

Study of the Role of Window Layer $\text{Al}_{0.8}\text{Ga}_{0.2}\text{As}$ on GaAs-based Solar Cells Performance

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Abstract

Numerical simulation of various structures of a solar cell plays a crucial role in the design, performance prediction and the comprehension of the physics involved in their operation. It also allows of better understanding the different ways to improve the solar cells efficiency before the manufacture of the practical cell. **Objectives:** In this study, numerical results were obtained using SCAPS-1D program in order to improve GaAs solar cells performance. **Methods:** The analysis deals with the role of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ -type window layer on overall electrical performance of solar cells. The variations of thickness and doping levels in this window layer were also investigated. **Findings:** By growing this layer at the GaAs surface, the efficiency increased from 17.23% to 27.37%. The simulation results showed that this window layer should be very thin and slightly doped to achieve good performances of the entire solar cells. **Improvements/Applications:** These results are interesting because they show how much the window layer is important in improving the efficiency of GaAs solar cells.

Keywords: Efficiency Improvement, GaAs, Numerical Simulation, SCAPS-1D, Solar Cell, Window Layer

1. Introduction

During recent years, Gallium Arsenide based solar cells have been widely used in particular for spatial applications, due to their suitable band gap energy of 1.42 eV¹, high conversion efficiency and their ability to resist to high space irradiations²⁻⁸. However, the major problem with the development of GaAs solar cells was the high recombination rate at the front surface which was detrimental to the carrier's collection⁹. Because of this, the first GaAs based solar cells had only achieved conversion efficiency in the order of 10%^{9,10}. This problem has been partially resolved by depositing at the GaAs

surface a window layer with large band gap energy¹¹. The use of a homojunction GaAs solar cell has not proved to achieve high efficient solar cells. It is therefore necessary to improve their performance by exploring other materials with similar properties to add at the top and/or bottom of the traditional structure. It has been shown that $\text{Al}_x\text{Ga}_{1-x}\text{As}$ thin film material with large band gap energy, acting like window layer and/or Back Surface Field (BSF) can help improving significantly the performance of this solar cells¹¹⁻¹³. As $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and GaAs materials exhibit similar crystalline parameters, few defects and recombination centers can therefore exist at the interface between them^{14,15}. This seemed to be useful because the conversion

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efficiency of these cells has passed 20% for the first time at the end of the year's 70¹⁴. Moreover, In_{0.5}(Al_{0.7}Ga_{0.3})_{0.5}P thin film used as back surface field in the design of GaAs solar cells improves the efficiency by 6% thanks to its high photo generation rate¹⁵. This kind of solar cells has achieved a good success of conversion efficiency around 20–25%¹⁶. Recently, these solar cells have achieved conversion efficiency of 28.8 ± 0.9%¹⁷ reported a power conversion efficiency of 34.01% for numerical simulations of front graded and fully graded AlGaAs/GaAs solar cell using SCAPS-1D simulation program¹⁸ achieved a power conversion efficiency of 29.7% for numerical simulations on GaAs single solar cells using Generic Algorithm reported a power conversion efficiency of 24.5% using TCAD 2D numerical simulations of GaAs solar cells^{19,20}. In²¹ achieved a power conversion efficiency of 27% using Silvaco Atlas of GaAs/InAs solar cells. In²² reported a value of 25.8% using PC1D numerical simulations on GaAs solar cells.

In this study, the main goal is first to simulate a homo-junction GaAs solar cell using SCAPS-1D program in order to evaluate the reasons of its efficiency limitations; then, using Al_xGa_{1-x}As type material like window layer to improve the solar cell efficiency; and finally, investigating the effects of thickness and doping levels of this window layer on the overall solar cell performances.

2. Simulation Program and Device Structure

2.1 Simulation Program

The simulations have been carried out using the SCAPS-1D program. SCAPS is a one-dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium²³. The program is freely available to the PV community and is easily downloaded. It was originally developed for all structures of the CuInSe₂ and CdTe family and since then, several extensions have improved its capabilities to implement other structures including thin films^{23,24}. New versions of the program have been improved especially to simulate characteristics of Alternative Current (AC) and Direct Current (DC) of hetero junction solar cells. Output parameters such as

J-V characteristics under dark and illumination can be extracted from results obtained by a SCAPS simulation²³. Moreover, important information like energy band diagram, electrical field distributions, free and trapped carriers populations, generation-recombination profile and individual carriers densities as a function of the position can also be extracted from SCAPS program²⁴. All this information is calculated by SCAPS on the basis of the Poisson's equation and the continuity equation for free electrons and holes given by the following expressions, respectively²⁵:

$$\frac{\partial}{\partial x} \left(\epsilon_0 \epsilon \frac{\partial \psi}{\partial x} \right) = -q \left(p - n + N_D^+ - N_A^- + \frac{\rho_{def}}{q} \right) \quad (1)$$

$$-\frac{\partial J_n}{\partial x} - U_n + G = 0 \quad (2)$$

$$-\frac{\partial J_p}{\partial x} - U_p + G = 0 \quad (3)$$

Where ψ is the electrostatic potential, n and p the free electron and free hole, N_D^+ and N_A^- ionized donor-like and ionized acceptor-like concentrations. J_n and J_p are the electron and hole current densities respectively. The term G is the optical carrier generation rate and U is the total recombination rate.

2.2 Device Structure and Material Properties

The basic structure, used for our simulations, is essentially composed of a homojunction npGaAs solar cell on which is deposited an Al_{0.8}Ga_{0.2}As n-type window layer to form the heterojunction. The lattice parameter difference between GaAs and Al_xGa_{1-x}As ($0 \leq x \leq 1$) is very small (less than 0.15% at 300 K), which promises an insignificant concentration of undesirable interface states²⁶; in many III-V ternary alloys, this parameter obeys Vegard's law. A schematic drawing of the solar cell structure is shown in Figure 1. The main physical parameters used in the simulations are presented in Table 1. These parameters have been chosen from literature, theory and in some cases reasonably estimated^{27–29}. Simulations have been done under illumination with the 1.5 G spectrum and a temperature of 300 K. The output parameters of the simulated solar cells have been recorded in the case of zero series resistance and very high shunt resistance.

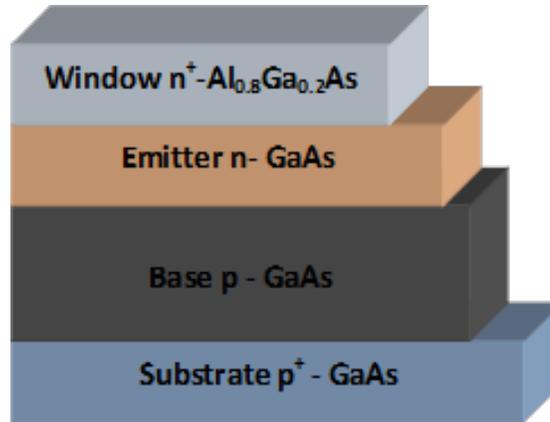


Figure 1. Basic structure of GaAs solar cells simulated in this study.

Table 1. Main material properties used in the simulation

Material	Window n+-Al _{0.8} Ga _{0.2} As	Emitter n-GaAs	Base p-GaAs	Substrate p+-GaAs
Thickness (μm)	0.02	0.1	2	0.5
Band gap energy (eV)	2.09	1.424	1.424	1.424
Electron affinity (eV)	3.74	4.07	4.07	4.07
Dielectric permittivity (relative)	10.6	12.9	12.9	12.9
CB effective density of states (cm ⁻³)	8 × 10 ¹⁹	1 × 10 ¹⁷	1 × 10 ¹⁷	1 × 10 ¹⁷
VB effective density of states (cm ⁻³)	1 × 10 ¹⁹	1 × 10 ¹⁹	1 × 10 ¹⁹	1 × 10 ¹⁹
Electron thermal velocity (cm/s)	2.3 × 10 ⁵	4.4 × 10 ⁵	4.4 × 10 ⁵	4.4 × 10 ⁵
Hole thermal velocity (cm/s)	1.4 × 10 ⁵	1 × 10 ⁵	1 × 10 ⁵	1 × 10 ⁵
Electron mobility (cm ² /Vs)	212	8500	8500	8500
Hole mobility (cm ² /Vs)	126	370	370	370
Donordensity N _D (cm ⁻³)	2 × 10 ¹⁸	2 × 10 ¹⁸	0	0
Acceptordensity N _A (cm ⁻³)	0	0	2 × 10 ¹⁷	2 × 10 ¹⁸
Absorption coefficient	SCAPS	SCAPS	SCAPS	SCAPS

3. Results and Discussion

3.1 Basic GaAs-based Solar Cell Simulation

The SCAPS-1D simulation program has been used to evaluate and to record output characteristics of the traditional n-GaAs/p-GaAs/p⁺-GaAs and the improved n⁺-Al_{0.8}Ga_{0.2}As/n-GaAs/p-GaAs/p⁺-GaAs solar cells (Figure 1). The resulting J-V characteristics and quantum efficiency results of n-GaAs/p-GaAs/p⁺-GaAs solar cell are shown in Figure 2. The calculated electrical parameters are presented in

Figure 2 (a). The simulated solar cell showed a conversion efficiency of 17.23%. As can be seen in Figure 2 (b), more than 80% of photons in visible range of the solar spectrum are absorbed by the material. But, as expected, there are losses induced by the recombination of charge carriers at the front surface due certainly to the high recombination rate of the GaAs surface, where we find pendant bonds which act like recombination centers. This problem has been partially resolved by the growth of a window layer at the GaAs surface.

The schematic energy band diagram at thermal equilibrium and illumination conditions for typical GaAs np

homojunction solar cell is illustrated in Figure 3. At equilibrium (Figure 3(a)), it can be seen that conduction band CB and valence band VB levels are well aligned with the Fermi level E_f , which define only the occupancy probability of different levels per electron³⁰. When the solar cell is illuminated (Figure 3 (b)), one can see besides CB and VB levels, quasi-Fermi levels for electrons F_n and for holes F_p . These levels are due to the fact that charge carriers have a thermal distribution of energy during the quasi-totality of their lifetime because of their interactions with the crystalline network³¹. Figure 4 depicts the generation and recombination rates in every layer of the cell. The generation rate is increased in the emitter and decreases slowly when entering the cell. On the other hand, the recombination rate is relatively low in all layers compared to the generation rate. Nevertheless, we can see at the np junction a non negligible recombination which can be assigned to the grain boundaries at the interface of the two materials.

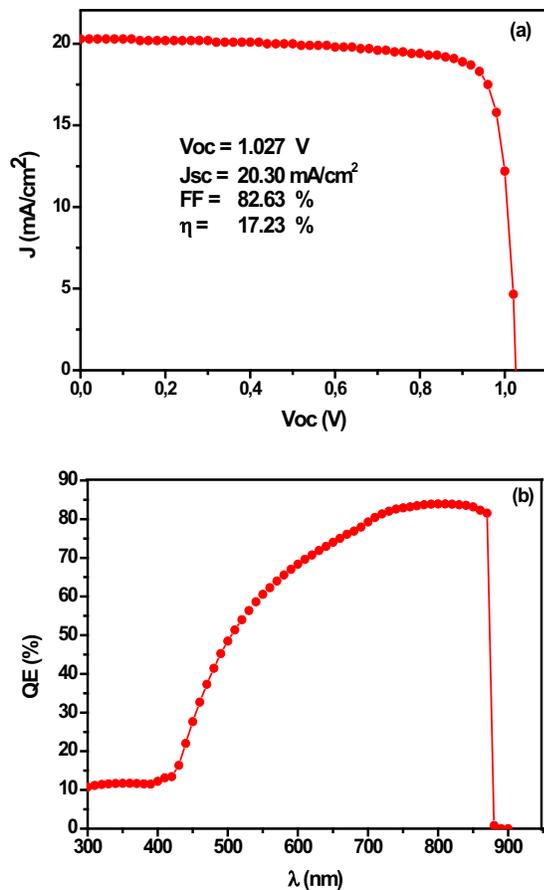


Figure 2. (a) J-V characteristics and (b) Quantum efficiency plots of the traditional simulated GaAs solar cells.

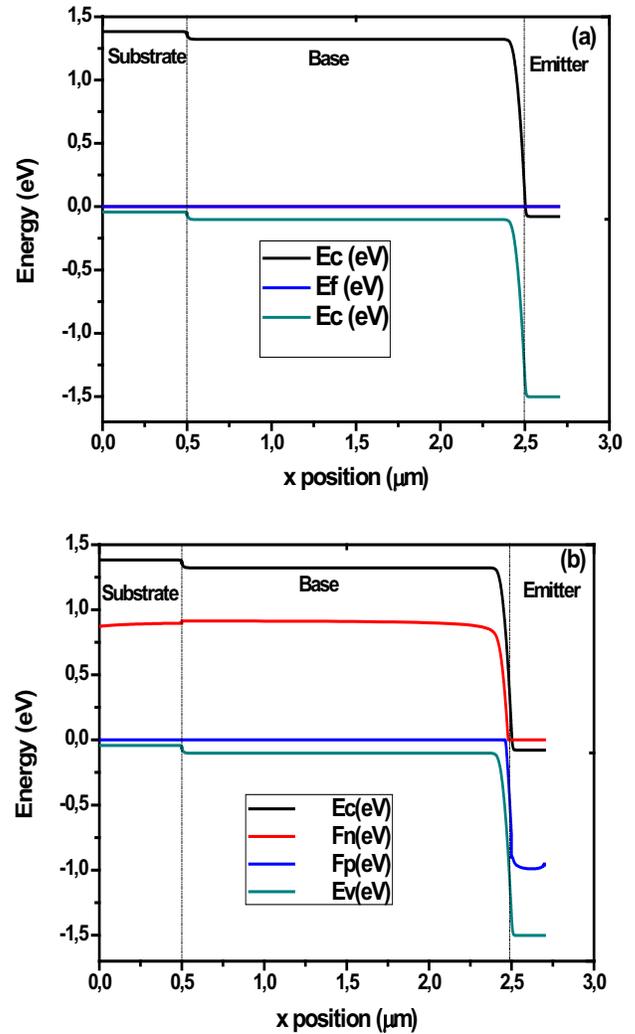


Figure 3. Energy band diagram calculated for GaAs solar cell: (a) at equilibrium and (b) under illumination condition.

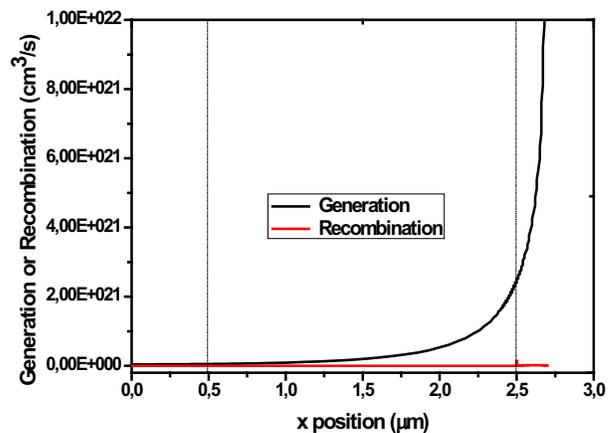


Figure 4. Generation-recombination profile in GaAs solar cell as a function of the illumination depth.

3.2 Al_{0.8}Ga_{0.2}As/GaAs Solar Cell Simulation

As shown in Figure 2 (b), there is a high recombination of free carriers at the front surface of the cell which can contribute to limit the efficiency of the solar cell. It had been suggested to put down the emitter a window layer, especially the Al_xGa_{1-x}As thin film material (in this study, $x = 0.8$ and band gap is about 2.09 eV because this typical x value of the window layer gives good results). The Al_xGa_{1-x}As window layer is transparent to photons with energies up to about 2.1 eV and cuts off the light gradually in the range 2.1-2.6 eV due to its indirect band gap. This layer not only must allow to minimize the recombination at the front surface of the cell, but also to make it more sensitive to photons with higher energies. J-V characteristics and quantum efficiency outputs of Al_{0.8}Ga_{0.2}As/n-GaAs/p-GaAs/p⁺-GaAs solar cell is shown in Figure 5. There is a significant improvement in the calculated electrical parameters when adding a window layer to the traditional GaAs solar cell as seen in Figure 5 (a). This improvement is mainly observed in the short current density and conversion efficiency values. With the use of Al_{0.8}Ga_{0.2}As-type window layer, photo-current has increased from 20.30 mA/cm² to 30.87 mA/cm² and conversion efficiency from 17.23% to 27.37%. This result is in good agreement with that of the experimental cell²¹.

This result was expected because by analyzing the quantum efficiency curve (Figure 5 (b)), there is almost not recombination at the front surface and the solar cell absorbs more or less 90% of the solar spectrum. Therefore, the window layer Al_{0.8}Ga_{0.2}As is almost transparent for the wide part of the solar spectrum and by this way improves the absorption of photo-carriers as shown in Figure 5 (b). Moreover, it reduced losses induced by recombination at the front, which improve the conversion efficiency. Nevertheless, it is important to note that the contribution of this layer in the generation of photo-carriers is negligible as it has large and indirect band gap energy of 2.09 eV. The schematic energy band diagram under illumination conditions for typical Al_{0.8}Ga_{0.2}As/n-GaAs/p-GaAs/p⁺-GaAs solar cell is illustrated in Figure 6. Figure 6 (b) shows well the discontinuity ΔE_c in the conduction band at the window-emitter interface. This discontinuity generally occurs in heterojunction solar cells and its essential goal is to limit the recombination

of photo-carriers at the window-emitter interface. The generation-recombination profile in every layer of the solar cell is shown in Figure 7. It can be seen in Figure 7 (a) that the generation rate in the solar cell with window varies more or less in the same way than in the solar cell without window. This confirms that the window layer does not contribute significantly in the generation phenomenon as stated above. In addition, the recombination rate is more increased at the np junction and the surface of the solar cell without window than that with window as shown in Figure 7 (b).

It is obvious that the window layer contributes much more to reduce the recombination in front surface than in the generation of photo-carriers.

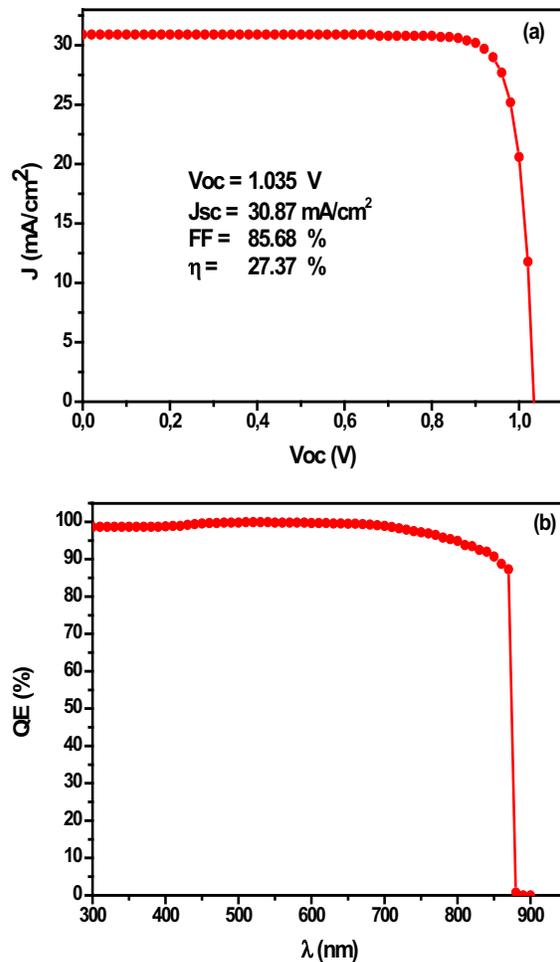


Figure 5. J-V characteristics and Quantum efficiency plots of the simulated Al_{0.8}Ga_{0.2}As/GaAs solar cells.

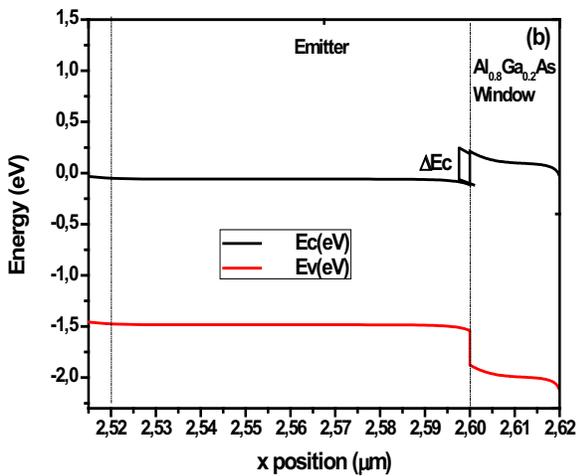
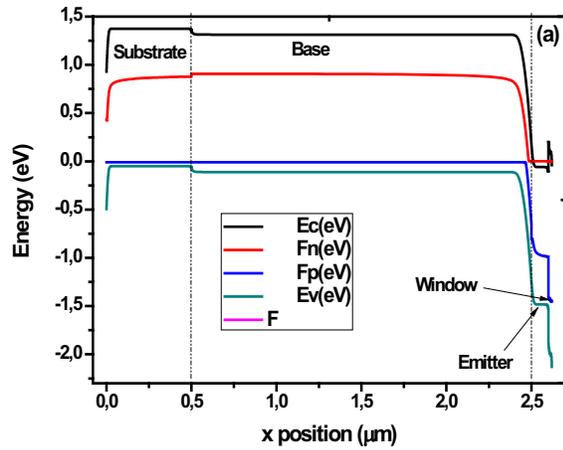


Figure 6. (a) Energy band diagram calculated for the Al_{0.8}Ga_{0.2}As/GaAs solar cell under illumination. (b) Enlarged view showing details of the conduction band offset ΔE_c at the window-emitter interface.

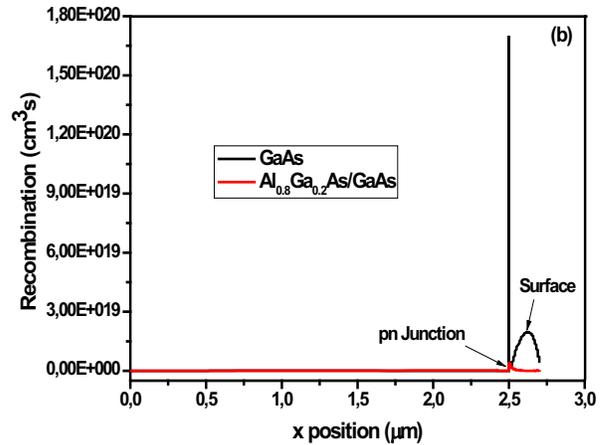
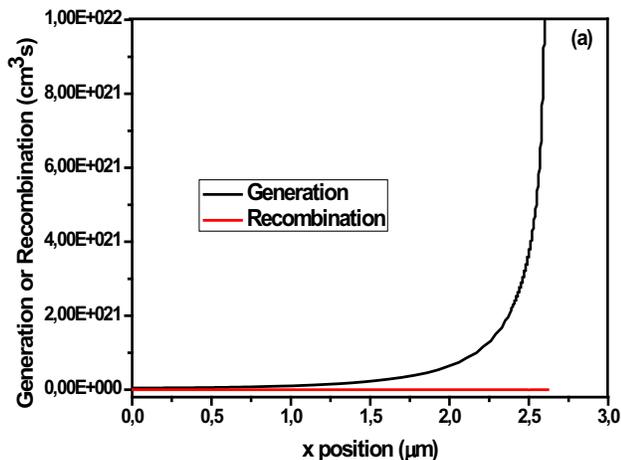


Figure 7. (a) Generation and recombination in Al_{0.8}Ga_{0.2}As/GaAs solar cell rates as a function of the illumination depth. (b) Recombination profile in GaAs solar cell with and without window.

3.3 Effect of the Al_{0.8}Ga_{0.2}As Window Layer Parameters

To investigate the effect that can have the window layer Al_{0.8}Ga_{0.2}As on the overall cell performance, some parameters such as thickness and doping levels have been varied from 0.01 μm to 0.1 μm and from 10^{14} to 10^{19} cm^{-1} , respectively. The variations of the calculated electrical parameters of the simulated solar cell as a function of the window thickness are shown in Figure 8 (a). It is seen that output parameters of the simulated solar cell decrease when the thickness increases. When the thickness increases, more photons are absorbed and the optical generation rate increases in the window. In addition, the increase in window's thickness would lead to decrease in the photons which have reached the absorber layer and contribute to photovoltaic conversion. The phenomenon can further the recombination of charge carriers and this reduces the solar cell electrical parameters values. This shows that, for GaAs based solar cells and because of the high recombination rate at the surface, the thickness of the window layer should be narrow. The Al_{0.8}Ga_{0.2}As compound has a large band gap of 2.09 eV, which means that only solar radiations with wavelength less or equal to $\lambda = 0.6 \mu\text{m}$ are absorbed. Solar radiations with wavelength more than $\lambda = 0.6 \mu\text{m}$ reach the GaAs interface and those having wavelength less than $\lambda = 0.87 \mu\text{m}$ are absorbed in the base. The optical generation rate therefore is very low

throughout the thickness of the window layer, especially if it is very thin. In addition, the layers with a high content in Al should be kept from the ambient air to avoid oxidation of Al. In most devices, the window layer is followed by a p-GaAs contactable capping layer to overcome this issue¹⁸.

In Figure 8 (b), are represented the effect of window layer doping on the output electrical parameters. We observed that the FF slightly increases when the doping increases whereas Voc, Jsc and conversion efficiency are nearly unchanged between 10^{14} and 10^{18} cm^{-1} and decrease beyond. The increase in FF value is negligible because the effect of series resistance has not been taken into account in our simulation. The increase of window layer doping reduces significantly its resistance. The increase of window layer doping increases the density of charge in the layer. When the layer is illuminated, due to the high density of charge rate, the optical generation rate increases and this can further the recombination process in the layer as stated above. Such a behavior can affect the values of Voc, Jsc and conversion efficiency.

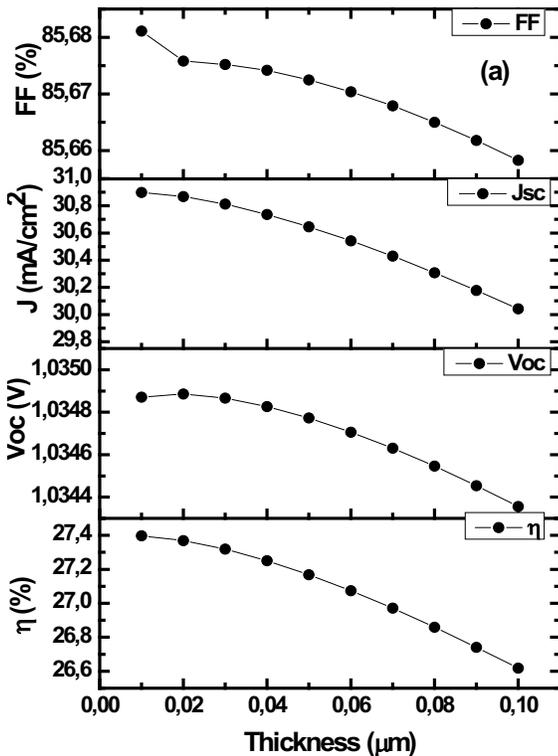
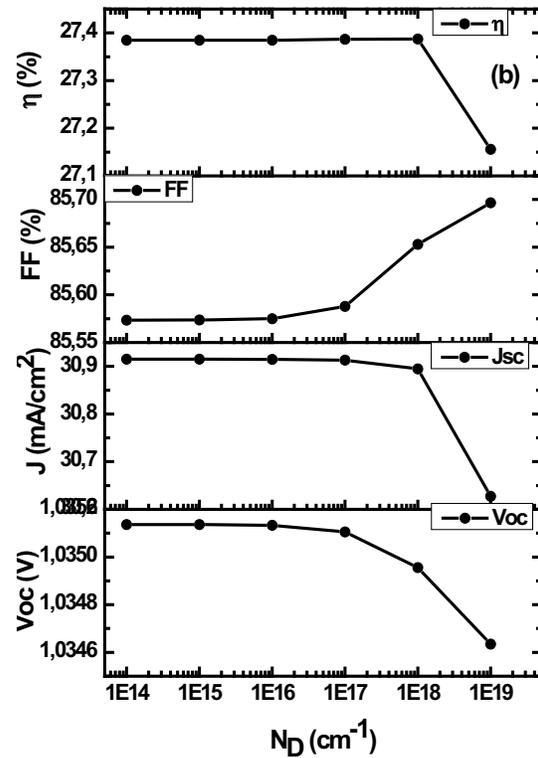


Figure 8. Calculated output parameters of the $\text{Al}_{0.8}\text{Ga}_{0.2}\text{As}/\text{GaAs}$ solar cell as a function of: (a) window thickness. (b) doping concentration of the window.

4. Conclusion

In this study, a homojunction solar cell was first designed and simulated. Then, a n-type window layer $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with $x = 0.8$ was used to improve the cell output parameters. Finally, some window layer parameters like thickness and doping concentration have been varied to investigate their effect on solar cell performance. The simulation results showed that $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ heterojunction solar cells achieve better conversion efficiency than the GaAs homojunction. This result is attributed to the reduction of the series resistance and the recombination velocity of photo generated carriers at the front surface of cell. The quantum efficiency curve revealed that the window layer is almost transparent in the wide part of the solar spectrum. The generation-recombination profile indicated that the window layer contributes much more to reduce

the recombination process than to generate the photo-carriers. We have also found that the window should be very thin to reduce series resistance in cell and also must be moderated doped. The conversion efficiency has moved from 17.23% for a GaAs homojunction solar cell to 27.37% for an Al_{0.8}Ga_{0.2}As/GaAs heterojunction solar cell. This result is in good agreement with experimental results. A thickness of 0.02 μm and a doping level in the order of 10¹⁸ of the window layer are found to be suitable in order to achieve good conversion efficiency in Al_xGa_{1-x}As/GaAs solar cells.

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