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## Optimization and Comparison between the efficiency of GaNAsSb and GaInNAs single solar cells deposited on GaAs

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### Abstract

In this work we study and optimize the single solar cell efficiency of  $\text{GaN}_x\text{As}_{1-x-y}\text{Sb}_y$  and  $\text{Ga}_{1-x}\text{In}_x\text{N}_y\text{As}_{1-y}$  deposited on GaAs. The solar cells are simulated, in the aim to find the best concentration of nitrogen and antimony for  $\text{GaN}_x\text{As}_{1-x-y}\text{Sb}_y$ , and indium and nitrogen for  $\text{Ga}_{1-x}\text{In}_x\text{N}_y\text{As}_{1-y}$  which gives us a band gap energy around 1 eV with a low strain and a maximum absorption, in fact we do not have only one value but a whole interval for both structures. In the second step we simulate the efficiency of both GaNAsSb and GaInNAs solar cells with the find concentration values in order to see which of the two structures will give a higher efficiency. We noticed that the results were obtained under AM1.5 illumination, 300 K and an ambient pressure. The two structures had a thickness of 300 nm. The N and P layers have a doping level of  $1.10^{15} \text{ cm}^{-3}$  and  $1.10^{16} \text{ cm}^{-3}$  respectively. This study gives us the possibility to produce multi-function solar cells.

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## Introduction

In 1999, Ungaro et al was proposed for the first time the growth of GaAsNSb for long wavelength applications [1]. Since then, only a few groups have studied this material system. In 2004, Yuen et al. looked at using GaAsNSb to replace GaAsN as the barrier layers in their InGaAsNSb quantum wells [2,3], but it was found that GaAsNSb quantum wells demonstrated poorer optical quality than InGaAsN (Sb) and thus their further work focused on GaAsN/InGaAsN(Sb) quantum wells only. Around the same time, Wicaksono et al also investigated the growth of GaAsNSb for infrared detectors and long-wavelength lasers [4, 5]. It was found that just like InGaAsN; The GaAsNSb has unique physical properties such as simultaneous reduction of band gap and lattice parameter [6-8] and potential applications in GaAs-based optoelectronic and photonic devices operating in the important telecommunication wavelength range of 1.3e155 m [8-10]. However, this last is characterized by a smaller value of band gap energy than with InGaAsN for the same nitrogen concentration [1,11,12]. Which allows us to avoid a formation of N-related defects which degrades the quality crystalline and of decrease the minority-carrier lifetime in the alloy [6,12]. These semiconductor alloys, based on the substitution of arsenic in GaAs with nitrogen (N) and the antimony (Sb), have lower band gap energy than GaAs, and optical properties that strongly depend on the composition alloy and the stress. In this work based on modeling and simulation we will determine the best concentration of nitrogen and antimony in  $\text{GaN}_x\text{As}_{1-x-y}\text{Sb}_y$ , and indium and nitrogen in  $\text{Ga}_{1-x}\text{In}_x\text{N}_y\text{As}_{1-y}$  that gives us the highest efficiency for each structure, and finally we will determine the best structure between the two.

### Nomenclature

$a_c, a_v$	are the conduction and valence-band hydrostatic deformation potentials.
$b$	is the valence band shear deformation potential .
$C_{11}, C_{12}$	are elastic stiffness constants.
$E_N$	is the localized nitrogen state energy (relative to the top of the valence band).
$V_{MN}$	is the matrix element describing the interaction between these two states.
$b_{\text{GaAsSb}}, b_{\text{InGaAs}}$	are “bowing” or “non-linear” parameter.
N	nitrogen
Sb	antimony
In	Indium
BAC	band anti-crossing model

## 2. Mathematical modelling:

One of the unique advantages of the  $\text{GaAs}_{1-x-y}\text{Sb}_x\text{N}_y/\text{GaAs}$  and  $\text{Ga}_{1-x}\text{In}_x\text{N}_y\text{As}_{1-y}/\text{GaAs}$  is that it can be grown lattice-matched to GaAs by carefully controlling the chemical compositions which gives us a growth of high quality materials. The lattice parameter of  $\text{GaAs}_{1-x-y}\text{Sb}_x\text{N}_y$  and  $\text{Ga}_{1-x}\text{In}_x\text{N}_y\text{As}_{1-y}$  respectively was calculated using Vegard’s law [13]. Outside the lattice matched the strained heterostructures are widely used in high performance devices ranging from quantum-well lasers to pseudomorphic field-effect transistors. Indeed, we have two types of the stress compressive strain if the lattice parameter of material epitaxial superior to that of substrate or, tensile strain in the opposite case. To calculate the strain in the  $\text{GaAs}_{1-x-y}\text{Sb}_x\text{N}_y/\text{GaAs}$  and  $\text{Ga}_{1-x}\text{In}_x\text{N}_y\text{As}_{1-y}/\text{GaAs}$  system we based on the following relationships [14]. The band gap of the  $\text{GaAs}_{1-x-y}\text{Sb}_x\text{N}_y/\text{GaAs}$  and  $\text{Ga}_{1-x}\text{In}_x\text{N}_y\text{As}_{1-y}/\text{GaAs}$  straining system can be calculated using a combination of solid model and BAC model as follows [15].

## 3. Resultants and discussion

Figure 1 illustrates (A) the variation of the strain as a function of Indium (In) and Nitrogen (N) for  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ , (B) the variation of strain the stress as function of N and the Sb for  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$ . The figure shows that the strain increases with (In, N) for  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$  and (N, Sb) for  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$ , also we notice that for both structures we have two types of strain, tensile strain for strictly positive values, and compressive strain for strictly negative values, so we get a lattice mesh for zero strain, each type of strain for both structures is obtained not only for a single composition but a range of concentrations of (In, N) for  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$  and (N, Sb) for  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$ . Figure 2 illustrate variation of band gap energy as a function of (A) (In, N) for  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ , (B) (N, Sb) for  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$ . The figure shows that the band gap energy decreases with the concentrations of

(In, N) for  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$  and (N, Sb) for  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$ , so the value 1 eV is obtained for a range of values that ranges between (0% to 40% for Indium with concentrations of 1% up to 2.8% nitrogen) for this range the values of levels energy  $E_{\text{ghh}}$ , the strain as well as the rang of absorption rates are shown in Table 1. Even for the  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$  structure, the 1 eV value is obtained for a range of values that varies between [1% up to 6% for N with varying concentrations of Sb between 2.7% to 2.9%] for this range the values of the energy levels,  $E_{\text{ghh}}$ , the strain and the absorption rang are shown in Table 2.

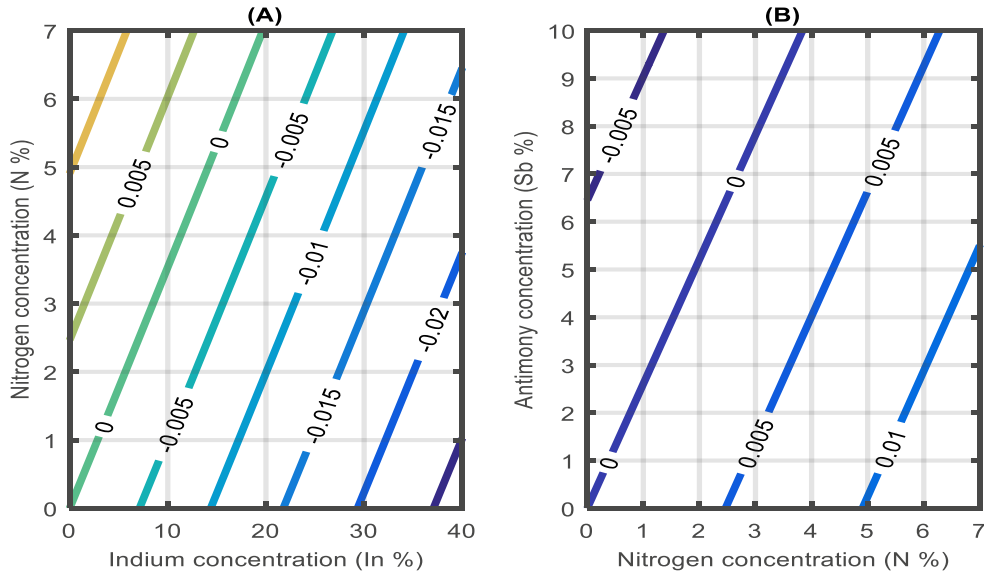


Fig. 1. variation of strain as a function of (A) In and N compositions for  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ , (B) N and the Sb compositions for  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$ .

Table 1. Values of levels energy  $E_{\text{ghh}}$ , the strain, the absorption rang as function of In and N compositions.

In (%)	N (%)	$E_{\text{ghh}}$ (eV)	$\epsilon_{\text{total}}$ (%)	$[\lambda_1, \lambda_2]$ ( $\mu\text{m}$ )
10	2.5	0.98	-0.21	[0.53-1.20]
20	1.9	1.00	-1.02	[0.53-1.20]
30	1.5	0.99	-1.76	[0.52-1.20]
40	1.0	0.99	-2.5	[0.52-1.20]

Table 2. Values of levels energy  $E_{\text{ghh}}$ , the strain, the absorption rang as function of N and Sb compositions.

N (%)	Sb (%)	$E_{\text{ghh}}$ (eV)	$\epsilon_{\text{total}}$ (%)	$[\lambda_1, \lambda_2]$ ( $\mu\text{m}$ )
1	2.7	0.99	-0.007	[0.53-1.20]
4	2.7	1.00	-0.6	[0.52-1.23]
4	2.8	0.99	0.6	[0.50-1.23]
6	2.8	1.00	1.0	[0.51-1.24]
6	2.9	0.99	1.0	[0.51-1.25]

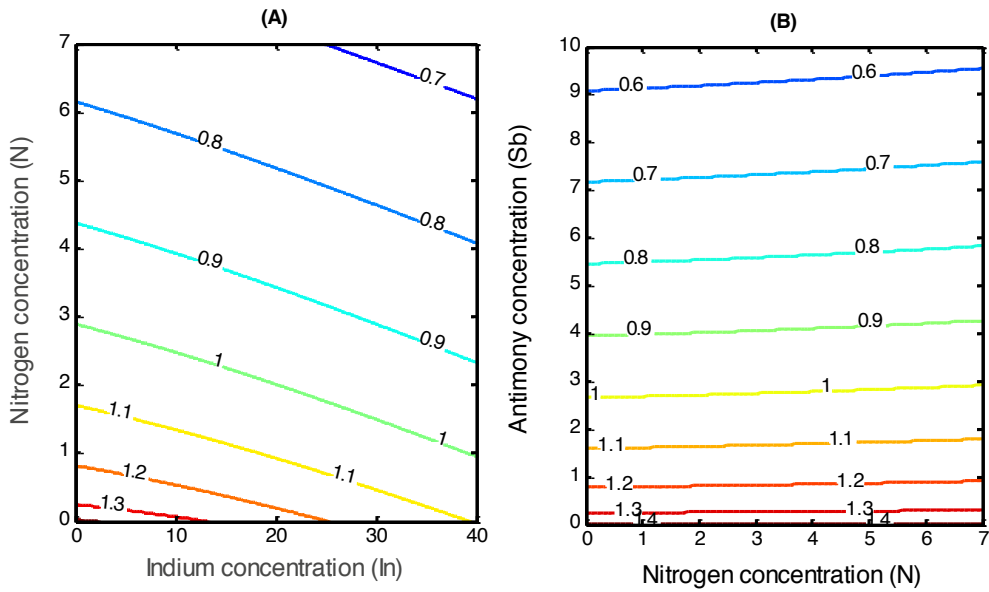


Fig. 2. variation of band gap energy as function of (A) In and N compositions for  $In_xGa_{1-x}As_{1-y}N_y$ , (B) N and Sb compositions for  $GaAs_{1-x-y}N_xSb_y$ .

Figure 3 illustrates (A) the efficiency values for each composition shown in Table 1 for the  $In_xGa_{1-x}As_{1-y}N_y$  structure. Figure 3. (B) illustrates the variation of the power as a function of the tension for the structures with the compositions also shown in Table 1. The figure shows us that the efficiency are close but the best one is 26.19% for the compositions (In = 30%, N = 1.5%).

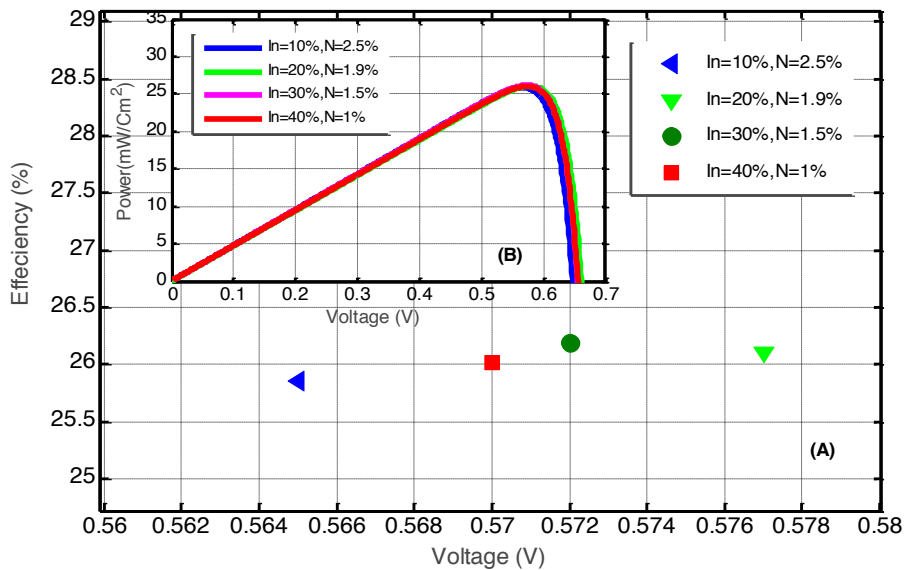


Fig. 3. (A) efficiency values for several composition. (B) variation of the power as a function of the voltage for the  $In_xGa_{1-x}As_{1-y}N_y$  structure.

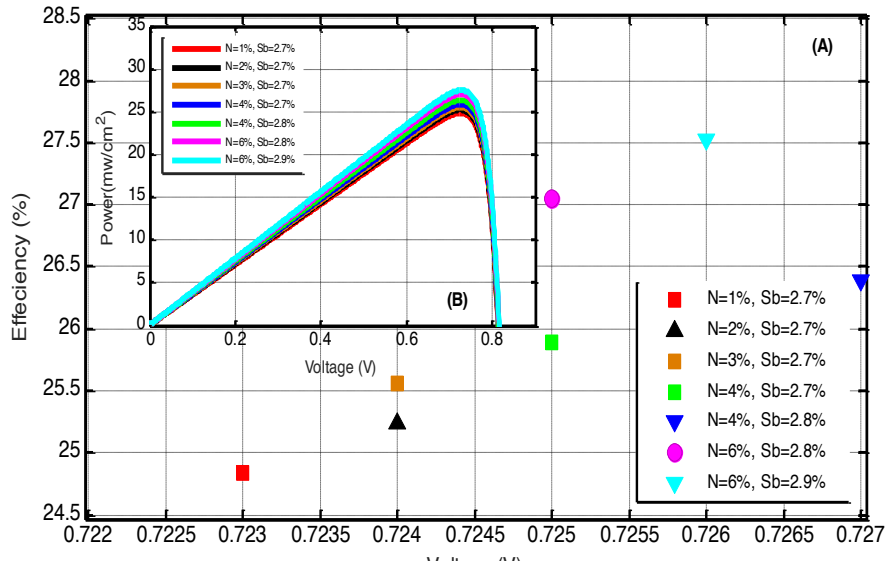


Fig. 4. (A) efficiency values for several composition. (B) variation of the power as a function of the voltage for the  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$  structure.

Figure 4 illustrates (A) the efficiency values for each composition shown in Table 2 for the  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$  structure. (B) illustrates the variation of the power as a function of the tension for the structures with the compositions also illustrated in table 2. The figure shows us that the varied efficiency between 24,84 is 27,52%, of such fate that they are increased with (N, Sb), the best efficiency is obtained for the compositions (N = 6%, Sb = 2.9%).

#### 4. Conclusion

This work shows the variation of some optoelectronic property as a function of In and N for structure  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ , and as a function of N and Sb compositions for  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$ . The results obtained show that the strain increases, thus the band gap energy decreases, with (In, N) for  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$  and with (N, Sb) for  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$ . The efficiency obtained are high compared to the other structures, the best one is 27.52% for the  $\text{GaAs}_{1-x-y}\text{N}_x\text{Sb}_y$  structure with the compositions (N=6%, Sb=2.9%) with a 1% strain and a range of varied absorption between  $[0.51\mu\text{m to } 1.25\mu\text{m}]$ , so this structure absorbs in the visible and near infrared range.

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