literature for quaternary materials and is justified by the fact that the band gap is large compared to the distance separating the valence sub-bands [8-10]. In practice, it means that the constant of coupling conduction-valence is disregarded.

3. Results and discussion

Fig .1 shows the variation of lattice mismatch versus nitrogen concentration for various antimony concentrations. For antimony incorporation (Sb) amount lower than 12% in GaInAsN quantum well structures, the lattice mismatch will increase with increasing antimony concentration which will lead to smaller compressive strain of less than 2%.

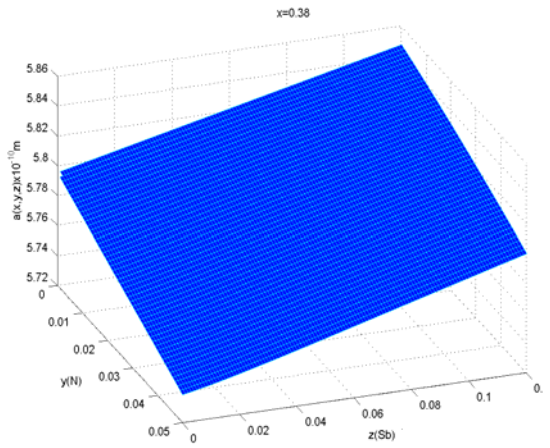

Fig. 1. Lattice parameter variation as a function of the concentration of N and Sb for In = 38%.

Fig. 2 shows the evolution of ΔE_C and ΔE_v as a function of the nitrogen and antimony concentrations. We notice that nitrogen increases ΔE_C while ΔE_v decreases. On the other hand, the antimony increases δE_v and decreases δE_c. A compromise must be chosen between the concentrations of N and Sb in order to have a good electronic confinement to decrease the leakage current.

Fig. 3. shows that for an alloy of 38% indium, 2.5% nitrogen and 2% antimony with a thickness of 6 nm and 2% mismatch of lattice parameter, we obtain conduction and valence band offset ratio of respectively Q_c=82% and Q_{hh}=18%. It can be noted that this structure will achieve a good electronic confinement, i.e. we will be able to minimize the leakage current and realize temperature-stable structures.

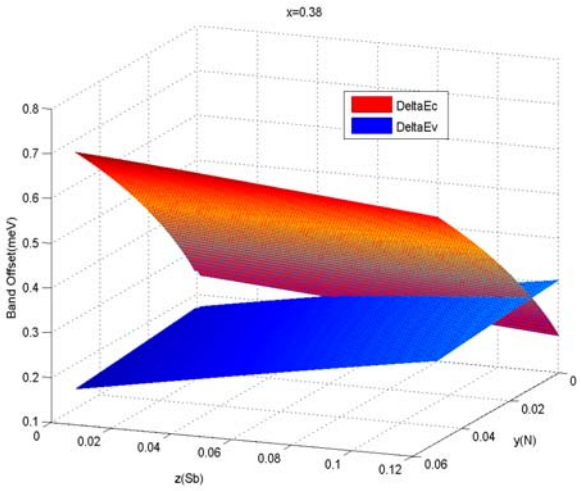

Fig. 2. Shift variation of the energy of conduction and valence bands as a function of N concentration and Sb for In = 38%.

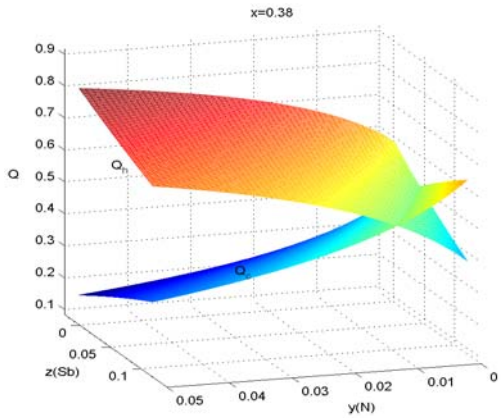

Fig. 3. Rate variation of carrier confinement of electrons and heavy holes concentration as a function of N and Sb for In = 38%.

Fig.4 shows the variation of the band gap energy as a function of N and Sb. Increasing the concentration of

nitrogen and antimony reduces the gap. For In = 38%, N = 2% and Sb =4% concentrations, the energy gap is Eg^{st} = 0.76eV. For a concentration of In = 38%, N = 3% and Sb =10% the gap E_g^{st} = 0.68eV. We can obtain a wavelength emission structure around 1.6µm.

In Fig. 5 we simulated a strained quantum well based GaInAsNSb / GaAs structure. The studied structure is composed of 30% In, 2.2% N and 1% Sb with an active region thickness L_W = 7.5nm and a strain ε = 1.7%. The quantized electron carriers energy for levels 1 and 2 is E_{e1} = 37.92meV, E_{e2} = 224.8meV respectively. For both levels of bearing heavy hole energy is E_{HH1}=-877.7meV, E_{HH2} = -912.1 meV. The rate of carrier confinement Q_C/Q_{HH} is 75/25. From these calculations we have determined the transition energy $E_{Tr.n} = E_{G\text{-}st} + E_{en} + E_{HHn}$. The transition energy levels 1 and 2 are 0.913eV and 1.12eV respectively. The emission wavelengths $\lambda_e = 1.24/E_{Tr}$ of two transitions $E_{e1\text{-}HH1}$ and $E_{e2\text{-}HH2}$ equal 1.3581µm and 1.1071µm respectively. From this study, we can vary the compositions of In, Sb and N to increase the emission wavelength for optical fiber communication applications.

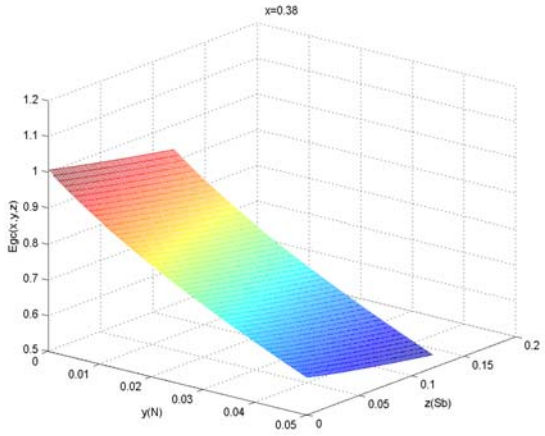

Fig. 4. Variation of the energy of the forbidden band as a function of N and Sb concentrations for In = 38%.

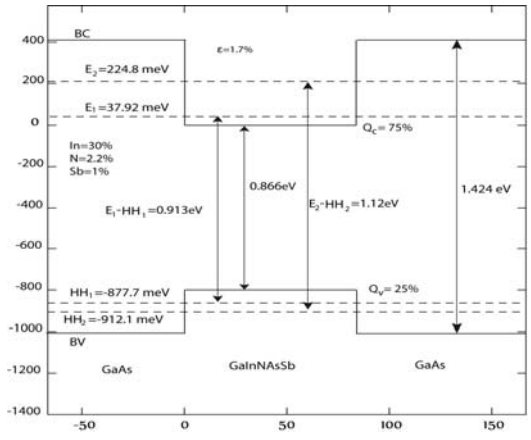

Fig. 5. Band lineup for single quantum well structure GaInAsNSb/GaAs emitting at 1.3581 µm.

4. Conclusion

In this paper we studied the strained quantum well structures based on GaInAsNSb/GaAs and using kp 8.8 method. The effect of nitrogen and antimony concentrations on the lattice parameter, the gap energy of the strips is taken into account. It was concluded that nitrogen increases the gap energy of conduction band decreases against the energy shift of the valence band. It is found that antimony has the opposite effect of nitrogen on the energy bands where we demonstrated that nitrogen and antimony decrease the energy gap. This study allowed us to find a balance between N and Sb rates in order to achieve reliable optoelectronic components operating at a wavelength of ~ 1.6µm.

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