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$GaAs_{1-x}N_x$ candidate material for a high efficiency based homojunction solar cell

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The GaAsN alloy has a great potential in the manufacture of the photovoltaic devices. A simple optimized GaAsN junction can reach conversion efficiency from > 20%, comparable with that reached by the best cells of die CISGS. Because the band gap of GaAsN can be modified from 1.4 eV to 3.4 eV by increasing the nitrogen content with multi-junction cells, it is theoretically possible to achieve the record performance 70% with this only material system, whereas the theoretical record in technology GaAs multi-junctions is less than 50%. The work presented in this paper concerns the study of photovoltaic cells based on GaAsN nitrided materials. The main objective is to optimize the front and base with their thickness and doping, on the electrical characteristic of the photovoltaic cell and subsequently its output parameters under solar illumination of AM1.5G. 54.1 % efficiency is predicted for this new $GaAs_{1-x}N_x$ based on a simple single solar cell. This structure can also provide a fundamental solar cell unit for developing very high efficiency IBSC solar cell.

Keywords: GaAsN; solar cell; homojunction; simulation; efficiency.

1. INTRODUCTION

III-V nitrides gallium nitride (GaN), aluminum nitride (AlN), and indium nitride (InN) and their alloys are semiconductor particularly attractive for applications in optoelectronics and microelectronics: Leds, Laser, solar cells, Schottky diodes, Hemts, SSDs [1-5]. Today the Synthesis of GaN is perfectly mastered [6-11].

Since the 1970s, nitride materials of elements III such as gallium nitride GaN and gallium arsenide GaAs and their alloys were presented as semiconductors for the development of optoelectronic devices. GaN alloys exhibit a direct gap adjustable hence their use in photovoltaics. Among these nitrided alloys, is interested in the GaAsN, a material that has great potential. The research into these materials has been triggered by observing in particular some of their characteristics: their direct bandgap, their high thermal conductivity, the field high breakdown, high mechanical stability, resistance to radiation. Their bandgap is originally one of the most attractive properties. Indeed, it varies between 1.42 eV for GaAs and 3.4 eV for GaN covering a range of wavelengths for semiconductors, from near infrared to the far ultraviolet

[12-15]. Among the alloys of GaN and GaAs, particular attention is paid to the ternary compound GaAsN (gallium arsenide nitride). This ternary compound is one of the more promising for optoelectronics. Indeed, it reveals a considerable interest in the of optoelectronic devices operating in the telecommunications fiber optic and photovoltaic cells. On the other hand, the alloy proves to be a good candidate for manufacturing a multitude of electronic devices such as resonant cavity Enhanced (RCE) photodetectors, light-emitting diodes (LEDs), heterojunction bipolar transistors (HBT), avalanche photodiodes (APD), solar cells or semiconductor lasers such as vertical cavity surface emitting lasers (VCSEL) [16].

GaN alloys exhibit a direct gap adjustable hence their use in photovoltaics. Among these nitrided alloys, is interested in the GaAsN, a material that has great potential [17, 18]. The GaAsN is a recently developed novel solar cell material for its promising tunable band gap of 1.42 eV to 3.4 eV for the realization of high efficiency solar cells [19-23].

However, when in the early 1990s, the synthesis of GaAsN alloys with a low nitrogen content become technically possible with the appearance of plasma cells [24, 25], a strong shift towards the infrared was observed from the absorption [25] and photoluminescence [24, 26] measurements, suggesting a decrease in $GaAs_{1-x}N_x$ band gap energy with incorporation of nitrogen. Theoretical work has supported these experimental results [27]. The alloy $GaAs_{1-x}N_x$ ($x < 0.05$) has in fact a giant curvature parameter b (bowing) [28, 29] Indeed, for GaAsN, b = 16 - 20 eV, the gap of the GaAsN and the value of b depend on the nitrogen composition (N). The gap decreases rapidly, while the bowing b decreases with the increase in the nitrogen (N) composition [30-31].

The work presented in this paper is focused on numerical simulations of GaAsN-based p–n junction solar cell structure. The main objective is to optimize the front and base with their thickness and doping, on the electrical characteristic of the photovoltaic cell and subsequently its output parameters under solar illumination of AM1.5G. Thus, starting from I-V curves, we have calculated the short-circuit current I_{SC}, the open-circuit voltage V_{OC} and the efficiency conversion. The aim of this work is therefore to determine the photovoltaic parameters, in particular the conversion efficiency using different concentrations of nitrogen incorporation x and finally to choose the one which results in the best efficiency.

2. DESIGN AND PHYSICAL PARAMETERS

2.1. Design of the solar cell

The structure studied based p-n junction solar cell, using the material GaAs1-xNx, is shown in Fig. 1. The structure is composed of the base substrate GaAs which served as a support for the growth of GaAs1-xNx, P-type layer which represents the base (with X_B as base thickness and N_A as base doping), N-type layer which represents the front or emitter (with X_E as front thickness and N_D as front doping) and contacts on the P region and the N region respectively. These contacts are ohmic type.

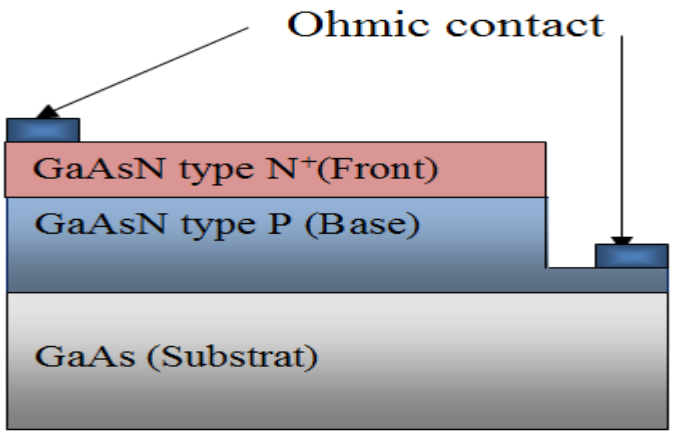

Figure 1 Presentation of the GaAsN based p-n junction solar cell.

One-dimensional Pc1D numerical simulation of $GaAs_{1-x}N_x$ based p-n junction solar cell is used in this work [32]. Pc1D is able to analyze, design and optimize structures intended for photovoltaic applications.

For each variation of the given parameter (x, X_E, N_D, X_B, N_A) we have generated the current voltage characteristics I(V) under the illumination AM1.5 G in order to extract the output parameters: the current of short circuit current I_{SC}, open circuit voltage V_{OC}, and conversion efficiency η of the cell.
With Pc1D the spectral response of $GaAs_{1-x}N_x$ based p-n junction solar cell as a function of the wavelength is also simulated.

2.2. Physical parameters

For the simulation, we studied the $GaAs_{1-x}N_x$ material with the nitrogen concentration x: 0%, 4%, 8%, 40% and 100%. Generally, the variation of the band gap width as a function of the composition of nitrogen is given by a quadratic interpolation [33].

$$E_g(GaAs_{1-x}N_x) = (1-x)\,E_g(GaAs) + x\,E_g(GaN) + x\,(1-x)\,b(GaAs_{1-x}N_x) \quad (1)$$

Where *x* is the stoichiometric coefficient evaluated in %. This coefficient corresponds to the quantity incorporating nitrogen into gallium arsenide, *b* is the parameter of curvature or bowing of the gap, E_g *(GaAs) = 1.42 eV* [34] and E_g *(GaN) = 3.4 eV* [35].

For our study, we have taken the experimental gap curve of the compound $GaAs_{1-x}N_x$ of the works of Ribeiro et al [36]. The choice of this value, x = 4%, 8% and 40%, is justified by the availability of its absorption coefficient (α) in the works of Teng and al [37].

Specific physical parameters of GaAs (x=0%), GaAs1–xNx (x=40%) and GaN (x=100%) are shown in Table 1. The physical parameters were also calculated for the values of x = 4% and 8% but are not shown in the table 1. The choice of the presentation of the physical parameters of x = 40% in Table 1 is justified by the best results presented in section 3 below.

Table 1 Specific physical parameters of $GaAs_{1-x}N_x$ for x= 0%, 40 % and 100%.

Physical Parameters	x = 0% GaAs	x = 40% $GaAs_{0.6}N_{0.4}$	x = 100% GaN
Band gap E_g (eV)[b]	1.422	1.4509	3.32
Electron affinity χ (eV)[a,c,d]	4.07	3.32	4.1
Electron mobility μ_n ($cm^2V^{-1}s^{-1}$)[a,c]	8500	2125	1000
Hole mobility μ_p ($cm^2V^{-1}s^{-1}$)[a,c]	400	378.378	350
Relative permittivity ε_r[a,c,d]	12.5	12.388	9.7
Intrinsic concentration n_i (cm^{-3})[a,c]	$3.1x10^6$	1.7×10^7	$4.4x10^{-7}$
Density of states in BC N_C (cm^{-3})[a,c]	4.335×10^{17}	7.93×10^{17}	1.452×10^{18}
Density of states in BV N_V (cm^{-3})[a,c]	1.28×10^{19}	1.55×10^{19}	1.994×10^{19}
Refractive index n[a,c,e,f]	3.6	2.099	2.15

[a]Ref. [33] Quay.; [b]Ref. [36] Ribeiro.; [c]Ref. [38] Boumesjed.; [d]Ref. [39] Vegard.; [e]Ref. [40] Yang.; [f]Ref. [41] Biswas.

3. RESULTS AND DISCUSSION

The simulation was carried out by optimizing the output parameters by varying the physical or technological quantities for five values of x: 0%, 4%, 8%, 40% and 100%. The value for x = 0% relates to the GaAs material, x = 100% for the GaN material and the choice of the three values x = 4%, 8% and 40% is justified by the availability of their absorption coefficients α in the work of Teng and al [37]. After analyzing all of our results, the best conversion efficiency for each of the values of x is: η (x = 0%) = 20.4%, η (x = 4%) = 44.6%, η (x = 8%) = 42%, η (x = 40%) = 54.1% and η (x = 100%) =1.03%. We have noticed that for low values of x the best results are obtained for x = 4% and for large values of x the best results are obtained for x = 40%, and between these two values the optimization is better for x = 40%.

The best technological parameters obtained for the front (emitter) and the base of the solar cell, optimized by simulation, for x = 40% ($GaAs_{0.6}N_{0.4}$) are: X_E= 0.1 µm with $N_D = 10^{16}$ cm^{-3} and X_B= 2.5 µm with $N_A= 5\times10^{17}$ cm^{-3}.

The best output parameters J_{SC}, V_{OC}, and η obtained of the p-n junction solar cell based on the $GaAs_{1-x}N_x$ material with three values of the x are summarized in the Table 2.

Table 2 Best output parameters of p-n single junction solar cell based on $GaAs_{1-x}N_x$ with the three values of x.

x (%)	0 GaAs	40 $GaAs_{0.6}N_{0.4}$	100 GaN
J_{SC} (mA)	28.3	69.9	0.494
V_{OC} (V)	0.898	0.923	2.210
η (%)	20.4	54.1	1.03

From this table, it should be noted that the $GaAs_{0.6}N_{0.4}$ p-n junction solar cell, a low-gap material, has a significantly higher efficiency than the GaN cell, a material with a large gap.

We observed that the $GaAs_{0.6}N_{0.4}$ (x = 40%) p-n junction solar cell gives high conversion efficiency when we choose the optimization we have done for the necessary parameters to the simulation.
Fig. 2 shows the simulated current-voltage characteristics of single p-n junction photovoltaic cells based on $GaAs_{1-x}N_x$ corresponding to x = 0%, x = 40% and x = 100%.

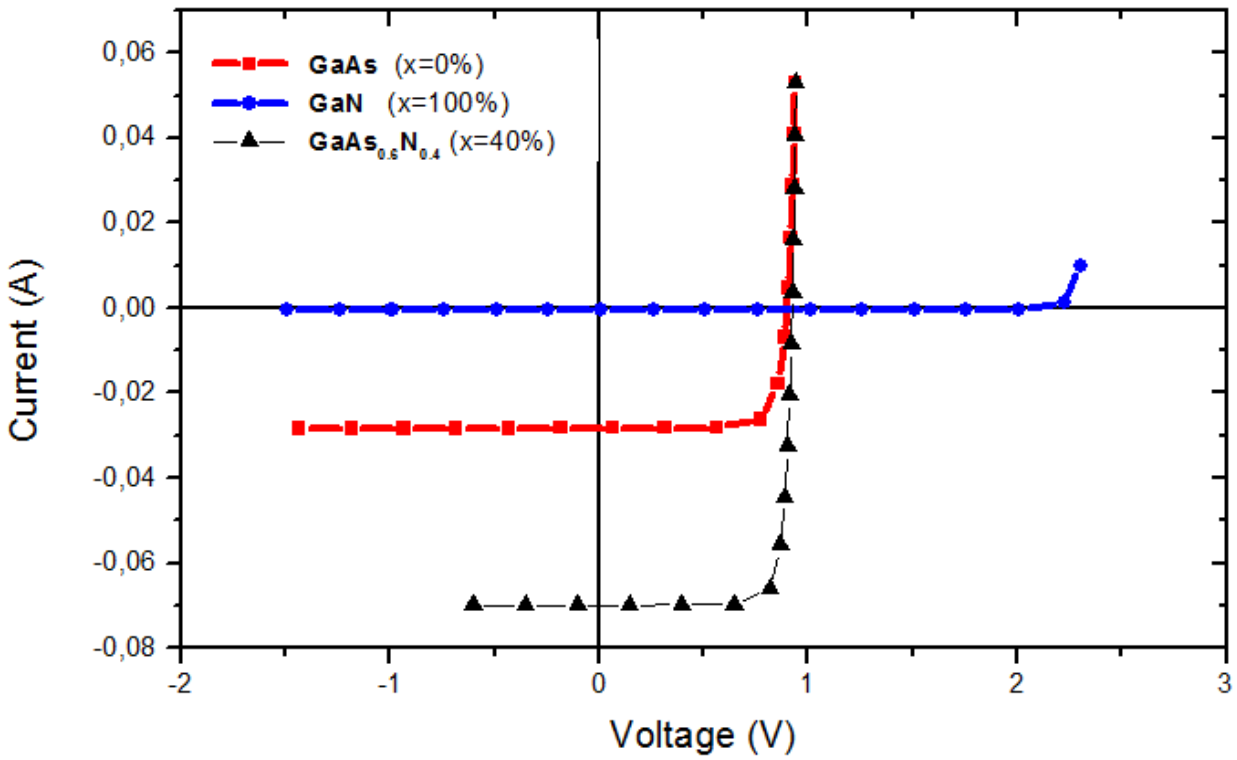

Figure 2 Current-voltage characteristics of the three p-n junction solar cells based on $GaAs_{1-x}N_x$ for x = 0%, x = 40% and x = 100%.

With Pc1D the spectral response as a function of the wavelength of the three p-n junction solar cells optimized is also simulated. Fig. 3 shows the spectral responses of the three solar cells optimized: p-n junction-GaAs solar cell, p-n junction-$GaAs_{0.6}N_{0.4}$ solar cell and p-n junction-GaN solar cell.

We observe in the near-infrared region, the quantum efficiencies of the GaAs and GaN homojunctions solar cells drop to zero. But we observe that the quantum efficiencies of the $GaAs_{0.6}N_{0.4}$ homojunction solar cell do not cancel. This indicates that there is absorption of low energy photons. This reflects the improvement in photocurrent of the $GaAs_{0.6}N_{0.4}$-p-n junction solar cell (see Figure 2). This phenomenon is well observed in GaAsN-Intermediate-Band Solar Cell **(**IBSC) [42].

4. CONCLUSIONS

The optimization of the solar cell based on $GaAs_{1-x}N_x$ p-n junction was made for a 40% of nitrogen incorporation (x). Our results which remain purely theoretical but which give an indication of the high

efficiency, 54.1%, which can be obtained in case an improvement in GaAsN technology is made. The spectral responses of the $GaAs_{0.6}N_{0.4}$ indicate that there is absorption of low energy photons. This reflects

the improvement in photocurrent. This phenomenon is well observed in IBSC solar cells based GaAsN. This work so can provide a fundamental solar cell unit for developing very high efficiency IBSC solar cell.

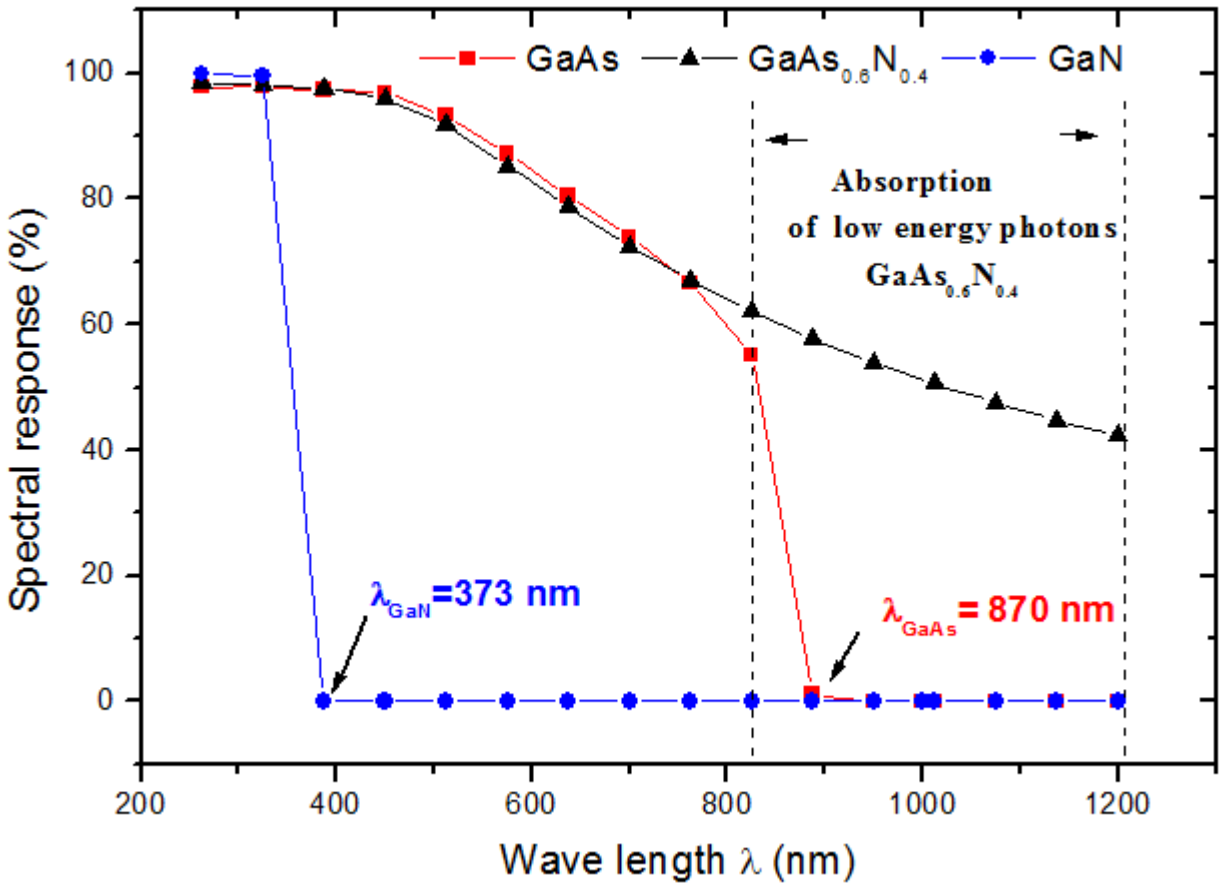

Figure 3 The spectral responses of the three p-n junction solar cell GaAs, $GaAs_{0.6}N_{0.4}$ and GaN.

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