Numerical study of InGaN based photovoltaic by SCAPs simulation

L. Boudaoud*, S. Khelifi, M. Mostefaoui, A. K. Rouabhia, N. Sahouane.

Unité de Recherche en Energies Renouvelables en Milieu Saharien, URER/MS, Centre de Développement des Energies Renouvelables, CDER, 01000, Adrar, Algérie

Abstract

The necessity to find new forms of renewable energy is very important and urgent nowadays. The renewable sources of energy derived from the sun are one of the promising options. The photovoltaic cells as one of renewable energy sources have been largely studied in order to obtain cheap, efficient and secure PV cells. The conversion efficiency is the most important property in the PV domain. Indium gallium nitride (InGaN) alloys offer great potential for high-efficiency photovoltaics. We present numerical simulations of GaN/InGaN heterojunction solar cells by SCAPs simulation. The calculation of characteristic parameters: short-circuit current density, open-circuit voltage, and conversion efficiency. So, these simulations study the effect of indium content and thickness in these parameters. While the maximum efficiency of a p-n GaN/InGaN heterojunction solar cell with 0.2 indium composition is 2.78%, above an indium composition of 20%, the modeled heterojunction devices do not operate as solar cells.

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Keywords: InGaN; GaN; Solar Cell; SCAPs simulations

1. Introduction:

Indium nitride (InN) is a promising material for near-infrared optoelectronics, high-efficiency solar cells, and high-speed electronics owing to its considerably narrow direct band gap (0.7–0.8 eV)\(^{1,2}\) and superior electron transport characteristics in nitride semiconductors\(^{1,3}\). Due to the direct band gap spanning from 3.4 eV (GaN, in the mid-UV), low effective electron mass, high absorption coefficients, and radiation tolerance, etc., InGaN alloy has drawn increasing research interests in super-high efficiency multi-junction solar cells and third generation
photovoltaics, such as quantum well solar cells (QWSCs)\textsuperscript{4,5} and intermediate band solar cells (IBSCs)\textsuperscript{5}. However, in spite of the advantages, challenges still remain (perhaps the most important one is the crystal quality of InGaN layers\textsuperscript{5}); InGaN-based solar cells are in their very early development stage\textsuperscript{6-9}. Although InGaN based solar cells offer tremendous potential for terrestrial as well as space photovoltaic applications, there are only a few reports on InGaN based solar cells. Furthermore, most reported InGaN solar cells have In contents lower than 15\% and band gaps near 3 eV, or larger, and therefore deliver diminishing quantum efficiency at wavelengths longer than 420 nm\textsuperscript{10-14}. In this paper, we present numerical simulations of InGaN heterojunction solar cells to provide guidelines for performance improvement through optimization of device structures given achievable material characteristics. Advanced electrical simulation of Nitriure indium gallium solar cells is illustrated by setting up a demonstration case in SCAPs (Solar Cell Capacitance Simulator), the solar cell simulation programme of the University of Gent. The performance of both GaN/InGaN heterojunction devices that are investigated through the calculation of characteristic parameters: short-circuit current density, open-circuit voltage, and conversion efficiency. These simulations study the effect of indium Content, and thickness of the InGaN absorbing layer.

2. Properties of In\textsubscript{x}Ga\textsubscript{1-x}N used in simulations:

The device consisted of a 110 nm p-type GaN layer (p-doping concentration 10\textsuperscript{15} cm\textsuperscript{-3}), an active region of n-InGaN/graded-InGaN layer 110-nm-(n+ doping concentration 10\textsuperscript{19} Cm\textsuperscript{-3}). The indium composition of the InGaN active layer was set to vary in the range [0.1-0.25]. The SCAPs package simulation program was used to operate the GaN/InGaN/g-InGaN solar cells.

Fig.1 demonstrates the schematic diagrams of the GaN/InGaN/graded-InGaN structures, which have been used in the simulation. The reflectivity of the front and back mirrors is equal to 0\%. All considered parameters are illustrated in table1. The most of the solar cell parameters used in this simulation are illustrated in Tale1.

Table1. The parameters values of the materials at 300 K\textsuperscript{15}.

| Parameters                                      | GaN   | InN   |
|------------------------------------------------|-------|-------|
| Band energy (eV)                               | 3.44  | 0.65  |
| Relative permittivity γ                         | 8.9   | 10.5  |
| Electron Affinity χ (eV)                       | 4.20  | 5.6   |
| Effective density of states the conduction band (Cm\textsuperscript{-3}) | 2 10\textsuperscript{17} | 810\textsuperscript{18} |
| Effective density of states in the valence band (Cm\textsuperscript{-3}) | 310\textsuperscript{17} | 310\textsuperscript{17} |
| Electron mobility μmaxe (cm\textsuperscript{2}V\textsuperscript{-1}S\textsuperscript{-1}) | 1000  | 1100  |
| Hole Mobility μ maxh (cm\textsuperscript{2}V\textsuperscript{-1}S\textsuperscript{-1}) | 170   | 340   |

To further analyze the degree of deviation from Vegard’s law, the Energy band gap of the In\textsubscript{x}Ga\textsubscript{1-x}N as a function of the indium composition x can be approximated using the following formula\textsuperscript{16}:

\[
E(In_xGa_{1-x}N) = xE(In) + (1-x)E(GaN) - bx(1-x)
\]  

(1)

Where b is the bowing parameter, which account for the non-linear fit of band gap energies, and is equal to 1.43 eV\textsuperscript{17}. In InGaN, electrical and optical properties changes with indium composition. In an ideal semiconductor, the absorption coefficient, \( \alpha \) (Cm\textsuperscript{-1}), as a function of energy can be expressed as\textsuperscript{18}:

\[
\alpha(E) = \alpha_0 \sqrt{\frac{E - E_g(x)}{E_g(x)}}
\]  

(2)

Where \( E_g(x) \) is the band gap of InxGa1-xN, E is energy photons and \( \alpha_0 \) of InxGa1-xN is assumed to be the same as that of GaN.
The electron and hole mobilities are calculated as a function of doping using\textsuperscript{19}.
\[ \mu_i(N) = \mu_{\text{min},i} + \frac{\mu_{\text{max},i} + \mu_{\text{min},i}}{1 + \left( \frac{n}{N_{g,i}} \right)^{\gamma_i}} \] (3)

Where \( i \) represents either electrons or holes, \( N \) is the doping concentration and are parameters \( \mu_{\text{min},i}, \mu_{\text{max},i}, \gamma_i, N_{g,i} \) specific to a given semiconductor\(^1\). In this respect, a typical structure of InGaN based thin film solar cell, as shown in Fig. 1, has been selected. In each simulation, only one of these parameters was varied, while the other was kept constant. We have studied the influence of these parameters on the conversion efficiency of the proposal cell.

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![Solar Irradiation AM1_5G](image)

Fig. 1. Schematic of GaN/InGaN/graded InGaN heterojunction solar cell

The efficiency of a solar cell was related to the short circuit current density \( J_{sc} \) and the open circuit voltage \( V_{oc} \) using the fill factor FF (equation (4)). As was known, the carrier concentrations would have a crucial effect on \( J_{sc} \) and \( V_{oc} \).

\[ \eta = \frac{J_{sc}V_{oc}FF}{P_{in}} \] (4)

However, \( V_{oc} \) of a p–n junction solar cell was given by the following equation:

\[ V_{oc} = \frac{k_B T}{q} \ln \left( \frac{J_{sc}}{J_0} + 1 \right) \] (5)

With

\[ J_0 = q n_i^2 \left( \frac{D_n}{L_n N_A} + \frac{D_p}{L_p N_D} \right) \]

Where \( L \) is the minority carrier diffusion length, \( D \) is the minority carrier diffusivity. The acceptor and donor concentrations are \( N_A \) and \( N_D \) respectively.

3. Simulation results

In Fig.2, the characteristics \( J_{sc} \) and \( V_{oc} \) with different In contents, and different thickness are shown. As can be seen, the curves have a similar trend. The short circuit currents densities \( J_{sc} \) increases as the thickness of the active region increases. As the thickness of the InGaN layer increases, the InGaN layer can absorb more photons, resulting in increased photogenerated current. Which are mainly attributed to the enhanced absorption of incident light due to the thickness of the absorber layer. Compared with In content, the optimized value is about 20%.

The open-circuit voltages \( (V_{oc}) \) for devices with \( x=0.1, 0.15, 0.2 \) and 0.25 are about 1.18, 1.82, 2.05 and 1.04 V, respectively. Contrary to \( J_{sc} \), \( V_{oc} \) slightly decreases as the thickness increases; this is mainly attributed to the enhanced absorption of incident light due to the reduction of the band gap of InGaN.
The solar cell efficiency and fill factor are presented in Fig.3. The efficiency conversion increases to reach maximum values. These values varied with Indium content in the absorber layer. So with the increasing of the composition $x$, the efficiency values increase and decrease dramatically when the composition is equal to 0.25 and the trend of the curve becomes like stairs appearance. The conversion efficiency $\eta$ represents the combined effects of $J_{sc}$ and $V_{oc}$. The efficiency improves as the thickness of the InGaN layer increases. This enhancement in efficiency mainly results from the increase in $J_{sc}$ because of the weaker influence of thickness on $V_{oc}$.

![Diagram showing the dependence of open circuit voltage and short circuit current on thickness with different composition of absorber layer In$_x$Ga$_{1-x}$N](image)

Fig. 2 The dependence of the open circuit voltage and short circuit current on thickness with different composition of absorber layer In$_x$Ga$_{1-x}$N

The Fig.3 illustrates the fill as function with the thickness. This parameter decreases when the content of the indium is equal to 0.1. But for $x=0.15$, in the beginning the values increase to attain a maximum for 450 nm and decreases. For the others compositions, the value of the fill factors increases.
Current versus voltage (I-V) characteristics of GaN/InGaN/InGaN solar cells with targeted Indium contents (x) of about 0.1, 0.15, 0.2, and 0.25 in the active region are shown in Fig. 4.
The values of Jsc increase with the increases of the composition but when Indium content exceeds 20%, this value was reduced sharply. This is the result of the energy band of the absorber layer is become smaller. This effect results in an abrupt drop in the current density, producing a reduction in the J–V curve for indium compositions of 25% as shown in Fig. 4. For an indium composition of 25%, the conversion efficiency dramatically reduces to 5.5%. And the device stops operating as a solar cell above an indium composition of 20%. The table 2 summarizes all the results obtained in this simulation. Ours results are in agreement with those published in the literature20.

Table 2 Characteristics of GaN/InxGa1-xN

| Sample | One sun 20 | 120 suns 20 | AM 1.5 global solar spectrum |
|--------|------------|-------------|-----------------------------|
|        | Simu | Meas | Simu | Meas | Our simulation InxGa1-xN |
|        | Voc (V) | Jsc (mA/Cm²) | FF | η % | x=0.1 | x=0.15 | x=0.2 | x=0.25 |
| x=0.1 | 2.786 | 1.9 | 2.91 | 2.19 | 1.34 | 1.72 | 2.65 | 1.04 |
| x=0.15 | 0.765 | 0.175 | 91.74 | 26.8 | 1.18 | 2.17 | 3.05 | 0.28 |
| x=0.2 | 94.76 | 63.7 | 94.95 | 74.0 | 68 | 60 | 47 | 52 |
| x=0.25 | 2.018 | 0.212 | 2.111 | 0.362 | 1.07 | 1.65 | 2.78 | 0.15 |

From the above discussion, the performance of the device (with In0.25Ga0.75N as active region) is much poorer than that of the device (In0.2Ga0.8N as active region). Because of the band energy of the second is higher than the first one, and is a direct consequence of reduced material quality when x exceeds 20%, which leads to a higher loss of the photogenerated charge carriers. In the ideal case, the absorption increases with the increase in the thickness of the absorber layer without any defects. With the increase in the thickness of the InGaN absorber layer, more photons can be absorbed, especially in an energy range of Eg(InGaN) ≤ E Photon ≤ E(GaN). However, it should be noted that when the thickness of the InGaN layer increases from 300 nm to 850 nm, the magnitude of the conversion efficiency of the device slightly increases. As the indium composition increases, this polarization-induced potential barrier becomes more prominent. The barrier height in the conduction band between the p-GaN and the n-InxGa1-xN layers increases when Indium content increases and the polarization-induced field that opposes drift transport increases21-23.

Conclusion
In conclusion, we numerically investigated the photovoltaic performance of p-GaN/ n-InGaN solar cells. Simulation
results show that short circuit current density, open circuit voltage, fill factor, and conversion efficiency strongly depend on Indium content, and thickness. Because of enhanced light absorption, Jsc increases for cells with larger thicknesses and 20% Indium compositions. In addition, Voc depends only slightly on the thickness of the n-InGaN layer. For an optimized p-GaN/n-InGaN heterojunction solar cell with a 850 nm thick absorbing layer and an indium content of 20%, the maximum conversion efficiency is 2.78%.

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