Simulation of the Electrical Parameters of Organic Photovoltaic Cells

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***Abstract*—** This work represents the modelling and simulation of organic solar cells using Quite Universal Circuit Simulator, QUCS. An equivalent circuit model constituted from one diode, a series and shunt resistance, and a photocurrent generator have been used. The simulated results as function of different parameters such as series resistance, temperature of the cell, the ideality factor and current saturation are given. The current density as function of voltage J-V characteristics of the organic cell obtained from the experimental results are compared to the simulated one, a value of 1.2 of the ideality factor is established.

***Keywords*—** Organic solar cells, temperature effect, ideality factor, simulations, QUCS.

1. INTRODUCTION

The Organic Solar Cells (OSCs) have attracted great attention due to their easy solution-processed preparation and material tunability, which could lead to light-weight, low-cost and large-area flexible solar products. Despite the shortcomings of their inferior device stabilities, their power conversion efficiencies (PCE) grow quickly with the development of new materials, and have surpassed 12% recently. There is urgent need to improve the device performance using better designs, technologies and models. The current-voltage characteristics of organic solar cells (OSC) is analyzed in terms of equivalent lumped parameter circuit at different level of insolation. In particular, starting from a circuital model based on a three-diode configuration, a set of formulas is proposed to describe the dependence of lumped circuit al parameters on irradiance intensity and consequently the behaviour of organic solar cells from dark to high irradiance conditions (Laudani et al. 2018). A new one-equation model based on a generalized equivalent circuit capable of accurately fitting ideal and non-ideal curves (De Castro et al. (2016)). To explain the S-shape current-voltage curves found in some experimental data a model is used (López-Varo et al. 2017). A simple and versatile electrical model for plasmonic solar cells is proposed (Kim et al. 2018). A numerical model that includes the 3D morphology of the blend in the simulator is developed. The model able to observe the charge and current density distribution across the blend at different working points. The effect of charge unbalance to solar cells performance is investigated (Gagliardi et al. 2018). Response surface methodology (RSM) is used to find optimal fabrication conditions for polymer solar cells. In order to optimize cell efficiency, the central composite design (CCD) with three independent variables polymer concentration, polymer-fullerene ratio, and active layer spinning speed was used. The variation in the device performance was explained by the best model. The experimental results are consistent with the CCD prediction, which proves that this is a promising and appropriate model for optimum device performance and fabrication conditions (Suliman et al. 2017). A Kinetic Monte Carlo model was developed to simulate the morphological variation of organic solar cells and its effects on photovoltaic parameters. This model is currently based on P3HT: PCBM system and can be easily extended to any low bandgap polymer solar cells. Other models can simulate three different parameters including domain size, donor-acceptor ratio and active layer thickness in the same model and predict the efficiency of organic solar cells on the variation of these parameters (Neupane et al. 2017). The microscale model consists of a system of partial and ordinary differential equations in an heterogeneous domain, that provides a full description of excitation/transport phenomena occurring in the bulk regions and dissociation/recombination processes occurring in a thin materials across the interface, the device performance is determined not only by the total interface length but also by its shape (De Falco et al. 2012). A mathematical model for OSCs consists of a system of nonlinear diffusion–reaction partial differential equations (PDEs) with electrostatic convection, coupled to a kinetic ordinary differential equation (ODE) is described (De Falco et al. 2010). The optical wave propagation in the 3D solar cell is simulated by Finite Difference Time Domain simulations. The influence of the nanowire dimensions on the quantum efficiency and short circuit current density of the solar cells is discussed, 3D model of solar cell allows for decoupling of electrical and optical properties (Knipp et al. 2017). Several models predict power conversion efficiencies in the range of 10–15%. A more general approach assuming device operation close to the Shockley–Queisser-limit leads to even higher efficiencies (Scharber et al. 2013). A novel building-block approach to equivalent circuit modelling of organic photovoltaic cells capable of simulating both optimal and degraded devices has been developed (Sesa al. 2018). The polaron-pair recombination are presented by an internal shunt resistance in the equivalent circuit model (Lee et al. 2018). The origin of S

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shape curve through an improved equivalent circuit model (ECM) is giving. The improved ECM involves a D:A junction as well as a rectifying junction to interpret the bias-dependent-recombination (Zuo et al. 2014) Two real models (single-diode and double-diode) are studied (Abbassi et al. 2018, Santiago et al. 2018 and Rhouma,et al. 2017). A fast and accurate method through utilizing combined analytical and numerical approach to determine the five parameters double diode model of photovoltaic modules is proposed. A rapid and accurate iterative numerical method is proposed to determine the value of series resistance. The proposed model can be useful for PV designers who require a fast, accurate and simple approach for modeling the PV modules (Yahya-Khotbehsara et al. 2018 and Chin et al. 2016). Factors that dominate the junction diodes in OSCs are discussed and suggestions for optimizing the junction diodes are proposed (Mao et al. 2017 and Mazhari (2006)). A novel explicit model is proposed to represent I-V expression of conventional double-diode model for photovoltaic (PV) cells. This model is based on two rules (Dehghanzadeh et al. 2017). A simulation study indicates that the conduction mechanism in the organic solar cell is strongly influenced by the excitonic diffusion. The performance of the opv device can be described by a two-diode-equivalent model (Cheknane et al. 2008). The opposed two-diode equivalent-circuit model consisting of a traditional one-diode photocell model and a parasitic diode with a parallel resistance is known to some how reproduce the S-shaped current-voltage curve of poor organic photocells (Tada, 2017). S-shape, in the current–voltage (*I*–*V*) characteristics, has been attributed to different physical phenomena such as poor quality of cathode-active layer interface or unbalance charge carrier mobilities. This non-ideal behavior can be electrically modelled including a second diode, in reverse bias, together with an extra shunt resistance in the traditional solar cell equivalent circuit (Romero et al. 2012). Light activation phenomenon in inverted bulk heterojunction (BHJ) organic solar cells (OSC) has been electrically modelled with a two-diode equivalent circuit. Current–voltage (*I*–*V*) characteristics show a highly pronounced S-shape that is gradually removed during light activation process. The circuit used to model *I*–*V* curves includes two diodes in forward and reverse bias together with two parallel resistances. The parallel of the reverse bias diode and its corresponding resistance models the electrical behaviour of the interlayer and photoconductivity are presented (Romero et al. 2014, Lattante et al. 2011 and Street et al. 2011). There are numerous studies that develop the mathematical modeling of photovoltaic cells and verified by software: Matlab ; 1D Amps, PC1D, matrix transfert. The model presented in this work is based on an equivalent circuit implemented in free software, Quite Universal Circuit Simulator (QUCS). QUCS uses a generic diode for adjust the current and voltage curve (I(V) curve at photovoltaic cell. Additionally, we can use equations to define the model of photovoltaic cell and represent its characteristic curves. The model of PV cell can be used to simulate a PV module, because PV module is an association of cells in serie and parallel.

In this study, a single diode model used to simulate organic photovoltaic cells is proposed. The simulated results are compared to the experimental one. The structure of the cell simulated is glass/ITO/ETL/active layer/HTL/Ag, ETL: electron transport layer, HTL: hole transport layer, the active layer is a mixture of an acceptor and donor organic materials.

2. STRUCTURE OF THE ORGANIC PHOTOVOLTAIC CELLS

The structure of the cells realized is glass/ITO/ZnO/P3HT:PCBM/Pedot/Ag . The structure is presented in figure 1. Zinc oxide (ZnO) is used as electron transport layer (ETL). Pedot is used as a hole transport layer (HTL), Poly(3-hexylthiophene) (P3HT) as donor and Phenyl-C61-butyric acid methyl ester (PCBM) as acceptor. The J(V) characteristics of the cells, with area 0.18 cm², are measured in the dark and under light intensity (100 mW/cm²). Figure 2 shows current density and power characteristics as function of voltage, Voc is the open circuit voltage. The measured parameters of the cell are shown in table 1.

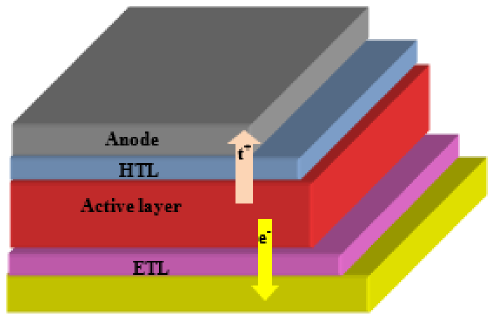

Fig. 1. Structure of the organic cells.

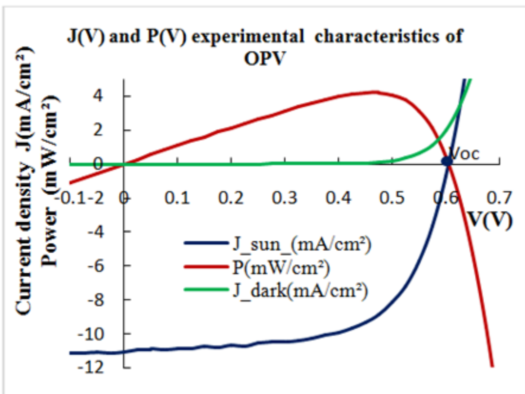

Fig. 2. Experimental J(V) and P(V) characteristics of inverted organic solar cells.

TABLE I: Experimental parameters of the organic solarCells

Voc (V)	Jsc (mA/cm²)	FF (%)	η (%)	Rs (Ω)	Rsh (Ω
0.59	11.02	65	4.22	39.54	3731.15

3. SIMULATION OF THE ORGANIC SOLAR CELLS

3.1 Equivalent circuit model used under QUCS

The circuit equivalent to a single diode used to model the electrical behavior of a photovoltaic cell based on P3HT: PCBM under QUCS is shown in Figure 3. This diagram allows us to compare the results obtained by experimental measurement with simulation results. By modifying the parameters of the circuit we can get closer to the experimental curves of the cell. The model works according to Schockley's equation. By introducing the experimental parameters of the cell into the model we obtain the desired characteristics.

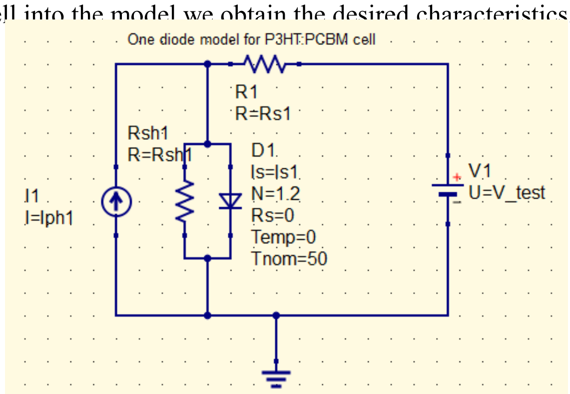

Fig. 3. Equivalent circuit model used under QUCs simulator.

3.2 Equations of the Model

The current of the diode is given by the equation (1). Where I is the output current of the photovoltaic cell, I_{ph} is the photocurrent generated, I_0 is the saturation current, R_s is a series resistance due to junction between the semiconductor and the metal contacts, R_{sh} is parallele resistance due to the linearity of the PN junction, n is the ideality factor of the diode, k_B is the Boltzmann constant, e is the elementary charge of electron and T is temperature in Kelvin.

$$I = I_{ph} - I_0\left(exp\left[\frac{e\,(V+I\,R_s)}{n\,k_B\,T}\right]-1\right) - \frac{V+I\,R_s}{R_{sh}} \quad (1)$$

The short circuit current I_{sc} is given using the equation (2).

$$I_{sc} = I_{ph} - I_0\left(exp\left[\frac{e\,I_{sc}R_s}{n\,k_B\,T}\right]-1\right) - \frac{I_{sc}R_s}{R_{sh}} \approx I_{ph} \quad (2)$$

The open circuit voltage V_{oc} is giving by equation (3).

$$V_{oc} = \frac{n\,k_B\,T}{e}\,ln\left[1+\frac{I_{ph}}{I_s}\right] \quad (3).$$

4. RESULTS AND DISCUSSIONS

4.1 Simulation of the temperature effect

In the laboratory when characterizing the organic cell, the cell is exposed to the radiation of the simulator which causes its heating, the temperature of the cell can increase up to 70°C. This thermal energy has effects on the transport of charges, on the photo-current generated, on the internal potential and on the total current of the organic cell. The influence of temperature on the performances of the cell appears in the current equation by the term V_T (V_T=k_BT/q) which represents the thermal potential; this potential represents the thermal agitation of the charges in the medium under consideration. Figure 4 shows the influence of temperature on the I (V) characteristics of the cell, the results obtained by simulation. When the temperature increases the open circuit voltage V_{oc} decreases and the short circuit current density J_{sc} remains almost constant. The power generation of the organic cells as function of temperature is shown in figure 5. The power generation decreases when temperature increases.

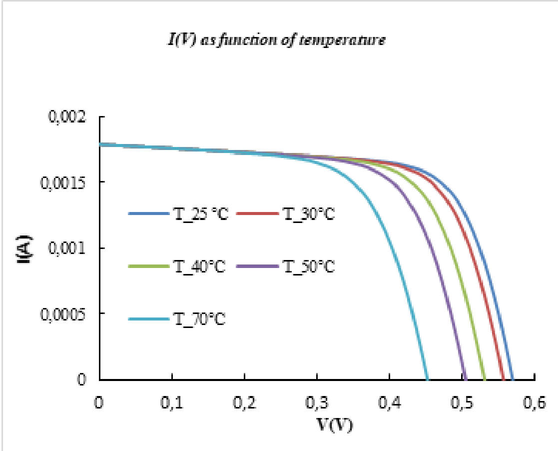

Fig. 4. Simulation of I(V) characteristics as a function of diode

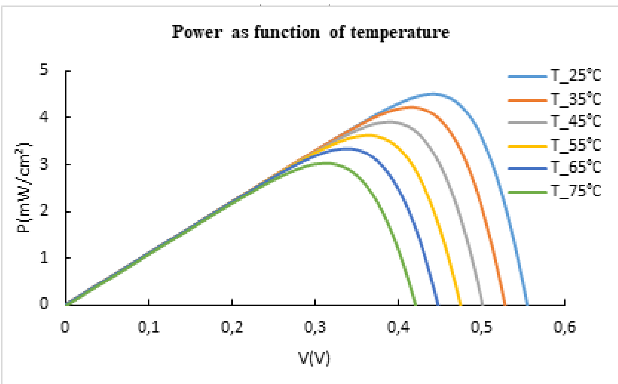

Fig. 5. Simulation of the power generation of the cell as function of temperature.

4.2. *Effect of the ideality factor*

In a silicon solar cell, the ideality factor n is considered equal to 1, which means that the recombination is band-band type, while in the organic cells it is considered to be close to 2, which corresponds to recombination assisted by the traps levels. From the experimental curves, we can still estimate an ideality factor by deriving the logarithm of the current of the organic cell in the dark. The value of n used in the simulations varies between 1.2 and 2. The ideality factor obtained by diode-equivalent model modeling for the inverted cell is shown in figure 6. When V=V_{oc} the obtained ideality factor n=1.2.

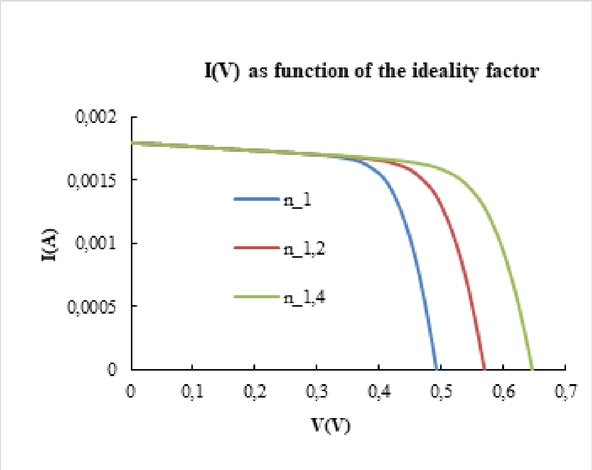

Fig. 6. Simulation of the I(V) characteristics as function of the ideality factor.

4.3 Effect of the series resistance

Series resistance is one of the parameters governing the operation of an organic solar cell. Figure 7 shows simulations of the effect of the variation of R_S on the J-V characteristics of the P3HT: PCBM inverted structure. The fill factor is significantly affected by increasing R_S of the cell. The results of simulations show that the characteristic J (V) with $R_S = 10\Omega$ is super imposed on the experimental curve.

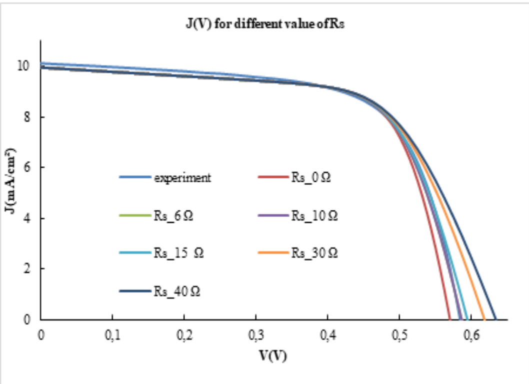

Fig. 7. Simulation of J(V) characteristics as function of the series resistance

5. IMPROVEMENT OF THE MODEL

The conversion efficiency of organic cells depends on the solar cells surface, as given in equation (4). The dependence of the parameters of the organic cells as a function of the cell surface can be simulated using equation (4).

$$\eta = FF\frac{V_{oc}\frac{I_{sc}}{S}}{\phi} \qquad (4)$$

Where V_{oc} is the open circuit voltage, I_{sc} the short circuit current, ϕ=1000 W/m² the standard power irradiation by square meter, S the solar cell surface and FF the fill factor.

An organic photovoltaic cell can be modeled by a three-junction model as shown in the figure 8.a. These junctions are: (1) the donnor/cathode junction, (2) the internally distributed donnor/acceptor junction and (3) the acceptor/anode junction. The Schottky organic/metal junctions correspond to direct paths from the anode to the cathode of the donnor and the acceptor, respectively. The use of the three-diode model provides simulation results closer to the experimental ones. Each junction will be represented by its equivalent circuit as shown in figure 8.b.

Using QUCS software, it is easy to simulate the degradation of organic solar cells by using the equation describing this phenomenon.

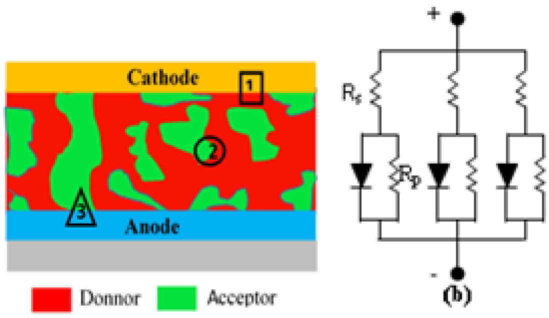

Fig. 8. (a) Schematic representation of the three junctions in organic solar cells: (1) the donnor/cathode junction, (2) the internally distributed donnor/acceptor junction and (3) the acceptor/anode junction, (b) equivalent circuit of the three junction model.

6. IMPROVEMENT OF THE PARAMETERS OF ORGANIC PHOTOVOLTAIC CELLS

The use of electrodes based on silver nanowires (AgNs) and three-layer electrodes of the type conductive transparent oxide/Metal/conductive transparent oxide, such as ZnO/AgNs/ZnO or WO_3/AgNs/WO_3. And the use of organic/inorganic/organic (OIO) electron transport layer improves cell performance. The inorganic material used is a transparent conductive oxide (TCO) such as SnO_2 or ZnO.
The disadvantage of organic photovoltaic cells is that it has a limited life. This is due to the decrease of their performance in the presence of oxygen and water. To improve stability and increase cell life, encapsulation is necessary.

7. CONCLUSIONS

The objective of this paper is to obtain by simulation, the electrical characteristics and the behavior of a photovoltaic system by using QUCS simulation environment this, according to the variations of the parameters of the model. The modeling results obtained on the QUCS environment using the single-diode model correspond to the experimental results; this allows us to conclude that the organic photovoltaic cell is equivalent to an electronic circuit composed of a current source, a diode, a series resistor and a parallel resistor, the calculated ideality factor of an organic solar cells is 1.2. The open circuit voltage of the cell decrease when temperature increases. Using QUCS software, we can also simulate the performance of the cells according to the geometry of the electrodes and as a function of the active surface of the cell.

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