Newton Raphson method used to model organic solar cells under Matlab software

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Abstract: - A circuit based simulation model for organic solar cells is defined. An electrical model is presented based on the Shockley diode equation. The general model was implemented on Matlab script file. Inverted organic cells were realized, characterized and modeled using single diode model. Simulated current density characteristic result was compared with the experimental current density characteristic for the solar cell realized and shows excellent correspondence of the model.

Key-Words: - Organic photovoltaic cell, Equivalent circuit, Newton Raphson method, Simulation, Matlab.

1 Introduction

Organic photovoltaic (OPV) is a relatively new technology that promises low-cost solar energy conversion and the possibility of novel applications. The Successful commercialization of this technology will require significant improvement in efficiency and lifetime [1, 2].

Modeling [2] is an important tool to understand the behavior of the device, and a correct model will help us in achieving highly efficient and stable solar cells. Fundamental understanding of the physical processes inside BHJ OPVs has also significantly progressed. After light absorption, the photo-generated excitons have to diffuse to the donor-acceptor interface to dissociate into electrons and holes via an ultra-fast charge transfer process [3]. Drift diffusion modeling of organic solar cells has demonstrated to be a powerful tool to explain the influence of various effects on the device performance and current-voltage characteristics (J-V curve), these simulations can be employed to define requirements of desired material properties. J-V characteristics are severely distorted by effect of the series resistance [4]. A carrier transport effect can be studied by a means of a simple equivalent circuit model directly derived from impedance spectroscopy analysis [5].

Drift diffusion simulations for a wide range of charge carrier mobilities and illumination intensities reveal significant carrier accumulation caused by poor transport properties, which is not included in the Shockley equation [8]. The conductivity of electrons and holes is given by $\sigma_{e,h} = e\,\mu_{e,h} \times n_{e,h}$. For a given mobility, the conductivity increases strongly under illumination due to the additional generation of charge carriers. The charge transport is affected by thermal annealing. An ideal solar cell may be modeled by a current source in parallel with a diode, in practice no solar cell is ideal, so a shunt resistance and a series resistance component need to be added to the replacement circuit. The current source represents the photocurrent I_{ph} generated within the illuminated cell. The series resistance R_s includes the ohmic contact contributions of the electrodes, the contact between the organic semiconductor and the metal and the resistivity of the active layer [6, 7]. This resistance has to be minimized for maximum solar cell efficiency. The shunt resistance R_P illustrates the potential leakage current through the device. R_p has to be maximized to reach high efficiency. The conventional circuit model used for inorganic solar cells , one diode model, has been used to interpret the behavior of polymer solar cells (PSCs) [10]. Single diode model, two diode model and three diode model are the most important model. The light contribution of these models is represented by a constant current source whereas the rest of the circuits correspond to the dark component. The equivalent circuit model suggested that series resistance increased as solar cell area became large and as a result the performance parameters such as short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (η) were reduced. Degradation of the performance with increased area is observed and analyzed in terms of the power loss density concept [11] in this work, one

diode model is used to simulate the J(V) characteristic of inverted organic solar cell. Simulated results were compared to the experiment results.

2 Materials and Methods

2.1 Struture of the device

When The structures of the devices manufactured are Glass/ITO/ZnO(NPS)/P3HT:PCBM/PEDOT(F010)/ Ag. The active layer based on a blend of poly(3-hexylthiophene) and fullerene is spin-coating on ITO/Zn(NP). ZnO NPS (were used to improve electron transport between ITO and the active layer. PEDOT(F010) were used as Hole transport layer The commercial ITO used in this study has a sheet resistance of 7 $\Omega/\square$ .Figure (1) shows the architecture of the cell realized.
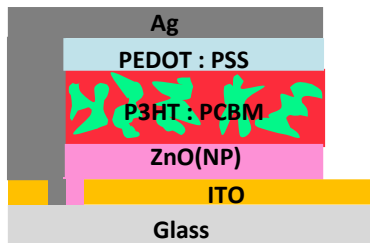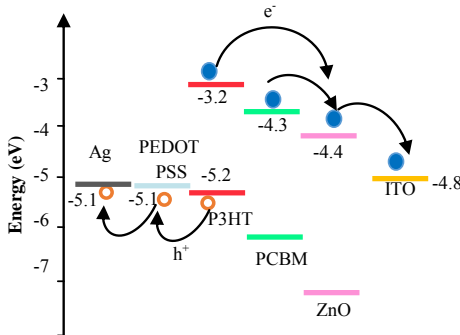
Fig.a

Fig.b

Fig.1. (a) Structure of the inverted organic solar cells for which the simulation will be performed and (b) energy levels diagram.

2.2 Equivalent circuit of the organic cell

Generally a solar cell is modeled using a circuit diode model as schematized in figure.2.
The circuit contains a diode, a current source I_{ph}, a serie resistor R_s and a shunt resistor R_p.
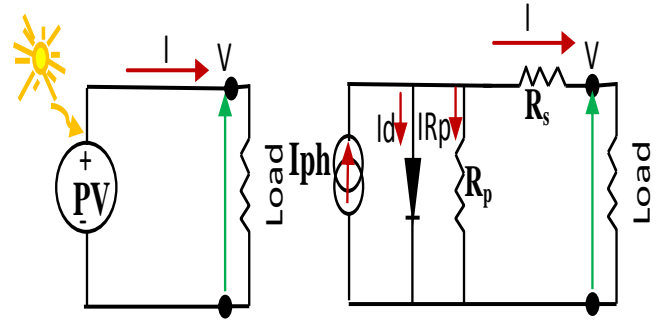
Fig.2. Equivalent PV cell used in the simulation.

2.3 Equations used in the simulation

From the equivalent circuit (fig. 2) the I(V) characteristic of the cell is given by:

$$I = -I_d + IR_p - I_{ph} \qquad (1)$$

$$I = I_s \left[\exp(\frac{e V}{n k_B T}) - 1 \right] + IR_p - I_{ph} \qquad (2)$$

Here I_d is the diode current (represents the dark current), V is the voltage, η is the diode ideality factor, I_s is the saturation current of the diode, k_B is the Boltzmann constant and T is temperature in degree Kelvin. This equation is further modified to model the organic photovoltaic cell as:

$$I = I_s \left[exp \left(\frac{e(V - I R_S)}{n k_B T} - 1 \right) \right] + \frac{V - I R_S}{R_p} - I_{ph} \qquad (3)$$

I_{ph} can be estimated with:

$$I_{ph} = \frac{I_{sc} G (1 + \alpha T)}{1000} \qquad (4)$$

G is the irradiation in W/m², α is the temperature coefficient of the I_{sc} and I_{sc} is the short circuit current of the current at cell voltage =0.
Further I_s is calculated with equation:

$$I_s = \frac{I_{ph}}{\exp\left(\frac{V_{oc} + \beta T}{k_B T}\right) - 1} \qquad (5)$$

where V_{oc} is the open circuit voltage (where current = 0), β is the temperature coefficient of the V_{oc}.
Various parameters will be approximated to a good accuracy from experimental or theoretical relations of organic devices. Results will be obtains for

P3HT:PCBM solar cells and will be verified with experimental values.

2.3.1 Open Circuit Voltage
At V_{oc} the resulting current density is zero. The open circuit voltage (V_{oc}) is given by:

$$V_{oc} = \left(\frac{nk_BT}{q}\right) ln\left(\frac{J_{ph}}{J_s} + 1\right) \tag{6}$$

2.3.2 Ideality Factor
In organic solar cells, the ideality factor (n) contains important information on the transport and recombination processes [8, 9] and can be determined via:

$$n = \left(\frac{k_BT}{e}\frac{d}{dV}\ln[J(V)/J_0]\right)^{-1} \tag{7}$$

For P3HT:PCBM solar cells ,the ideality factor depends on the recombination mechanism . The ideality factor of the dark current BHJ is dominated by the fastest transporting material in the blend. The non-ideality is caused by deeply trapped carriers, of which the effect is neutralized under illumination, so that the ideality factor under illumination is a reliable indication of the recombination mechanism taking place [9].

2.3.3 Series Resistance
Initial value of series resistance R_{s0} is obtained from the slope of the IV curve in dark at the voltage=V_{oc}.
Thus $R_{s0} = \frac{dV}{dJ}$ at $V = V_{oc}$
Since during absence of light there is the photovoltaic current (Iph = 0), and assuming that parallel resistance is high that ignoring IRp the eq1 (I=IRp+Id-Iph) reduces to: I=Id.
The equation can be more evaluated as:

$$I = I_s\left[exp\left(\frac{eV}{nkT}\right) - 1\right] \tag{8}$$

This current depends on the diode's ideality factor n. Total series resistance can now be calculated as given by the relation:

$$R_s = R_{s0} - \frac{1}{\frac{eI_s}{nkT}exp\left(\frac{eV_{oc}}{nkT}\right)} \tag{9}$$

where I_s is the saturation current given by the relation as:

$$I_s = \frac{I_{ph}}{exp\left(\frac{eV_{oc}}{nkT}-1\right)} \tag{10}$$

Iph can be calculated as:

$$I_{ph} = I_{sc}\frac{G}{1000} \tag{11}$$

where G is the irradiation in W/m².

2.4 Construction of the model

Using Newton's method to finally sum up the results, that approximates behavior of the device:

$$I = I - \frac{I_{sc}-I- I_s\left(exp\left(\frac{V+I*R_S}{nkT}\right)-1\right)}{-1-I_s\left(\frac{eR_S}{nkT}\right)exp\left(\frac{V+I*R_S}{nkT}\right)} \tag{12}$$

where V is the voltage that has generated by sweeping from zero to at least V_{oc}, for measuring the current at all those value of voltages for the IV plot. The equation is put in a loop for repetition for at least 5-10 times, so as to get more accurate values.

2.4.1 Calculating of Effeciency
We can calculate the fill factor (FF) and efficiencies using following using expression:

$$FF = \frac{V_n-\ln(V_n-0.72)}{V_n+1} \tag{13}$$

Where V_n is the normalized V_{oc} and is calculated as:

$$V_n = \frac{eV_{oc}}{nkT} \tag{14}$$

3 Results and Discussions
The equations can now be put into Matlab, as a simple program. The material properties and other conditions are fed input to generate the characteristics of the particular device.
Fig. 3.a shows the simulation results and fig.3.b the experimental J(V) characteristics of an organic solar cell with structure ITO/ Zn(NP)/P3HT:PCBM/PEDOT (F010)/Ag. The results obtained by simulation correspond to the experimental results. The short circuit current J_{sc} measured is 11mA/cm² it is the same as the J_{sc} obtained from simulation 11 mA/cm². The single diode model is an important tool to study the performance of the OPV and we can improve the model by adding different parameters to the model. In order to obtain accurate results it is necessary to take in consideration the electrical and physical properties of the active layer and the electrodes such

as the series resistance which depend in the thickness of the active layer and the mobility which depend on temperature and field effect. The total series resistance R_s between two contacts [7] can be expressed by the following equation:

$$R_s = R_{bulk} + R_{contact} = \rho_{bulk} \times d + R_{contact}$$
(15)

where R_{bulk} ($\Omega.cm^2$) is the bulk resistance of the active layer itself, $R_{contact}$ ($\Omega.cm^2$) is the specific contact resistance between the active layer and the electrode, ρ_{bulk} ($\Omega.cm^2$) is the resistivity of the active layer and d is the thickness of the active layer.

The voltage drop V_{tr} required for the charge carrier transport through the active layer is given by:

$$V_{tr} = J \, R_{tr}$$
(16)

where R_{tr} is a transport resistance is a non ohmic resistance related to the charge-carrier conductivities and the thickness of the photoactive layer [8]. It is necessary to implement these equations in the program.

Fig. 3. J(V) characteristics of organic solar cells: (a) simulation results using one diode model, (b) experimental J(V) characteristics of inverted organic solar cell with structure: ITO/Zn(NP)/P5HT:PCBM/PEDOT(F010)/Ag.

4 Conclusion

One diode model is simple but efficient to optimizing the OPV performances. With this model, based in Shockley equation, we can study the efficiency of the cell as function of different parameters such as: temperature, series and shunt resistances, ideality factor, gap of the materials used. The model of PV cell can be used to simulate a PV module, because module is an association of cells in series and parallel. The model PV module can use to study mismatch effects due to different electrical characteristics of PV cells. The single diode equivalent circuit usually is used to illustrate the characteristics of solar cells

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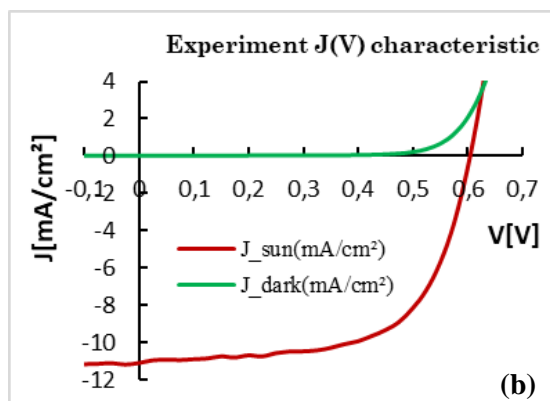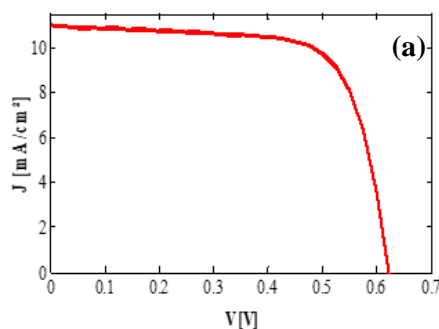
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