Numerical simulation of highly photovoltaic efficiency of InGaN based solar cells with ZnO as window layer

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$In_xGa_{1-x}N$, as one promising nitride semiconductor alloys for modern optoelectronic devices, has received extensive attention in recent years. However, due to its powerful modulation of energy band gap from UV to visible spectra (0.7-3.4 eV) and its interesting absorption coefficient can range from 10^3 to 10^5 cm^{-1}, depending on the material properties, it can be considered as a potential candidate for high efficiency solar cells. The actual efficiency reached is (30.38%) [1]. In order to enhance more the efficiency, we perform in this work, a device modeling and numerical simulation using SCAPS software. We optimize the photovoltaic characteristics of a solar cell based on $In_xGa_{1-x}N$. This cell is mainly composed of indium gallium nitride semiconductors for both buffer and active layer p-$In_xGa_{1-x}N$/i-$In_xGa_{1-x}N$ and the window layer contains of n-ZnO. The optimization of the various optoelectronic parameters allows improving performance of the solar cell, in addition to absorbing as much solar radiation as possible. The main photovoltaic parameters of the analog device: open circuit voltage, short circuit current density, fill factor and conversion efficiency (η) were compared and analyzed.
We have reached the conversion efficiency of 26.11% for a thickness of 1450 nm and an n-doping of 3×10^{18} cm^{-3} in the active layer ($In_{0.3}Ga_{0.7}N$). This study investigates the great potential of InGaN solar cells and can be used for the design and manufacture of high efficiency III-nitride based solar cells.

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Keywords: SCAPS, $In_xGa_{1-x}N$, Photovoltaic parameters, Efficiency

1. Introduction

The energy efficiency of solar cells has experienced a considerable increase in photovoltaic using different materials. The new semiconductor material considered for solar cells is the ternary "Indium gallium nitride". This alloy is a composition that has been extensively researched since 2002 as a potential photovoltaic material. It was initially studied for light-emitting diode (LED) and UV sensor applications [2]. The ternary alloy InGaN, in particular have become promising candidates for photovoltaic applications, thanks to its large and direct gap of prohibited energy varies between (0.7 and 3.4 eV) which covers from infrared to ultraviolet. Fluctuations in the arrangement of InN and GaN inside InGaN, the band gap of this semiconductor material can be changed. Subsequently, a high efficiency solar cell can possibly be created by having a few InGaN intersections [3,4]. In addition, it has attractive photovoltaic properties such as high radiation tolerance, high mobility and a high absorption coefficient allowing thin layers of material to absorb most of the solar spectrum [5]. Other advantages of $In_xGa_{1-x}N$, this material is a semiconductor belonging to the category of nitrides-III, its structure is wurtzite, a hexagonal structure it could achieve high efficiency at low cost [2].

In 2007, the single junction performance of the $In_{0.65}Ga_{0.35}N$ solar cell was successfully modeled by Zhang and al achieved a conversion efficiency of 20.28 % [6]. In 2008, Shen et al. have obtained for the similar $In_{0.65}Ga_{0.35}N$ solar cell higher efficiency (24.95 %) due to the adoption of the density of states (DOS) model, providing more information about

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recombination/generation in semiconductors than the lifetime model, and neglecting the defect effects [7]. Benmoussa et al. simulated an InGaN solar cell (x= 52) using AMPS-1D software and published an efficiency of 22.99 % in 2013 [8]. A. Mesrane and F. Rahmoune obtain the maximum conversion efficiency around 26.5 % of the single junction $In_{0.622}Ga_{0.378}N$ (1.39 eV) solar cell with the best structure parameters in 2015 [3].

In 2018, a work carried out by Y. Marouf focuses on $In_xGa_{1-x}N$ p-n homojunction solar cell, initially, performed by changing in content, thickness and doping concentration of the emitter. An improvement of the conversion efficiency has been observed by adding an $In_xGa_{1-x}N$ and a wide band gap window layers to the optimized cell, showing an efficiency of 19.62 % using SILVACO / ATLAS software [9].

In this paper, SCAPS software is used to simulate the device performance of InGaN solar cell under the standard conditions (AM1.5 G, 1000 W/m² and 300 K). The aim of this simulation work is to obtain the maximum conversion efficiency of solar cell with the best structure parameters. So, we have successfully simulated and developed a new structure consists essentially of $In_{0.3}Ga_{0.7}N$ in the active layer; our purpose is to improve the energy efficiency of the device by optimizing different optoelectronic parameters. The photovoltaic parameters open circuit voltage V_{oc}, short circuit current Jsc, filling factor FF, efficiency η of different layers under varied (thicknesses, doping concentration and the composition x of indium) are measured.

2. Modeling and simulation

2.1. Solar cell structure

Our study focuses on $In_xGa_{1-x}N$ solar cell structure which is presented schematically in Figure 1; this pin-structure is formed by a p-type of $In_{0.53}Ga_{0.47}N$ as a buffer layer, i-type of $In_{0.3}Ga_{0.7}N$ in the active layer and the windows layer n-type of ZnO as showing below.

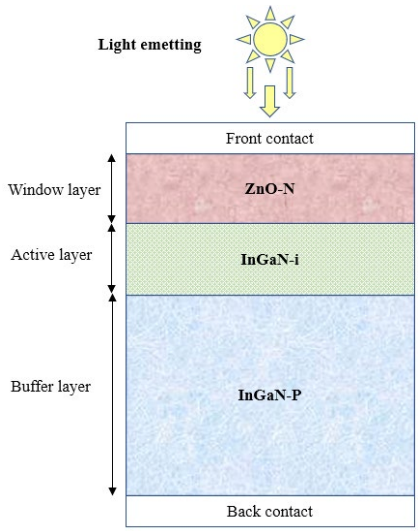

Fig. 1. The studied solar cell pin-type structure based on indium gallium nitride $In_xGa_{1-x}N$.

We have used SCAPS software to simulate our new solar cell, it's often used for modeling and simulation of solar cells; it is a very important way to find possibilities of existence of a new structure and optimizing the different physical parameters to obtain optimal energy efficiency. SCAPS is a one-dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium. The software has the ability in solving the basic semiconductor equations, the Poisson equation and the continuity equations for electrons and holes [10,11].

First of all, we have described our basic structure in SCAPS software which is shown in figure 2, and then we introduced the optoelectronics parameters of each layer by numerical calculations based on rich bibliographic research.

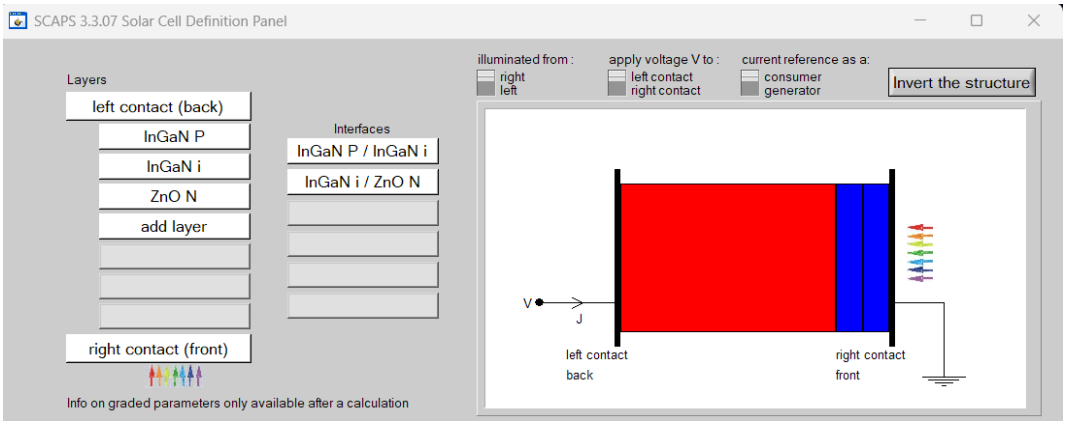

Fig. 2. Simulation of $In_xGa_{1-x}N$-based solar cell and the presentation of different layers.

2.2. Relationships and parameters of $In_xGa_{1-x}N$ material:

As mentioned above, the attractive characteristics of the nonpolar $In_xGa_{1-x}N$ ternary alloys make it a useful candidate for solar cells fabrication. In order to run numerical simulation calculations, the baseline parameters of the solar cell have to be defined to be used as inputs for SCAPS software. The band gap of the $In_xGa_{1-x}N$ layers can be calculated using Eq. (1) [12]. Calculations showed that all III-Nitride materials in the wurtzite phase have a direct band-gap.

$$E_g(In_xGa_{1-x}N) = x.E_g^{InN} + (1-x).E_g^{GaN} - b.x.(1-x) \quad (1)$$

where $x = (0,1)$; $E_g^{InN} = 0.7\ eV$; $E_g^{GaN} = 3.4\ eV$; and $b = 1.43$ is the bowing factor.

Similarly, the optoelectronic parameters used in our modeling for the $In_xGa_{1-x}N$, such as the relative permittivity (ε_r); the electron affinity (χ) and the effective conduction and valence densities of states (N_c) and (N_v) are estimated using the following equations as function of the indium composition (x) [13]:

$$\varepsilon_r(In_xGa_{1-x}N) = 14.6x + 10.4(1-x) \quad (2)$$

$$\chi(In_xGa_{1-x}N) = 4.1x + 0.7\left(3.4 - E_g\right) \quad (3)$$

$$N_c = \left(0.9x + 2.3(1-x)\right) \times 10^{18} \quad (4)$$

$$N_v = \left(5.3x + 1.8(1-x)\right) \times 10^{19} \quad (5)$$

Additionally, for the calculation of the electron and holes mobilities μ_n and μ_p, we used the Caughey-Thomas mobility model, in which the carrier mobilities dependence on the doping density and the electric field strength are derived. Hence, the mobility of electrons and holes μ_n, μ_p are given respectively by the following relation [14]:

$$\mu_{n,p}(N) = \frac{\mu_{n,p}^{max} - \mu_{n,p}^{min}}{1+\left(N/Ng_{n,p}\right)^{\gamma_{n,p}}} + \mu_{n,p}^{min} \quad (6)$$

Where N is the total doping density and $\gamma_{n,p}$ and $Ng_{n,p}$ areempirical parameters. The following table shows the value of the parameters used in the equation (6) for modeling the mobility of electrons and holes [15].

Table 1 .The parameters used in the equation (6) to modeling the mobility of electrons and holes.

Parameters	GaN	InN
$\mu_n^{min}(cm^2v^{-1}s^{-1})$	55	33
$\mu_n^{max}(cm^2v^{-1}s^{-1})$	1000	1100
γ_n	1	1
$Ng_n\ (cm^{-3})$	2×10^{17}	8×10^{18}
$\mu_p^{min}(cm^2v^{-1}s^{-1})$	3	3
$\mu_p^{max}(cm^2v^{-1}s^{-1})$	170	340
γ_p	2	2
$Ng_p\ (cm^{-3})$	3×10^{17}	3×10^{17}

Using these data, $\mu_{n,p}(N)$ is firstly calculated for GaN and InN materials and mobilities for InGaN layers are then linearly interpolated for electrons and holes as follows [16]:

$$\mu_n(In_xGa_{1-x}N) = 524x + \mu_n(GaN) \quad (7)$$

$$\mu_p(In_xGa_{1-x}N) = 6.5x + \mu_p(GaN) \quad (8)$$

Table 2. Main parameters of materials used in the simulation.

Parameters	(Tampon layer) p-InGaN	(Active layer) i-InGaN		n-ZnO
Thickness (nm)	400	50	Varied	50
Bandgap (eV)	1.61	2.39	Eq 1	3.3
Electron affinity(eV)	5.35	4.8	Eq 2	4.45
Dielectric permittivity	12.46	11.45	Eq 3	9
CB-effective density of states (cm^{-3})	1.558×10^{18}	1.922×10^{18}	Eq 4	2.2×10^{18}
VB-effective density of states (cm^{-3})	3.655×10^{18}	2.745×10^{18}	Eq 5	1.8×10^{19}
Electron thermal velocity(cm/s)	10^7	10^7	10^7	10^7
Hole thermal velocity (cm/s)	10^7	10^7	10^7	10^7
Electron mobility ($cm^2v^{-1}s^{-1}$)	1287.72	1151.48	Eq 6	100
Hole mobility ($cm^2v^{-1}s^{-1}$)	184.45	182.75	Eq 6	31

In this section, we present a numerical study for p-$In_xGa_{1-x}N$/i-$In_xGa_{1-x}N$/n-ZnO newly proposed structure. The energy conversion of a solar cell depends on the density of the short

circuit current (I_{sc}), open-circuit voltage (V_{oc}), the Fill Factor (FF) and (P_{in}) is the incident power of the solar spectrum of the solar cell as follows:

$$\eta(\%) = \frac{FF \times V_{oc} \times I_{sc}}{P_{in}} \quad (9)$$

The filling factor (FF) can describe the overall behavior of a solar cell. This factor is a measure of the quality of a solar cell; it is the ratio of the available power to the maximum power point (P_m) divided by the open circuit voltage (V_{oc}) and the short-circuit current (I_{sc}):

$$FF(\%) = \frac{P_m}{V_{oc} \times I_{sc}} \quad (10)$$

3. Simulation results and discussion

The simulations were performed at 300 K and an incident solar radiation of 1000 W/m^2 (AM1.5 G). Firstly, we started the simulation from the basic model corresponding to the parameters given in Table 2. With respect to the physical parameters used, we varied subsequently the thickness, the indium composition (x) and the doping concentration for each layer in order to improve the efficiency of InGaN based solar cell. The performance of the optimized solar cell was finally assessed. The detailed procedure and calculation are illustrated in the following.

Firstly, from the basic model, we optimized the thickness of active layer ($In_xGa_{1-x}N$) showed in Figure 1, by varying it between 50 and 1650 nm. Figure 3 represents the parameters of the cell (η, FF, $J_{sc,}$ V_{oc}) as function of the thicknesses.

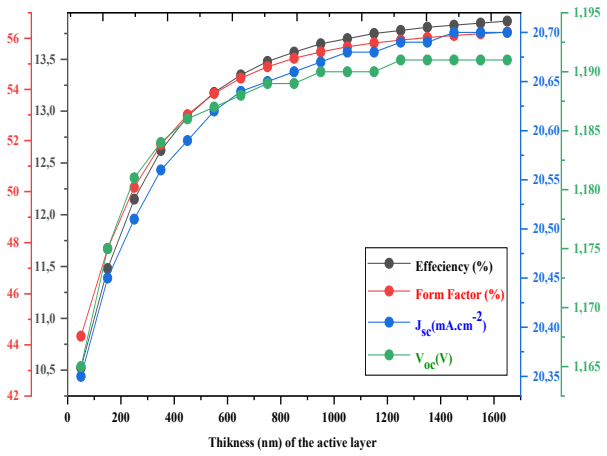

Fig. 3. The efficiency, the form factor, the short circuit current and the open circuit voltage as a function of the thickness of the active layer (i-$In_xGa_{1-x}N$).

Figure 3 shows the proportional relationship between the parameters of the cell (η , FF, $J_{sc,}$ V_{oc}) as function of the variation of the thickness of the active layer up to 1450 nm; beyond that, we notice a slight increase of the photovoltaic parameters of the solar cell (efficiency and form factor); the current and the voltage are 20.7 mA/cm^2 and 1.191 V respectively. The increase of the efficiency is due to better absorption of photons and therefore to an increase in the number of electron hole pairs created. However, if the thickness becomes too large, part of the photogenerated charges recombine before being collected. Since for specific applications such as in the space, we can take a thickness around 1450 nm using the best efficiency 13.83 %.

So, the following parameter presents the variation of the N-type doping concentration of the active layer. We varied the doping between $7 \times 10^{17} cm^{-3}$ and $10^{19} cm^{-3}$. Electrical measurements on nitrides show a high concentration of electrons, usually on the order of $10^{18}\ cm^{-3}$, giving them an intrinsically N-type character [17,18].

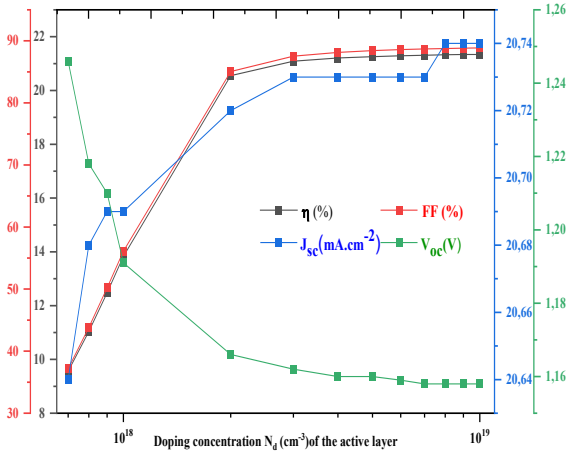

Fig. 4. The parameters of the cell (FF, J_{sc}, V_{oc}) as function of the doping concentration of the active layer.

We notice in figure 4 that the efficiency increases when the doping concentration increases up to a concentration of $3 \times 10^{18} cm^{-3}$ which is suitable for an energy conversion of 21.09 % and it is almost constant beyond this concentration, same for Form Factor, Current density and open circuit voltage decreases as function of the variation of doping concentration. The conversion efficiency increases rapidly from 9 to 21 %. This indicates that the doping of the absorbent layer has an important effect on the efficiency of the cell. This is due to the fact that the increase in doping generates a strong electric field at the p-InGaN/i-InGaN junction.

Then, we optimized the Indium composition (x) of the active layer ($In_xGa_{1-x}N$); we varied the energy band gap between 2.19 eV and 2.39 eV. Figure 5 represents the parameters of the cell (η , FF, V_{oc}, I_{sc}) as function of the variation of the indium composition (x):

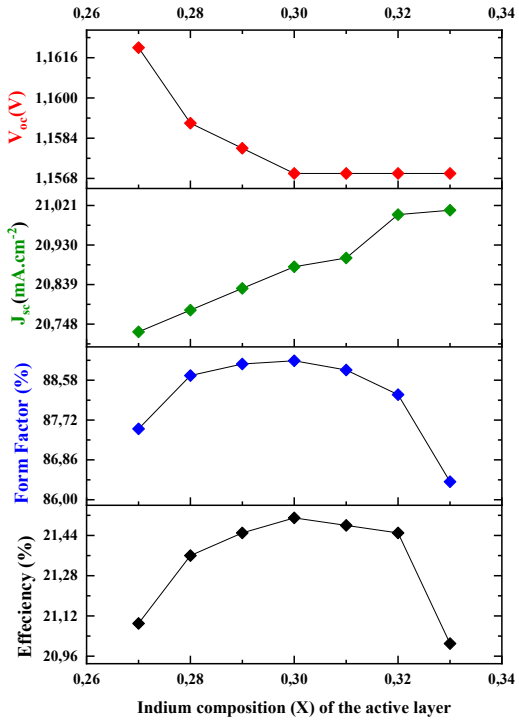

*Fig. 5. The efficiency, the form factor, the short circuit current and the open circuit voltage as a function of the composition (**x**) of Indium of the active layer.*

The composition (x) of the Indium is varied between 0.27 and 0.33. This interval allows us to have significant results from our simulation. We notice in Figure 5 a slight increase of the efficiency up to $x = 0.3$. There is a minor reduction beyond this point, both in the form factor and overall performance. However, the short circuit current and open circuit voltage remain relatively stable. These findings emphasize the significance of the active layer gap selection, as it is a critical parameter.

We have fixed the optimal values of the active layer (Thickness, doping concentration and composition (x) of Indium) and completing the optimization of the buffer layer (p-$In_xGa_{1-x}N$).

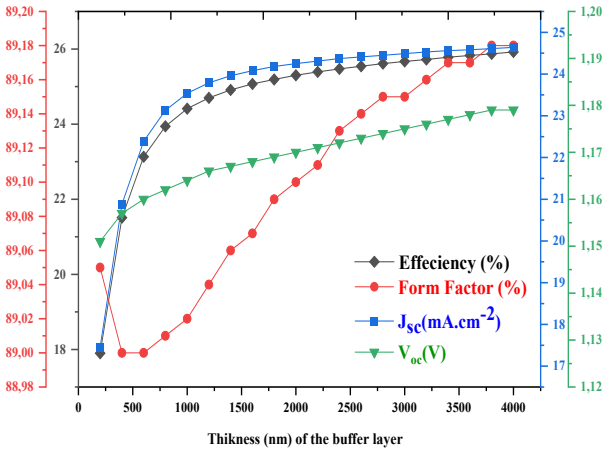

Fig. 6. Efficiency, J_{sc}, FF and V_{oc} as a function of the thickness of the buffer layer.

In Figure 6, we can observe that when the thickness of the buffer layer increases, the efficiency and the J_{sc} increase slightly and then almost stabilized from a thickness of 3000 nm. The form factor FF and the V_{oc} are almost constants at the values of 89% and 1,1 V respectively with a low variation. It is therefore not necessary to develop absorbers beyond 3000 nm. There is a major structural defect; we take half of field thickness between 2000 nm and 4000 nm. There is a low induced potential resulting from the weak electric field at the junction. So, the thickness of buffer layer is a critical parameter.

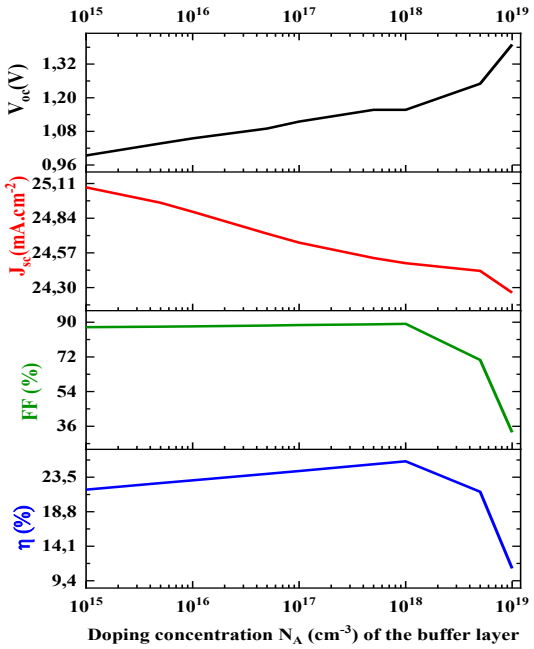

Fig. 7. The photovoltaic parameters of the cell (η , FF, J_{sc}, V_{oc}) as function of the doping concentration of the buffer layer.

So, the following parameter presents the variation of the doping concentration of the buffer layer on the parameters of the cell (FF, $J_{sc,}$ V_{oc}); we did vary the doping between $(10^{15} - 10^{19})cm^{-3}$ in the buffer layer which is p-type doped. We notice in Figure 7 that the efficiency increases when the doping concentration increases up to the value of $10^{18}cm^{-3}$ which is suitable for an energy conversion of 25.67 % while the form factor remains practically constant at this concentration.

Figure 8 shows the parameters of the cell as a function of the composition (x) of Indium. We vary the concentration between $x = 0.48$ and $x = 0.58$. We obtained better results for the optimum value of $x = 0.54$. The composition of the Indium of the buffer layer is a critical parameter.

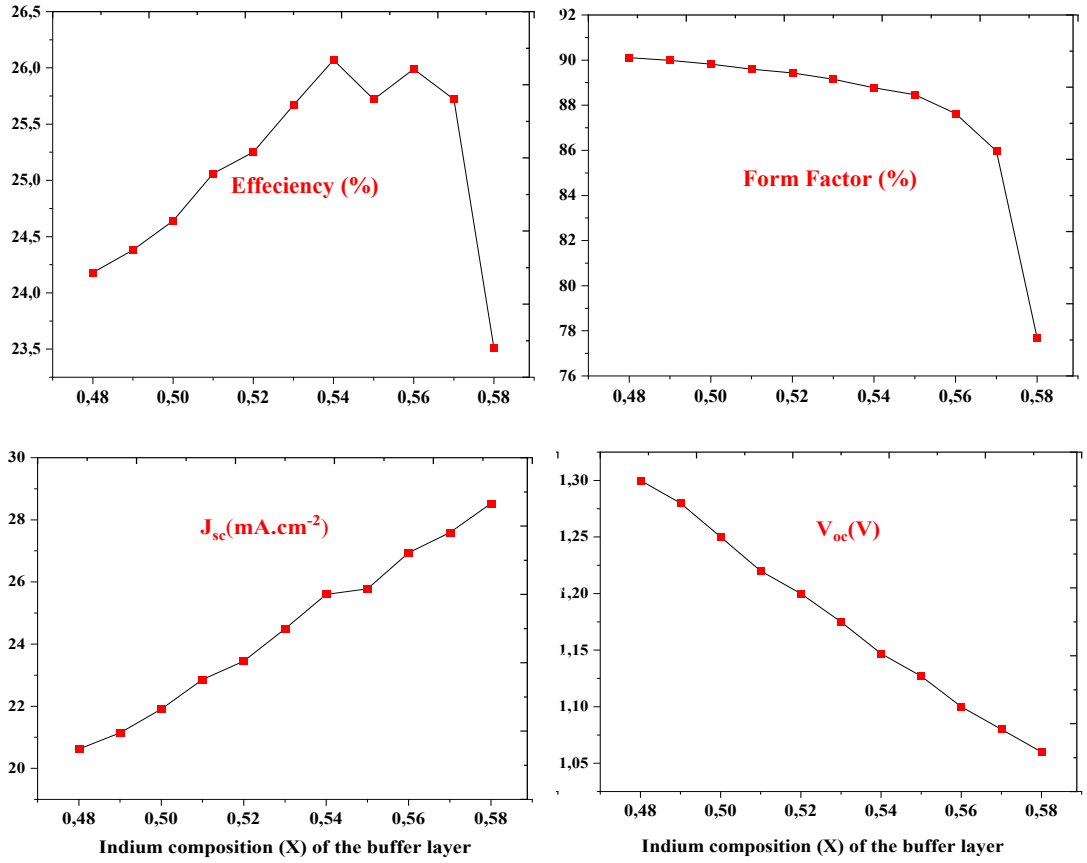

Fig. 8. The efficiency, the form factor, the short circuit current and the open circuit voltage as a function of the composition x of Indium of the buffer layer.

Using the optimal parameters of the buffer layer and the active layer, we completed the optimization of the window layer n-ZnO

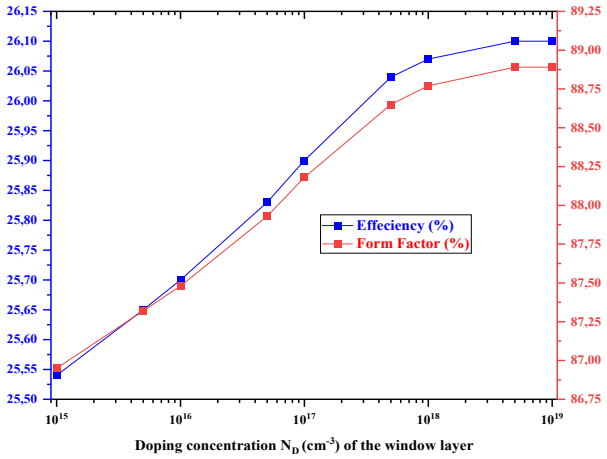

Fig. 9. Doping concentration (cm^{-3}) of the window layer.

We can see from the figure 9 that the efficiency and the form factor increase when the doping concentration increases up to a maximum value corresponds to more than 26 %. The short circuit current and the open circuit voltage almost constant as function of the variation of doping concentration.

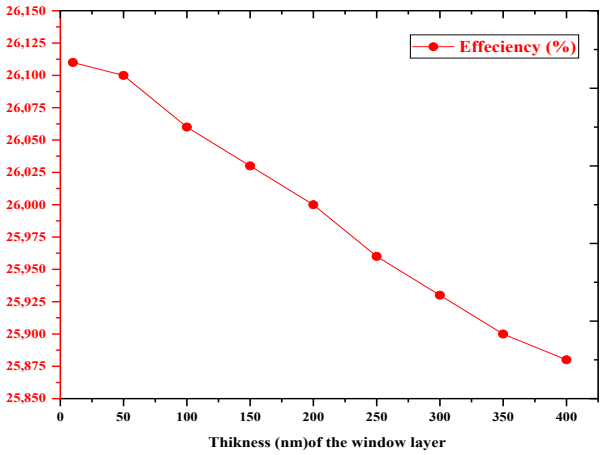

Fig. 10. The efficiency as function of the thickness of the window layer (ZnO).

At this step, we varied the thickness of the window layer between 10 nm and 400 nm. We can clearly see in the figure 10 that the optimum is present around 10 nm corresponding to the best compromise between absorption of photons, collection of current. In order to improve the performance of the InGaN based solar cell; the thickness, the doping concentration and the composition x of indium were optimized for each layer. Our results show that the efficiency increased remarkably from 10.52 % to 26.11% with an enhancement more than 100 %. The simulation results are shown in Figure 11.

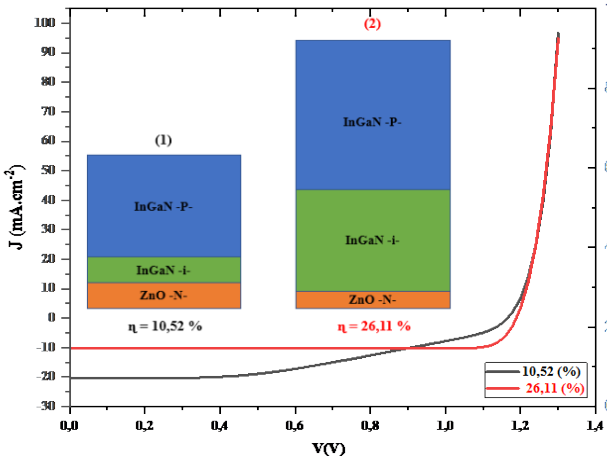

Fig. 11. The current-voltage characteristic of input structure and optimized structure based on $In_xGa_{1-x}N$.

4. Conclusion

$In_xGa_{1-x}N$-based solar cell was studied and simulated by SCAPS-1D simulator using 1-sun AM1.5 illumination. This new cell structure consists mainly of indium gallium nitride in buffer layer and active layer, the window layer is formed by zinc oxide p-$In_xGa_{1-x}N$/i-$In_xGa_{1-x}N$/n-ZnO. According to the numerical simulations carried out, we have optimized different optoelectronic parameters to improve the performance of the solar cell; we obtained the best results for a thickness of 1450 nm of active layer, n-doping 3×10^{18} cm^{-3} and 30% of indium concentration; we have reached an energy efficiency of 26,11%. The numerical simulations in this paper may be helpful for experimental studies of solar cell and the improvement of cell performance.

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