Vol. 12(12), pp. 532-537, December 2018
DOI: 10.5897/AJEST2018.2565
Article Number: 7F49C0B59479
ISSN: 1996-0786

http://www.academicjournals.org/AJEST

African Journal of Environmental Science and Technology

*Full Length Research Paper*

# Study by numerical simulation of a PN solar cell in 3C-SiC / Si

**M. Toure[1*], B. Berenguier[2], D. Kobor[1], L. Ottaviani[2] and M. Pasquinelli[2]**

[1]Laboratoire de Chimie et de Physique des Matériaux (LCPM), UFR Sciences et Technologies, Université Assane Seck de Ziguinchor, BP 523, Ziguinchor, Sénégal.
[2]IM2NP (UMR CNRS 7334) – Université Aix-Marseille, Case 231 - 13397 Marseille Cedex 20, France.

Received 3 September 2018; Accepted 29 October 2018

**The optimization of the solar cell includes the study of the influence of parameters such as cell thickness, doping levels and profiles, contact configuration and optical confinement on the output to obtain a structure leading to the best performance. The optimal parameters depend on the structure of the solar cell, the quality of the substrate material (lifetime, mobility), the quality of the ohmic contacts, the speed of recombination, etc. The cell to be studied has a structure composed of an n-type gap material ($Eg_{3C\text{-}SiC}$=2.36 eV) as a window layer and a small gap material ($Eg_{Si}$ = 1.12eV) as a substrate. The manufacture of a cell based on 3C-SiC / Si is expensive because 3C-SiC is a material that does not exist in the natural state, hence the interest of numerical simulation in order to determine the most important parameters for the operation of heterojunction solar cells (3C-SiC / Si), to minimize losses and to optimize the physical and geometrical parameters of the cell in order to obtain maximum efficiency. The most important recombination sources are Shockley-Read-Hall recombinations in the substrate, Auger recombinations and recombinations on the front of the cell. To study the influence of the various parameters, we first defined a reference solar cell with a set of fixed parameters, then we varied the parameters one by one (the others remaining fixed) in order to analyze their influences. On the characteristics of the solar cell, we obtained a Voc of 0.633 6 V, a short-circuit current of 37.82 mA / cm$^2$, a form factor of 83.38%, which gives us a yield of 19.98%.**

**Key words:** Solar cells, numerical study, heterostructure, silicon carbide, Silicon.

## INTRODUCTION

One of the methods used to exploit solar energy is to use photovoltaic cells that convert the energy carried by the incident radiation into a continuous electric current. This conversion is based on the photovoltaic effect generated by the absorption of photons. Part of the absorbed photons generates electron-hole pairs that are separated by an electric field created in the space charge area of a p-n junction. One way to amplify this current is to reduce the thickness of the first insolated area that absorbs some of the incident light.

An actual trend is to build a band shape wavelength collection also called multi-junctions solar cells, where

*Corresponding author. E-mail: tourempci@hotmail.fr.

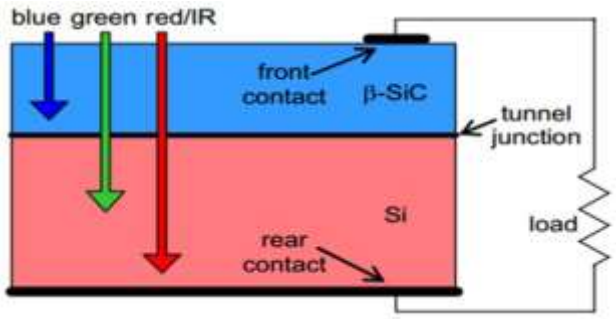


**Figure 1**. Structure of the tandem cell based on 3C-SiC / Si.

several single junctions made of different materials with different band gaps are superposed, each one collecting a part of the spectra. Thus, III-V compounds are currently dominating the multi-junction field, with a 40.7% efficiency world record for GaInP/GaInAs/Ge triple junction cell (Yastrebova, 2007). However, Silicon and its alloys are still a field of interest for producing multi-junction cells. High development degree of silicon technology, lower cost of fabrication and non-toxicity are good arguments to follow this way. In case of tandem cell, the optimal band gap for the top junction would be between 1.6 and 1.8 eV, but few materials compatible with silicon are presently available meeting this requirement (Toure et al., 2014).

3C silicon carbide (3C-SiC), with 2.36 eV band gap could be a potential replacement material. SiC is known for his ability to resist high radiation level, making it suitable to work in solar concentrators. The opportunity to make 3C-SiC/Si tandem cells has been studied theoretically (Heidarzadeh et al., 2014; Richards et al., 2003), leading to a theoretical efficiency of 26%.

In particular, in this study of numerical simulations, we propose a solar cell tandem based in inorganic material, a bilayer solar cell of 3C-SiC on a substrate in silicon. The advantage of the difference in the network parameter between 3C-SiC and silicon, that is to say the low recombination of the carriers in the SiC / Si interface, leads to the harvesting of the maximum wavelength of the spectrum AM 1.5. A solar cell including a bandgap at 1.12 eV and a wider bandgap at 2.3 eV leads to the harvesting of the solar spectra photons added to the UV wavelengths photons.

Toure et al. (Toure et al., 2014) have done a first study which allowed us to evaluate the potential of the heterojunction 3C-SiC / Si for a photovoltaic application. The conclusion of this study is that the performances of the cells are deteriorated by SRH recombination phenomena which hut the current density, the open-circuit voltage as well as the quantum yield in the infrared domain. These recombinations could come from the deterioration of the diffusion length of the silicon during the deposition of 3C-SiC at high temperature.

Being a material that does not exist in the natural state and is expensive, it is essential to conduct numerical simulation studies to see which parameters act to improve the performance of the 3C-SiC / Si cell.

In order to predict the cell's performance, we used the SCAPS simulation software. SCAPS (Solar Cell Capacitance Simulator) by adopting the structure of Richards et al. (2003) (Figure 1) to determine the most important parameters for the operation of heterojunction solar cells (3C-SiC / Si), minimize losses and optimize the physical and geometrical parameters of the cell in order to obtain maximum efficiency.

**Presentation of the numerical model**

In Figure 2 we presented the structure of solar cell. To simulate the solar cell device under the light, Maxwell electromagnetic equations are solved. The Maxwell equation solver leads to the electromagnetic field strength which allows us to obtain the generation rate (G) of the electron-hole pair by the following equation:

$$G = G_n = G_p = \frac{\eta}{\hbar\nu}\left[-\nabla\frac{1}{2}\Re\left(\vec{E}\times\vec{H}\right)\right] \quad (1)$$

Where η, is the quantum yield assumed the unity, ħν the photon energy (ħ being the quantum Planck constant, ν the wave frequency), $\nabla\frac{1}{2}\Re\left(\vec{E}\times\vec{H}\right)$ the power density (related to the time averaged Poynting vector) according to the electric field $\vec{E}$ and the magnetic field $\vec{H}$.

To compute the solar cell device, the electromagnetic results are injected in the electrical simulation regarding the physical phenomena inside the device. Thus, generation rate is introduced in the following continuity and Poisson Equations 2, 3, 4 in order to determine the evolution of the charge carrier density and the electric field inside the solar cell device:

$$\frac{\partial n}{\partial t} = G_n - R(n,p) - \frac{1}{q}\nabla\left(-q\,n\,\mu_n\nabla\phi - k_B T\mu_n\nabla n\right) \quad (2)$$

$$\frac{\partial p}{\partial t} = G_p - R(n,p) - \frac{1}{q}\nabla\left(q\,n\,\mu_p\nabla\phi - k_B T\mu_p\nabla p\right) \quad (3)$$

$$\Delta\phi = -\frac{\rho(x,y,z)}{\varepsilon_0\varepsilon_{SC}} \quad (4)$$

Where, n, p are electron and hole densities ($cm^{-3}$), $G_n$ $G_p$ electron and hole generation rates ($s^{-1}.cm^{-3}$), R(n,p) the carrier recombination rate ($s^{-1}.cm^{-3}$), q the elementary charge (C), $\mu_n$, $\mu_p$ electron and hole mobilities ($cm^2.V^{-1}.s^{-1}$), Φ the potential (V), $k_B$ the Boltzmann constant ($J.K^{-1}$), T the temperature (K), ρ the charge density ($cm^{-3}$), $\varepsilon_0$ the vacuum permittivity constant ($m^{-3}.kg^{-1}.s^4.A^2$), $\varepsilon_{SC}$ the semiconductor permittivity constant. It is important to emphasize these continuity equation expressions are coupled to recombination physical phenomena such as the SRH

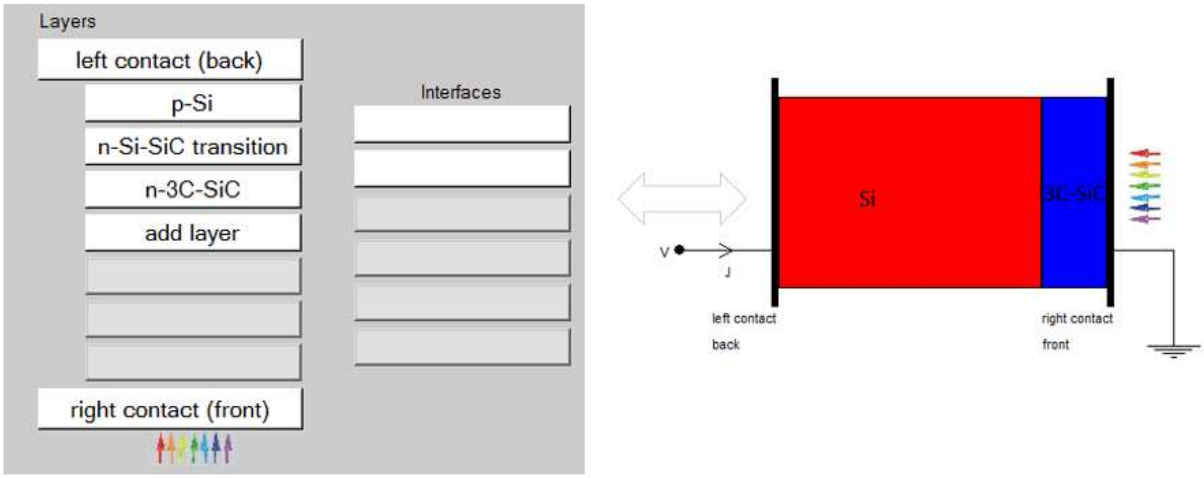


**Figure 2.** Structure of the 3C-SiC / Si solar cell.

**Table 1.** Value of life time and mobility in SiC.

| **Life time** | **180 ns et 3 µs (Ichimura et al., 1997; Ščajevn , 2014)** |
|---|---|
| Mobility | 20 cm²/V. s (Nishino et al., 1983 ) 100 cm²/V. s (Ščajevn et al., 2013) |

recombination-generation rate R (n,p). The $\tau_n$ and $\tau_p$ are electron and hole lifetime. For both simulation window, in particular on the both sides of the solar cell device, are imposed the Neumann boundary conditions sides. All simulations are performed at room temperature (300 K). The bandgap $E_G$ of the 3C-SiC has a width of 2.3 eV and 1.12 eV for the silicon whereas work function $\chi$, are respectively equal to 4.05eV and 3.85eV.

In the SCAPS literature was introduced by the references (Niemegeers and Burgelman, 1996; Burgelman et al., 2000), its algorithms are amply detailed in (Niemegeers et al., 1998), and its applications of the simulation can be consulted in the references (Niemegeers and Burgelman, 1997; Burgelman et al., 1999).

The optimization of the solar cell includes the study of the influence of the parameters such as the thickness of the cell, the levels and the doping profiles, the quality of the material, the substrate (lifetime, mobility), the configuration and quality of the ohmic contacts, the recombination speed, the optical confinement in order to obtain a structure leading to the best performance.

## RESULTS AND DISCUSSION

In order to predict the cell's performance, we used the SCAPS simulation software. SCAPS (Solar Cell Capacitance Simulator) is a one-dimensional numerical simulation software for solar cells developed by the Department of Electronic and Computer Systems (ELIS) at the University of Gent in Belgium. Several researchers have contributed to the development of this software: Alex Niemegeers, Marc Burgelman, Koen Decock, Johan Verschraeagen, Stefaan Degrave (Decock et al., 2011; Burgelman and Marlein, 2008; Verschraegen and Burgelman, 2007; Degrave et al., 2003; Niemegeers and Burgelman, 1996). This allows from the fundamental parameters of the materials used to calculate the performance of the cells, such as the internal quantum efficiency as well as the current-voltage curves under illumination. The difficulty of this study was to be able to simulate the 3C-SiC.Si on SCAPS because it was originally developed for the CuInSe2, CdTe family cell structures and to obtain the SiC-3C parameters, in particular the lifetime and mobility in this material given in Table 1. According to the literature, this can vary according to the quality of the material (Ichimura et al., 1997; Ščajevn, 2014). However, several extensions have improved its capabilities to become applicable to crystalline solar cells (of the Si and GaAs family), as well as amorphous solar cells (a-Si and Si micro-morphs).

So we did four simulations. In the first case, we set an intermediate lifetime in SiC: 1.3 µs. The current-voltage curves under AM0 are shown in Figure 3a and the quantum yield curves in Figure 3b for the four doping levels.

The simulation of current-voltage curves under illumination shows that these doping levels do not affect the characteristics of our cells. In all cases, the open circuit voltage is of the order of 0.57 V, short-circuit current 46.5 mA / $cm^2$, the form factor is 81%, which gives us a performance of 16.8%. This shows that the weakest doping is sufficient to establish a large area of space charges in the silicon. As regards the internal quantum efficiency (QE), it can be observed that the most important doping induces a considerable drop in the

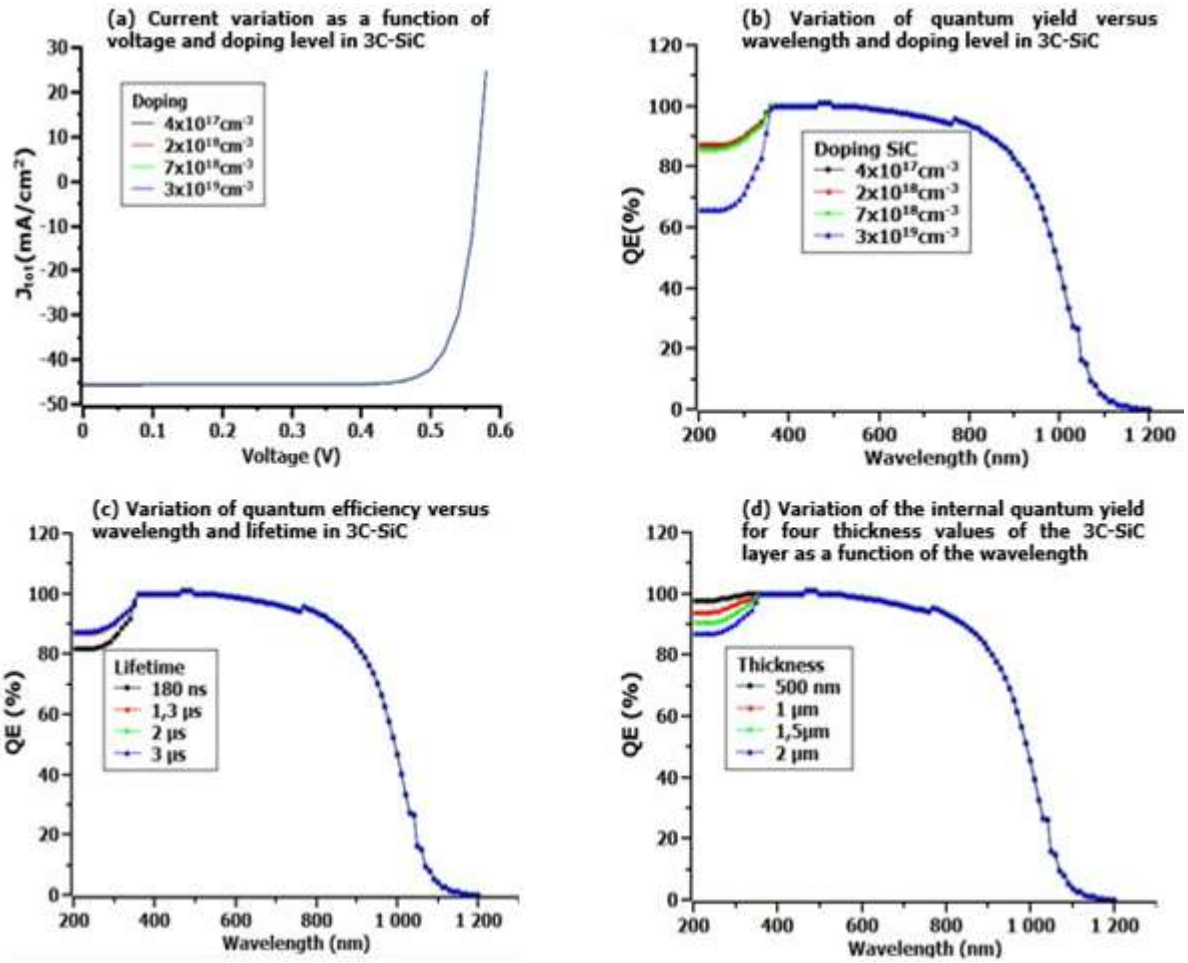


**Figure 3.** Variation in the doping rate of the service life and thickness of the SiC layer.

efficiency at the shortest wavelengths in the range 200 to 400 nm.

This decrease could be due to a decrease in carrier collection that could come from a narrowing of the space charge zone in SiC. For the rest of the simulations, we used 2x1018 $cm^{-3}$ doping for the SiC layer. In a second step, we tested the influence of the lifetime on the quantum yield and the results are represented in Figure 3c.

From 200 to 400 nm, we have a quantum efficiency variation of about 80% for 180 ns and about 88% for the rest. Above 400 nm, the curves are confounded for all lifetimes, because the diffusion length is sufficient to ensure the collection of loads even with a service life of 180 ns. The parameters Voc, Jsc, FF, η are identical.

Thirdly, we varied the thickness of the SiC layer in Figure 3d, keeping the doping at a value of 2x1018 $cm^{-3}$ and the lifetime at 1.3 µs. The quantum yield in the UV rises significantly as the thickness of the layer decreases as the space charge area approaches the surface. Finally we have decreased the life time in silicon logarithmic way. We can observe in Figure 4a that the quantum efficiency remains constant in the UV. This component comes indeed from the silicon carbide layer. On the other hand, it is significantly degraded in the infrared part generated by silicon. With regard to the current-voltage characteristics in Figure 4b, we see that the open circuit voltage as well as short-circuit current fall as the service life decreases. This result therefore makes it possible to envisage the use of a substrate of very good quality.

These simulation results allowed us to detect optimal values given in Table 2 for some parameters that will allow us to optimize the performance of our 3C-SiC / Si heterojunction cell. The results of the simulation with these parameters are given in Figure 5a and Figure 5b.

The simulation of the current-voltage curves under illumination with the optimum parameters gives us an open circuit voltage is the order of 0.633 6 V, short-circuit current 37.82 mA / $cm^2$; the form factor is 83, 38%, which gives us a return of 19.98%. The external quantum efficiency is determined not only by the thickness of the substrate and the window layer but also by an important parameter which is the diffusion length. a deterioration of the parameters of our cells by recombination phenomena

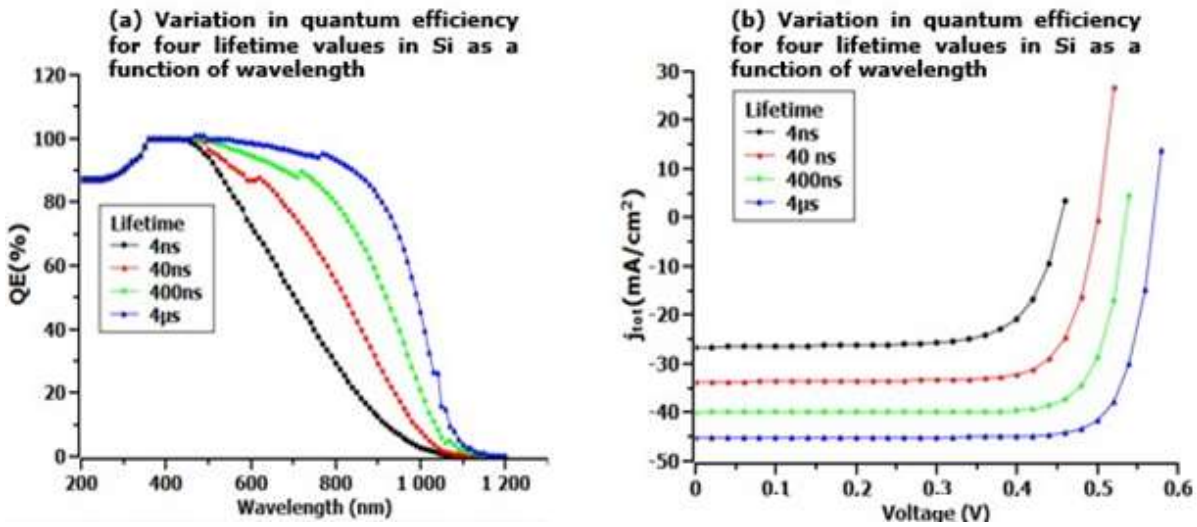


**Figure 4.** Variation in the life of the Si layer.

**Table 2.** Optimum parameters for the heterojunction cell.

| Settings | Optimum value |
|---|---|
| Doping of the 3C-SiC layer | $2x10^{18}cm^{-3}$ |
| Lifetime in 3C-SiC | 1,3 µs |
| Electron mobility in 3C-SiC | 100 cm²/V. s |
| The thickness of the 3C-SiC layer | 500 nm |
| Si substrate doping | $2x10^{16}cm^{-3}$ |
| Lifetime in the Si | 4 µs |

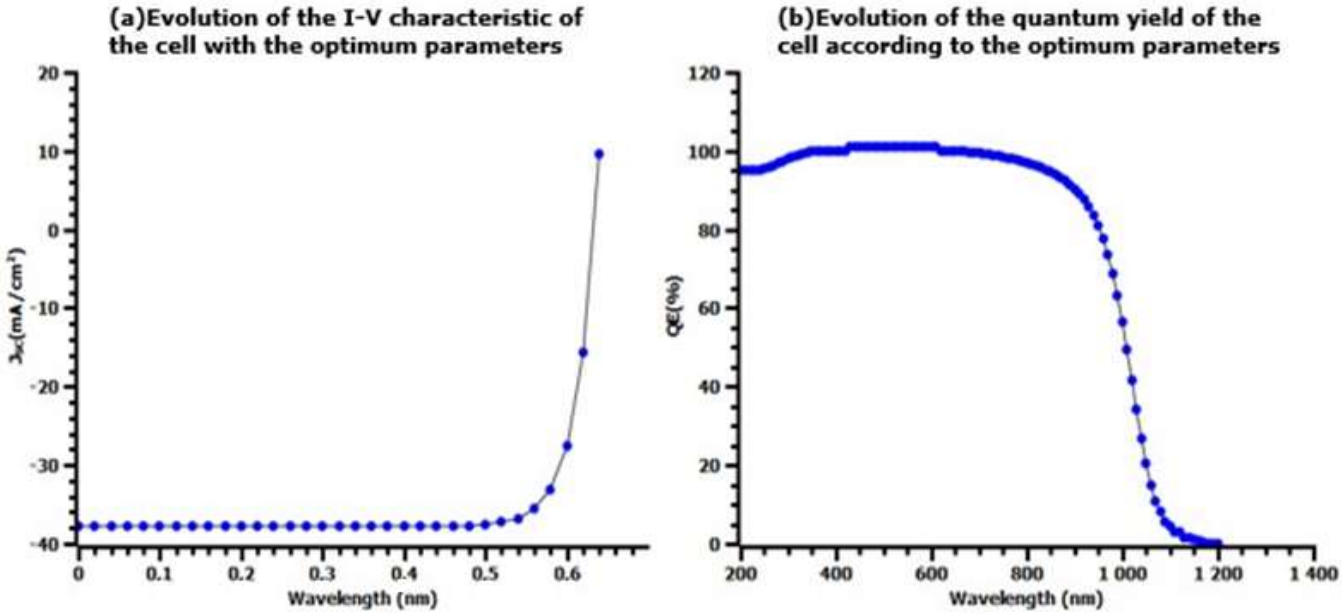


**Figure 5.** Evolution of I-V characteristic and the quantum yield of the cell according to the optimum parameter.

was noticed. These same remarks were made by Biondo et al. (2014) by performing a numerical simulation study using the Finite Difference Time Domain (FDTD); they in turn concluded that the SRH recombination phenomena inside the junction are responsible for the deterioration of the current density and the open-circuit voltage.

## Conclusion

In this paper, we studied the influence of the parameters of the 3C-SiC / Si solar cell on its efficiency using numerical simulation under SCAPS. The aim of the study was to optimize the geometrical and doping parameters of the window layer as well as the substrate as a function of the wavelengths in order to obtain a maximum yield. The numerical simulation shows that the 3C-SiC / Si structure requires the use of a substrate of good electronic quality, a very thin window layer of the order of 500 nm for 3C-SiC and a rate of doping of the order of 1018. This study also makes it possible to highlight the main parameters influencing the performance of the cell. We deduce the optimal conditions for achieving satisfactory conversion efficiencies of about 20%.

Any other simulation must be done by including more parameters of 3C-SiC that until now are not very well known as those of silicon.

## CONFLICT OF INTERESTS

The authors have not declared any conflict of interests.

### REFERENCES


Biondo S, Vervisch W, Ottaviani L (2014). Optical and electrical simulations of solar cell based on silicon and silicon carbide. Materials Science Forum pp. 778-780; 1050-1053.

Burgelman M, Nollet P, Degrave S (1999). Electronic behavior of thin film CdTe solar cells", Applied Physics A69:149-153.

Burgelman M, Nollet P, Degrave S (2000). Modeling polycrystalline semi-conducteur solar cells Thin Solid films. pp. 361-362; 527-532.

Burgelman M, Marlein J (2008). Analysis of graded band gap solar cells with SCAPS. Proceedings of the 23rd European Photovoltaic Solar Energy Conference. pp. 2151-2155.

Decock K, Khelifi S, Burgelman S (2011). Modelling multivalent defects in thin film solar cells. Thin Solid Films 519:7481-7484.

Degrave S, Burgelman M, Nollet P (2003). Modelling of polycrystalline thin film solar cells: new features in SCAPS version 2.3. Proceedings of the 3rd World Conference on Photovoltaic Energy Conversion. Osaka. pp. 487-490.

Heidarzadeh H, Baghban H, Rasooli H, Dolatyari M, Rostami A (2014). A new proposal for Si tandem solar cell: Significant efficiency enhancement in 3C–SiC/Si, Opt. - International Journal for Light and Electron Optics 125(3):1292-1296.

Ichimura M, Tajiri H, Morita Y (1997). Excess carrier lifetime of 3c-SiC measured by the microwave photoconductivity decay method. Applied physics letters 70(13):1745-1747.

Niemegeers A, Burgelman M (1996). Numerical modelling of ac-characteristics of CdTe and CIS solar cells. Proceedings of the 25th IEEE Photovoltaic Specialists Conference. Washington DC. pp. 901-904.

Niemegeers A, Burgelman M (1997). Effects of the Au/CdTe back contact on IV – and CV –characteristics of Au/CdTe/CdS/TCO solar cells. Journal of applied Physics 6:2881-2886.

Niemegeers A, Gillis S, Burgelman M (1998). A user program for realistic simulation of polycrystalline heterojunction solar cell: SCAPS-1D, Proceedings of the 2nd World Conference on photovoltaic Energy Conversion (Wien, Österreich, July 1998), JRC, European Commission. pp. 672-675.

Nishino S, Powell JA, Will HA (1983). Production of large-area single-crystal wafers of cubic SiC for semiconductor. Applied Physics and Letters 42:5.

Richards BS, Lambertz A, Corkish RP, Zorman CA, Mehregany M, Ionescu M, Green MA (2003). 3C-SiC as a future photovoltaic material. in Proceedings of 3rd World Conference on Photovoltaic Energy Conversion 3:2738-2741.

Ščajevn P (2014). Application of excite-probe techniques for determination of surface, bulk and nonlinear recombination rates in cubic SiC. Materials Science and Engineering: B 185:37-44.

Ščajevn P, Karaliūnas M, Kuokštis E, Jarasiūnas K (2013). Radiative and nonradiative recombination rates in cubic SiC. Journal of Luminescence 134:588-593.

Toure M, Berenguier B, Ottaviani L, Pasquinelli M, Palais O, Di Lauro P, Kobor D (2014). New 3C Silicon Carbide on Silicon Hetero-Junction Solar Cells for UV Collection enhancement. MRS Proceedings, 1693, Mrss14-1693-dd08-04. doi:10.1557/opl.2014.611.

Verschraegen J, Burgelman M (2007). Numerical modeling of intra-band tunneling for heterojunction solar cells in SCAPS. Thin Solid Films 515:6276-6279.

Yastrebova NV (2007). High-efficiency multi-junction solar cells.Avr-2007. (Accessed: 25-Mar-2014), http://sunlab.site.uottawa.ca/pdf/whitepapers/ HiEfficMjSc-CurrStatus & Future Potential.pdf.