International Journal of Innovation and Applied Studies
ISSN 2028-9324 Vol. 43 No. 4 Oct. 2024, pp. 1126-1133

http://www.ijias.issr-journals.org/

SCAPS-based numerical simulation of an organic heterojunction OTC/ED/EA solar cell

S. Tuo[1], K. J. Datte[2], S. A. Yapi[3], and D. Kone[3]

[1]Faculty of Sciences and Technologies, Université de Man, Man, Côte d'Ivoire

[2]Department of sciences and Technologies, Ecole Normale Supérieure, Abidjan, Côte d'Ivoire

[3]UFR SSMT, Université Felix Houphouët Boigny, Abidjan, Côte d'Ivoire

ABSTRACT: In this study, we propose a simple structure of an organic heterojunction solar cell of OTC/ED/EA type. Material energy values are used for the first time. The study concerns a numerical simulation using SCAPS. Under standard conditions: AM1.5 and T = 300K, the cell parameters are: V_{oc} = 1.186V, J_{sc} = 14.314mA/cm^2, FF = 88.57% and Eff = 15.04%. The effects of parameters such as thickness, energy band gap, ND and NA charge carrier density of state, of the active layers were observed. It appears that, apart from the ND density of state, all the other material parameters influence the values of the cell parameters. It is still necessary to limit the value of NA to avoid degenerated cells. The influence of temperature has also been studied. It was found that when the temperature increases, the performance of the cell decreases. This work is essential because it provides the scientific community with data to make organic solar cells more efficient.

KEYWORDS: solar cell, ED, EA, charge carrier, thickness, temperature.

1 INTRODUCTION

The need for energy is increasingly crucial. Energy is at the heart of the development of nations. African countries, faced with their galloping demography and their need for industrialization, need to have abundant energy. As for developed countries, they need to consolidate their energy needs. Thus, a lot of efforts are made in research as well as in policies to diversify energy sources, but particularly renewable sources that are environmentally friendly. In this context, solar photovoltaic is an interesting solution if we manage to diversify active materials and deposition techniques at lower cost. Indeed, most of the solar panels marketed so far are made from silicon ([1], [2]). However, silicon is widely used in electronic devices. This leads to its scarcity and consequently its cost [2]. Faced with this situation it is necessary to develop other materials, especially organic ones, to address the problem of silicon abusive. Organic materials are particularly interesting because they are abundant, diversified, flexible and easy to obtain ([3], [4], [5]).

Simulation is an interesting technique that allows apprehending the behavior and performance of a physical system. A photovoltaic cell is a physical system that by receiving light wave produces electricity. All the physical mechanisms taking place in the cell are governed by equations. These include the phenomena of charge generation, recombination and diffusion. Numerical programs can be designed to solve these equations. The photovoltaic cell is a stack or blend of active materials. The most efficient solar cells in terms of efficiency are made of inorganic materials. The efficiency can exceed 26% [6]. However, organic solar cells would be interesting if they could compete with inorganic solar cells in terms of conversion rates. Indeed, organic materials are light, easy to obtain and less expensive ([7], [5]) reported yields of 16% with organic solar cells. Many works are published to improve the conversion efficiency ([4], [8], [9], [10], [11]). It all depends on the choice of materials and their properties. Our work aims at studying the influence of the properties of the active layers of the solar cell by simulation. SCAPS is a powerful tool to simulate the influences of the parameters of the photovoltaic cell ([12, [13]). However, it is true that the experimental results do not necessarily reproduce the results of the simulation. This is due to the complex manufacturing processes that introduce defects and impurities. However, this does not detract from the effectiveness of the

simulation in providing the scientific community with manufacturing possibilities. In this work the simulation concerns a solar cell with stacked layers of organic materials of the OTC/ED/EA type. More precisely in this study, we want to simulate the influence of the donor and acceptor materials respectively. ED and EA constitute the active layers. The OTC material constitutes the optical window. These materials have adjustable properties. This means that we can vary for example the energy gap, the LUMO, HOMO values, the carrier densities of states.

2 METHODOLOGY

The physics of semiconductors is quite classical. The phenomena of generation, recombination of charge carriers are governed by equations. The Poisson and continuity equations are fundamental equations in semiconductors. Based on these equations (Eqn 1- Eqn 5), it is possible to develop algorithms to describe and simulate the physical phenomena at the interface and in materials. This is what SCAPS does [14]. Indeed, SCAPS is a powerful program for the simulation of solar cells. It is understood that the solar cell is a superposition of layers of active materials and charge collection electrodes. Figure 1 shows the structure of the solar cell to be simulated.

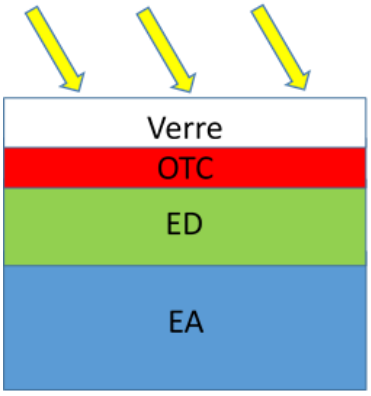

Fig. 1. Structure of the OTC/ED/EA solar cell

$$\frac{\partial^2\psi}{\partial^2 x} = -\frac{q}{\varepsilon}(p - n + N_D^+ - N_A^-)$$ Eqn 1: Poisson Equation

$$\frac{\partial n}{\partial t} = \frac{1}{q}\cdot\frac{\partial J_n}{\partial x} + G - U$$ Eqn 2: Continuity equation for electrons

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\cdot\frac{\partial J_p}{\partial x} + G - U = 0$$ Eqn 3: Continuity equation for holes

$$J_n = qD_n\cdot\frac{\partial n}{\partial x} - q\mu_n\cdot n\cdot\frac{\partial \psi}{\partial x}$$ Eqn 4 : Electron diffusion current

$$J_p = -qD_p\cdot\frac{\partial p}{\partial x} - q\mu_p\cdot p\cdot\frac{\partial \psi}{\partial x}$$ Eqn 5 : Hole diffusion current

With ψ: Electric potential, ρ: Charge density, N+D: Trap density of ionized donors, N-A: Trap density of ionized acceptors, n electron density, p: hole density, q: electric charge, ε: permittivity. Jn (p): electron (holes) current, G: Generation rate, U: Recombination rate. Dn (p): electron (hole) diffusion constant, µn (p): electron (hole) mobility

SCAPS was developed at the Department of Electronics and Information Systems (ELIS) of the University of Ghent in Belgium supervised by Dr. Marc Burgelman [15]. This program is free to download and is compatible with almost all Windows versions. It was originally developed to simulate CdTe or $CuInSe_2$ solar cells. However, it has been improved to take into account heterojunction thin film solar cells, even organic ones. 3310 version was used to integrate the Gaussian type defect levels. This

version allows to have the J(V) curves under darkness and under illumination, the energy band diagrams, the charge carrier densities, the generation and recombination profiles. It is possible to determine the energetic values of materials by electrochemistry [16]. By integrating these values into the SCAPS program, one can see the influence of the ED donor material layer or EA acceptor material layer on the cell parameters. Table 1 gives the standard values of the parameters of the material layers of the cell.

Influence parameters of interest are the thickness Ep, the gap energy Eg, the charge carrier density. We can also see the influence of temperature. Only one parameter varied at a time, the other parameters are kept constant. A similar study was done by [7]. The radiation spectrum chosen is the AM1.5 standard and the default operating temperature is 300K.

Table 1. Standard parameters of the cell in the simulation

Parameters	Materials		
	OTC	**ED**	**EA**
Thickness (nm)	5,000	200	1000
Gap energy (eV)	3,8	1,7	1,5
Electronic Affinity (eV)	4.6	4.8	5,2
Dielectric Permittivity	10,000	10,000	10,000
Effective density of states in BC (cm-3)	4.10^{+18}	2.10^{+18}	2.10^{+18}
Effective density of states in BV (cm-3)	9.10^{+18}	9.10^{+19}	2.10^{+18}
Thermal velocity of the electrons (cm/s)	1.10^{+7}	1.10^{+7}	1.10^{+7}
Hole thermal velocity (cm/s)	1.10^{+7}	1.10^{+7}	1.10^{+7}
Electron Mobility (cm^2/V.s)	2.10^{*2}	2.10^{+2}	2.10^{+2}
Hole mobility (cm2/V.s)	1.10^{+2}	1.10^{+2}	1.10^{+1}
Donor density ND (cm-3)	5.10^{+17}	1.10^{+15}	0
Donor density ND (cm-3)	0	0	5.10^{+17}

3 RESULTS AND DISCUSSION

J(V) curve in Fig. 2 is the curve simulated with the standard values from Table 1 above, and at temperature T = 300K. Under these conditions, the cell parameters are such that V_{oc} = 1.186V, J_{sc} = 14.314mA/cm^2 FF = 88.57% and Eff= 15.04%. The voltage has been varied between 0 V and 1.200 V and it can be seen that the current increases with the voltage. This means that the current depends on the voltage and the load carrying mechanisms. Thus, at high voltages, there is an increase in the number of photo-generated charge carriers, which leads to an increase in current. These good results are certainly also due to the good agreement between the energy levels between the donor and acceptor materials. Indeed, the electronic affinities of ED and EA are respectively 4.8 eV and 5.2 eV.

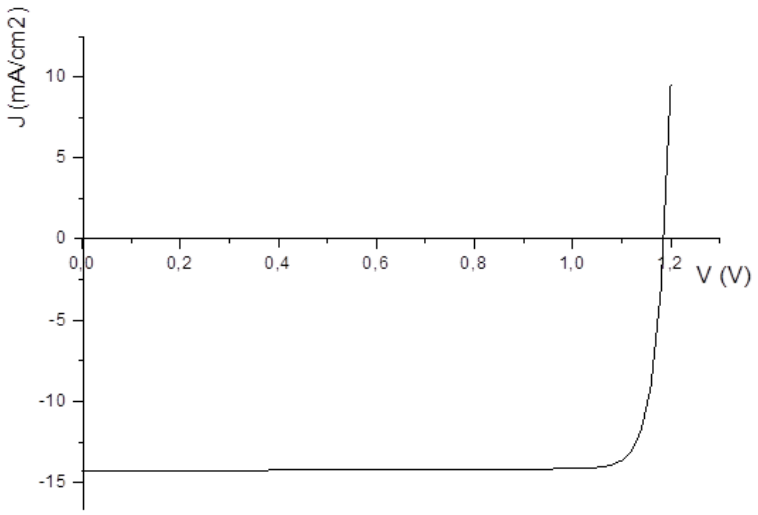

Fig. 2. J(V) curve of the simulated solar cell under standard conditions

These interesting results led us to investigate the influence of the variation of the properties of both active materials on the one hand and the influence of temperature on the other hand.

3.1 VARIATION OF THE THICKNESS OF THE ACTIVE LAYERS

It is known that the mobility of electrons is greater than holes ones [19]. So, it is logical to make the electron-accepting layer (layer whose fermi level is close to the valence band) thicker than the donor layer (layer whose fermi energy is close to the conduction band). So that there is a large number of charge carriers reaching the opposite electrode without recombination. In this view, the thickness of EA is 1000 nm and that of ED is 200 nm (Table 1). Thus, by maintaining the thickness of EA at 1000 nm, the thickness of the ED layer was first varied from 100 nm to 1000 nm (Figure 3a) in steps of 100 nm. There is an increase in Voc from 1.173 V to 1.198 V. The short circuit current increases from 10.987 mA/cm^2 to 21.732 mA/cm^2. Form factor FF increases from 77.11% to 89.69. Regarding the efficiency, it increases with the increase of ED thickness from 9.94 % to 23.36 %. The increase in thickness increases the number of absorbed photons. It is then logical to observe the increase of the current J_{sc} and the open circuit voltage V_{oc} by increasing the thickness of ED. This also increases efficiency as all parameters increase.

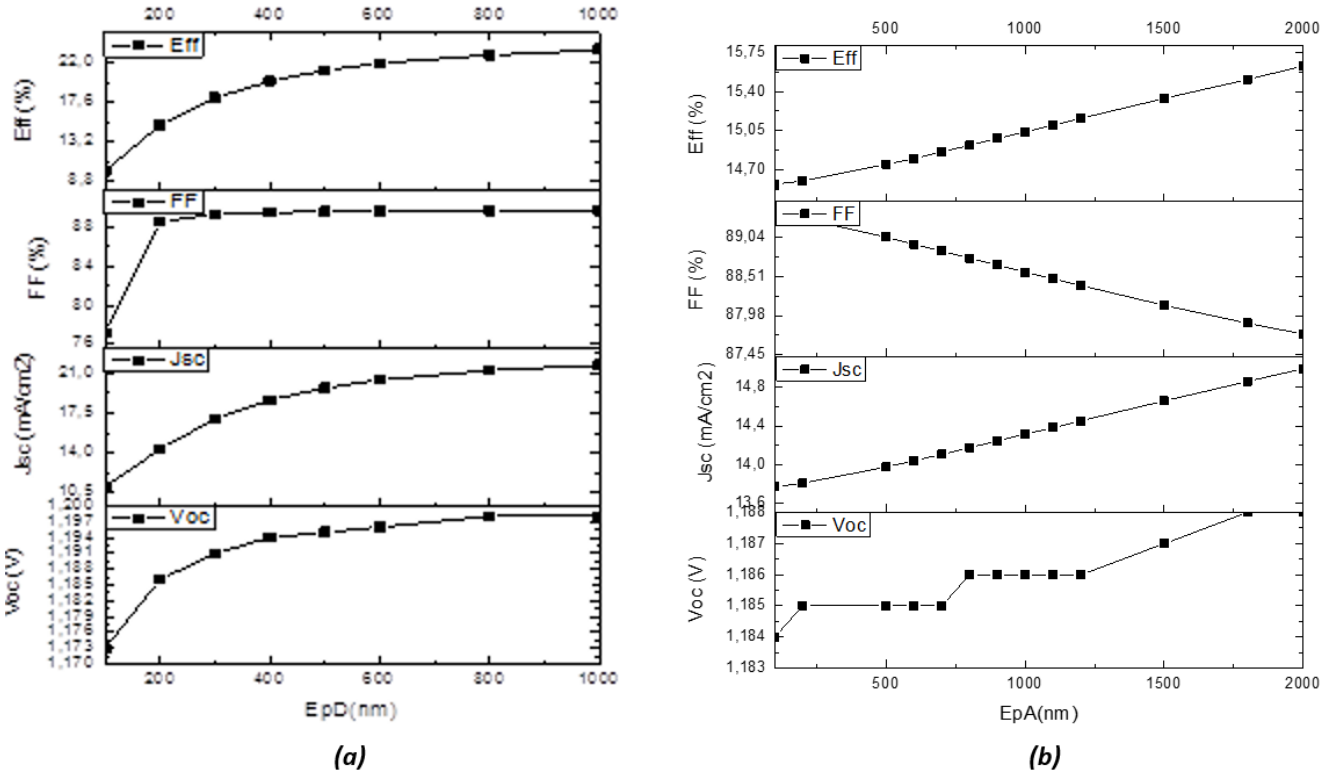

Fig. 3. Variation of the parameters Voc, Jsc, FF and Eff as a function of thickness: (a). ED, (b). EA

In the same way the thickness of EA varied from 100 nm to 2000 nm in steps of 100 nm, maintaining the thickness of ED at 200 nm (Fig. 3b). It can be seen that Voc increases slightly from 1.184 V to 1.188. Jsc also increases slightly from 13.766 mA/cm^2 to 14.998 mA/cm^2. Form factor FF decreases from 89.36 % to 87.73 %. However, the efficiency increases from 14.57 % to 15.63 %. The decrease in FF form factor could be explained by the fact large thicknesses induce resistive components that affect the form factor. Thus, it appears large thicknesses of EA do not affect the Voc whereas this is not the case for an increase in the thickness of ED. But the efficiency of the solar cell is related to the thickness of EA and ED. Therefore, for a better compromise of efficiency the ED layer should not be too thin and also the EA layer should not be too thick. This study proves that better efficiencies would be obtained from thicknesses of ED = 1000 nm and EA = 2000 nm.

3.2 ENERGY BAND GAP VARIATION

In another time the energy band gap Eg of ED varied from 1.2 eV to 2.0 eV. Fig. 4 shows the variation of solar cell parameters as a function of energy band gap. It can be seen short-circuit current Jsc, form factor FF and efficiency Eff decrease, while the

open circuit voltage Voc varied little from 1.11 V to 1.12 V when Eg varied between 1.2 eV and 1.5 eV. Then from Eg = 1.5 eV to 2 eV, Voc increased up to 1.60 V. Current decrease can be explained by the fact long wavelength photons are not absorbed by wide band gap materials. Thus, a small amount of electron-hole pairs is observed. This affects the efficiency of the cell since all parameters decrease.

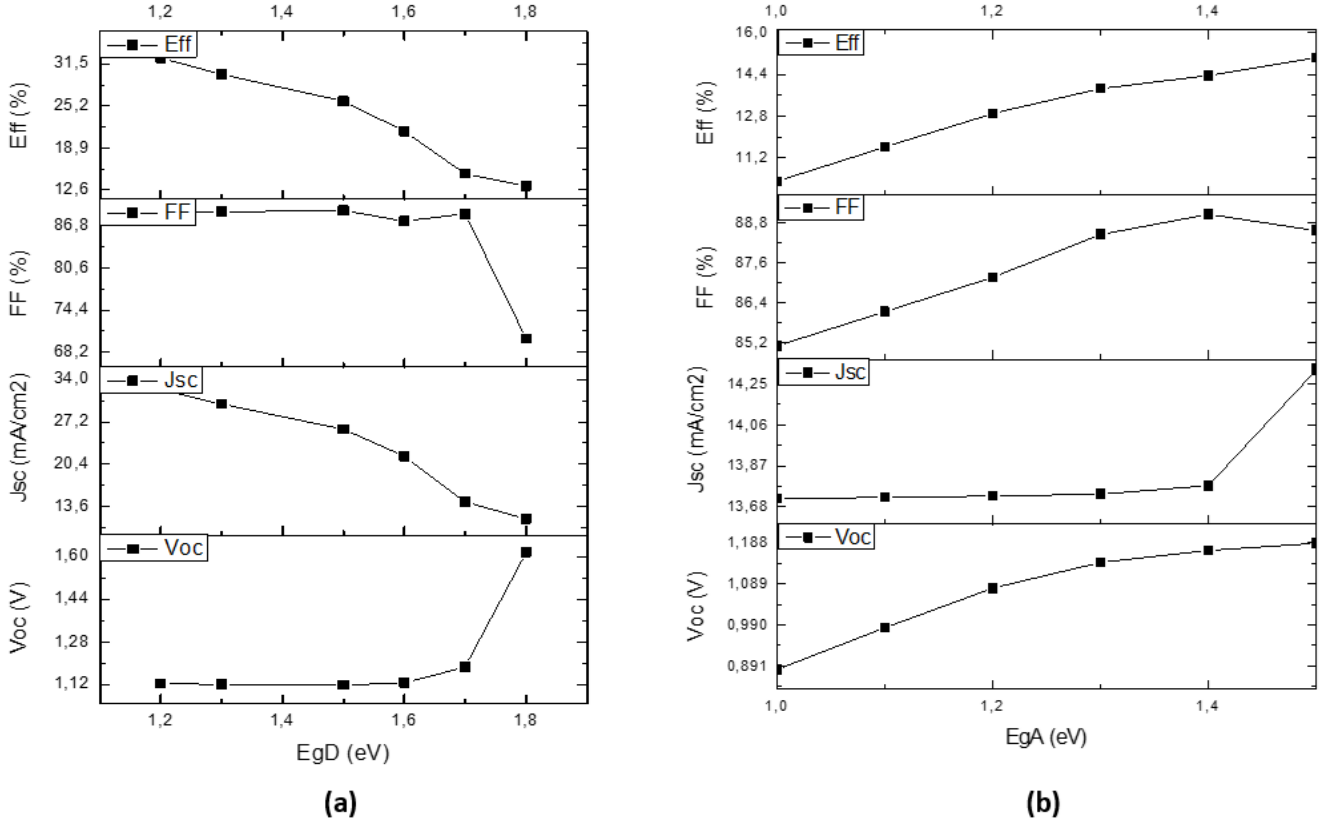

Fig. 4. Variation of the parameters Voc, Jsc, FF and Eff as a function of Eg: (a). ED and (b). EA

3.3 DOPING OF DONOR AND ACCEPTOR MATERIALS

In addition, we were interested in the doping of the active layers. Fig. 5 shows the influence of active layer doping on solar cell parameters. The doping of organic materials is different from inorganic materials ones. Here, it is a question of doping active layers of organic materials by raising HOMO level for the donor and lowering LUMO level for the acceptor. This is done by increasing the concentration of donor atoms ND for the donor and NA for the acceptor by adding specifics molecules. It can be seen the variation in ND does not affect the cell parameters since they all remain practically constant. Only the NA variation affects the parameters of the cell as confirmed by Joel et *al* [14]. Indeed, for a donor HOMO value, the process of generating free charges is governed by LUMO level value of the acceptor. We can see that Voc increases with NA up to 1.1017 cm^{-3}. Above this value of NA, problems of convergence arise. This supposes that doping must not exceed a certain value in order not to obtain degenerated semiconductors. Short-circuit current J_{sc} decreases as the charge carrier density increases. This can be explained by recombination phenomena that take place at high charge carrier densities. Thus, the collection of charge carriers by the electrodes decreases, which causes the Jsc to decrease.

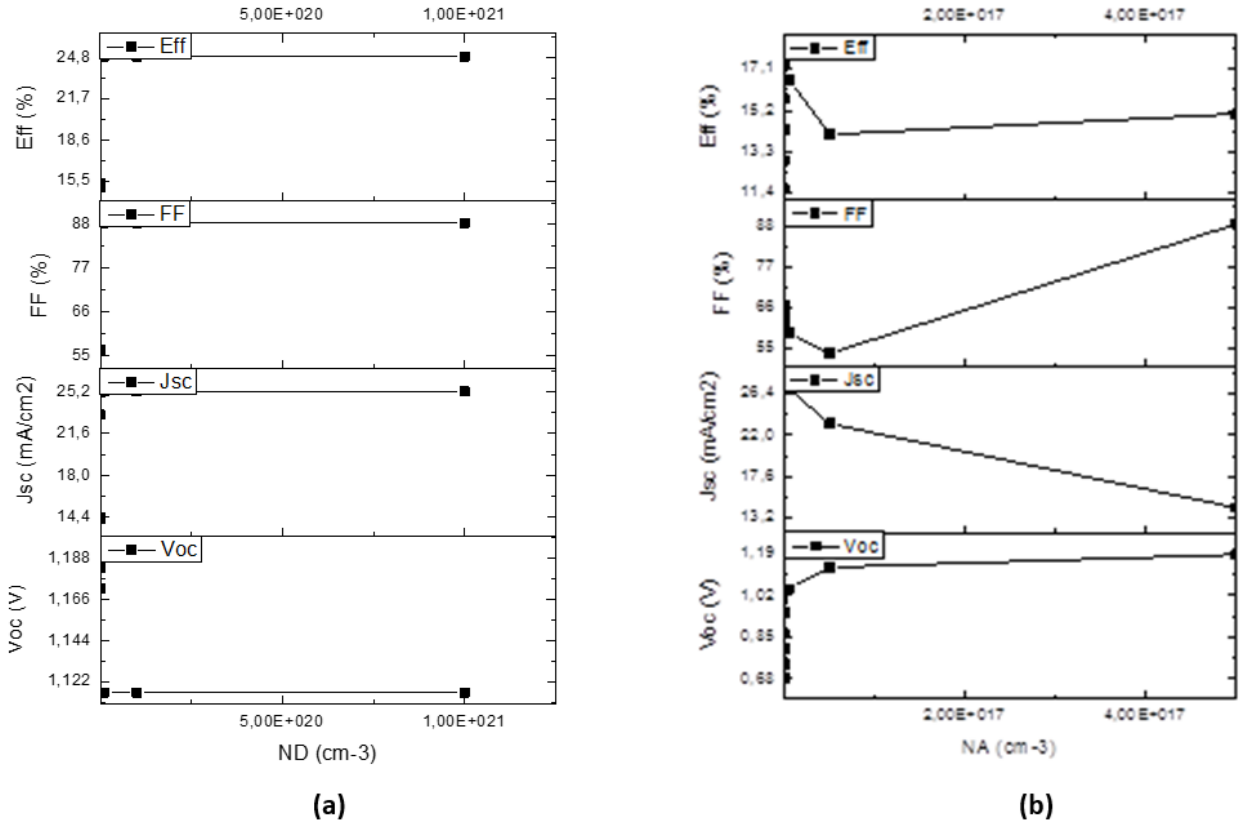

Fig. 5. Variation of the parameters Voc, Jsc, FF and Eff as a function of the state density of the charge carriers: (a). ND and (b). NA

3.4 TEMPERATURE VARIATION

The cell has to operate under various climatic conditions. It is therefore essential to study the influence of temperature on the stability of the cell. Thus, we have varied temperature from room temperature, 300 K to 400 K and even below 300 K, in steps of 10 K. Fig. 6 shows the influences on temperature on the parameters of the solar cell. A decrease in Voc, FF and Eff is observed as the temperature increase. Only short-circuit current increases with temperature. Indeed, when the temperature increases, the energy band gap of the semiconductor decreases and thus more photons have enough energy to generate electron-hole pairs, which justifies the increase of Jsc. On the other hand, the increase in temperature causes the electrons to gain more energy and become unstable. Then they are more likely to recombine with the holes before reaching the area of charge space. This contributes to decrease the values of Voc, FF and Eff.

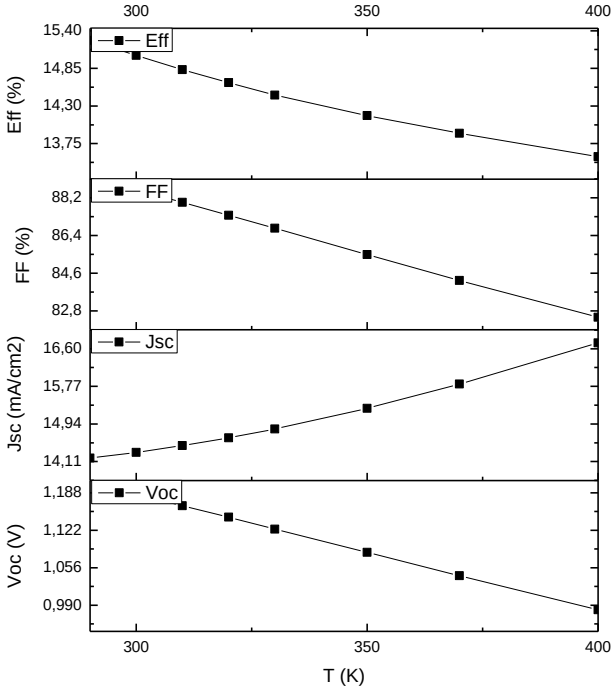

Fig. 6. Variation of the parameters Voc, Jsc, FF and Eff as a function of temperature T

4 CONCLUSION

In this study the influence of properties such as thickness, energy band gap, carrier concentration of the active layers of the organic solar cell was investigated. The simulation results showed that the cell parameters depend on the thickness, energy band gap and carrier density of the active layers. However, the study showed that the carrier density of the donor material does not have a significant effect on the cell parameters. For a good compromise it is preferable not to slice the electron donor layer too thinly and not to widen the acceptor layer too much. In addition, the performance of the cell degrades with increasing temperature.

ACKNOWLEDGMENT

The authors sincerely thank Dr. Marc Burgelmann and his team at the University of Gent, Belgium, for providing the scientific community with this simulation program.

DISCLOSURE STATEMENT

The authors declare that there are no conflicts of interest.

REFERENCES

[1] Maulid Kivambe, Brahim Aissa and Nouar Tabet, Emerging Technologies in Crystal Growth of Photovoltaic Silicon: Progress and Challenges, Energy Procedia 130 (2017) 7–13.

[2] V.V. Tyagi, Nurul A.A. Rahim, N.A. Rahim, Jeyraj A./L. Selvaraj, Progress In solar PV technology: Research and achievement, Renewable and Sustainable Energy Review 20 (2013) 443–461.

[3] Brishty Deb Choudhury, Bernabe Ibarra, Federico Cesano, Yuanbing Mao, Muhammad N. Huda, Aminur Rashid Chowdhury, Carolina Olivares, M.Jasim Uddin, The photon absorber and interconnecting layers in multijunction organic solar cell, Solar Energy, Volume 201, 1May 2020, pages 28-44.

[4] Jianqiang Qin, Lixiu Zhang, Zuo Xiao, Shanshan Chen, Kuan Sun, Zhigang Zang, Chenyi Yi, Yongbo Yuan, Zhiwen Jin, Feng Hao Yuanhang Cheng, Qinye Bao, Liming Ding, Over 16% efficiency from thick-film organic solar cells, Science Bulletin 65 (2020) 1979–1982.
[5] Jean-Pierre M. et Thierry T., Vers l'optoélectronique organique bas coût, Journée électronique 2005 - Optique intégrée et photonique, Volume 4, 2005.
[6] Yuqiang Liu, Yajuan Li, Yiliang Wu, Guangtao Yang, Luana Mazzarella, Paul Procel-Moya, Adele C.Tamboli, Klaus Weber, Mathieu Boccard, OlindoIsabella, Xinbo Yang, Baoquan Sun, High-Efficiency Silicon Heterojunction Solar Cells: Materials, Devices and Applications, Materials Science and Engineering: R: Reports, Volume 142, October 2020, 100579.
[7] A.M. Ali, D.A. Said, M. Khayyat, M. Boustimi, R. Seoudi, Improving the efficiency of the organic solar cell (CuPc/C60) via PEDOT: PSS as a photoconductor layer doped by silver nanoparticles, Results in Physics 16 (2020) 102819.
[8] Jianqiang Qin, Lixiu Zhang, Zuo Xiao b, Shanshan Chen, Kuan Sun, Zhigang Zang, Chenyi Yi, Yongbo Yuan, Zhiwen Jin, Feng Hao, Yuanhang Cheng, Qinye Bao, Liming Ding, Over 16% efficiency from thick-film organic solar cells, Science Bulletin, August 2020.
[9] L. Cattina, S. Ouro Djobo, C. Sanchez, M. Morsli, J.C. Bernède, The influence of the HOMO energy level of the organic electron donor on the effectiveness of the anode buffer layer in photovoltaic solar cells, Energy Procedia 31 (2012) 89 – 95.
[10] M.Hssein, S.Tuo, 1, S.Benayoun, L.Cattin, M.Morsli, Y.Mouchaal, M.Addou, A. Khelil, J.C. Bernède, Cu-Ag bi-layer films in dielectric /metal/dielectric transparent electrodes as ITO free electrode inorganic photovoltaic devices, Organic Electronics (2016).
[11] W. Abdelaziz, A. Zekry, A.Shaker, M. Abouelatta, Numerical study of organic graded bulk heterojunction solar cell using SCAPS simulation, Solar Energy, Volume 211, 15 November 2020, Pages 375-382.
[12] Aseena S, Nelsa Abraham, V.Suresh Babu Optimization of layer thickness of ZnO based perovskite solar cells using SCAPS 1D, MaterialsToday: Proceedings, October (2020).
[13] R.T. Mouchou, T.C. Jen, O.T. Laseinde, K.O. Ukoba, Numerical simulation and optimization of p-NiO/n-TiO 2 solar cell system using SCAPS, April (2020).
[14] Joël Hervé NKUISSI TCHOGNIA, Bouchaib HARTITI, Jean-Marie NDJAKA, Abderraouf RIDAH 1 et Philippe THEVENIN, Performances des cellules solaires à base de Cu2ZnSnS4 (CZTS): une analyse par simulations numériques via le simulateur SCAPS, Afrique SCIENCE 11 (4) (2015) 16 – 23.
[15] El Hassane Ihalane, Lahoucine Atourki, Hassan Kirou, Ahmed Ihlal, Khalid Bouabid, Numerical study of thin films CIGS bilayer solar cells using SCAPS, MaterialsToday: Proceedings, Volume 3, Issue 7, 2016, Pages 2570-2577.
[16] M. Burgelmann, P. Nollet, S. Degrave, Modelling polycrystalline semiconductor solar cells, Thin Solid Films, 361 (2000) 527-532.
[17] Juliusz Sworakowski, How accurate are energies of HOMO and LUMO levels in small-molecule organic semiconductors determined from cyclic voltammetry or optical spectroscopy?, Synthetic Metals Volume 235, January 2018, Pages 125-130.
[18] Juliusz Sworakowski, JózefLipiński, KrzysztofJanus, On the reliability of determination of energies of HOMO and LUMO levels in organic semiconductors from electrochemical measurements. A simple picture based on the electrostatic model, Organic Electronics, Volume 33, June 2016, Pages 300-310.
[19] T. Ghorbani, M.Zahedifar, M.Moradi, E.Ghanbari, Influence of affinity, band gap and ambient temperature on the efficiency of CIGS solar cells, Optik, Volume 223, December 2020, 165541.