

THE EFFECT OF TEMPERATURE AND ACTIVE LAYER THICKNESS ON THE PERFORMANCE OF ORGANIC SOLAR CELL:BULK HETEROJUNCTION

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ABSTRACT:

In this work, General-purpose Photovoltaic Device Model (GPVDM) software was used to investigate the performance of a bulk heterojunction solar cell with P3HT:PCBM as its active layer. GPVDM is a free general-purpose tool for simulation of light harvesting devices. The model solves both electrons and holes drift-diffusion, and carrier continuity equations in position space to describe the movement of charge within the device. The model also solves Poisson's equation to calculate the internal electrostatic potential. Recombination and carrier trapping are described within the model using the Shockley-Read-Hall (SRH) formalism, the distribution of trap states can be arbitrarily defined. The software gives an output that contains the Current-Voltage (I-V) characteristic curves. A study of the effect of active layer thickness and temperature on the performance of the solar cell device was carried out. At the optimal thickness of 220 nm, the devices were found to have power conversion efficiency up to 6.28%. On other hand the fill factor (FF) decreases as the thickness increases. The FF is highest at active layer thickness of 220 nm. The effect of device temperature was also investigated and the optimal working temperature was found to be 300 K, where power conversion efficiency and FF are 6.28% and 0.808375 respectively.

Keywords: P3HT:PCBM, Fill-factor, Conversion Efficiency, Maximum power point.

1. INTRODUCTION

Which one type of structure has been widely investigated to optimize its configuration. At the beginning, a BHJ (Bulk Heterojunction) structure was made out of ITO/MEH-PPV: C60(10:1 in weight)/Ca by Yu et al. [01]. Later on, the C60 material was replaced by PCBM(6,6-phenyl C61-butyric acid methyl ester) because of its higher solubility [02]. These cells exhibited an efficiency of about 3% under a 200mW/cm² illumination [03]. Alem et al. , at their turn, fabricated a PV device made of ITO/PEDOT:PSS(poly(3,4-ethylenedioxythiophene)poly(styrenesulfonate))/MEH-PPV(Poly[2-methoxy,5-(2'-ethyl-hexyloxy)-p-phenylene vinylene]):PCBM (1:5)/LiF/Al (lithium fluoride/aluminium) [04]. The obtained efficiency were around 2,9% under AM 1.5 illumination. Their conclusion was that the introduction of the PEDOT:PSS layer, the mass ration D/A, and the solvent had direct effect on PV cell parameters. Other materials of the PPV (p-phenylenevinylene) family have been investigated in this BHJ structure MDMO-PPV (poly[2-methoxy-5-(3',7'- dimethyloctyloxy)-p-phenylenevinylene]) has been used with various derivative of fullren (C60, PCBM or C71) in a mass ratio 1:4 for BHJ. Obtained efficiency ranges from 2,5 to 3,3% [05] [06], [07], [08]. Later on, PPV and materials were replaced by P3HT by Sariciftci group [09]. The BHJ structure of OPV (Organic Photovoltaic) made of P3HT:PCBM ((poly(3-hexyl thiophene):(6,6-phenyl C61-butyric acid methyl ester)) in a weight ratio 1:2 reached an efficiency of 3,5% [09]. A similar cell fabricated by Waldauf et al. exhibited a 3,8% efficiency [10] under standard illumination. When P3HT:PCBM weight ratio was lowered to 1:08, the OPV cells efficiency reached 5% [11] [12]. As PCBM, perilènemixed with conjugated polymer was used in BHJ configuration. For this structure, it is also possible to make use of two polymers in photo active layer to improve light absorption, and that, by lowering energy levels in the materials (for a better correspondence to solar spectrum).

BHJ structures were designed to be made of small molecules (donor / acceptor) by some research groups [13] [14]. BHJ made of (CuPc, C60) (Copper phthalocyanine, buckminsterfullerene) exhibited conversion efficiency of 2.5%. Other generations of BHJ cells were fabricated with discotic liquid crystal to obtain higher free carriers mobility. Other research groups in their work in fabricating solar cells in molecular (or macromolecular) scale [15] [16][17] [18] [19], using new organic materials.

The investigation / carried with these materials allowed a better analysis of charge transfer in materials with D/A properties. So far, Research results are presented to take into account not only PV results and studied possible PVO structures, but also characteristics. These parameters include morphology, absorption, energy levels, and concentration. It is to be noticed that some works were carried out on effects of type or size of substrate used on PV performance. Flexible OPV were fabricated by replacing ITO/glass substrate with ITO / PET.

On the other hand, Al-Ibrahim et al. [20] have carried out works on flexible BHJ structure based on compound film MDMO-PPV-PCBM (1:3). An efficiency of 3% was measured over a surface of whatin air.

For the same configuration and under the same conditions, works were carried out for materials that are derived from PAT (P3HT, P3OT₂et P3DDT) and from PCBM. But measured efficiencies were low (between 0,59% and 1,54%) [21] [22]. PVO cells based on mixture MDMO-PPV:PCBM in bigger size (6 cm x 6 cm, and expanded to 10 cm x 15 cm) fabricated by Brabec et al, exhibited a 1,2% under 488 nm monochromatic illumination, at 10 mW/cm² [23], [24].

PV cell J-V characteristics showed the effect of contact material, carriers drift-diffusion, carriers generation and recombination.

2. THEORETICAL BACKGROUND

The main electrical parameters of a solar can be analyzed by studying its current-voltage characteristics curve. Some of these parameters are: short circuit current (I_{SC}), open- circuit voltage (V_{OC}), maximum power point voltage (V_{max}), maximum power point current (I_{max}), maximum power point (P_{max}), fill factor (FF) and power conversion efficiency (η).

2.1. Fill factor

The "fill factor" (FF) is a parameter which, in conjunction with V_{OC} and I_{SC} , determines the maximum power from a solar cell. The FF is defined as the ratio of the maximum power from the solar cell to the product of V_{OC} and I_{SC} so that:

$$FF = \frac{P_{max}}{V_{oc}I_{sc}} \quad (1)$$

The FF is a measure of the "squareness" of the solar cell and is also the area of the largest rectangle which will fit in the IV curve. The FF is illustrated below (Fig -1).

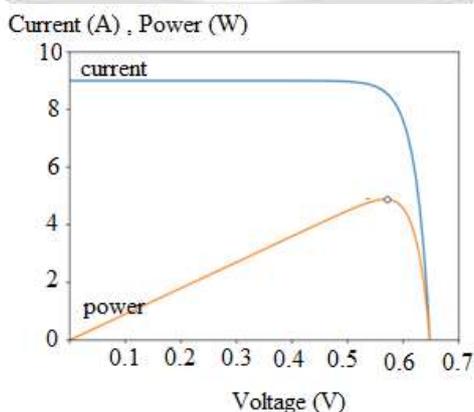


Fig -1: An IV -curve where the intersection with the y-axis corresponds with the I_{SC} and the intersection with the x-axis corresponds with the V_{OC} . [25]

Graph of cell output current (red line) and power (blue line) as a function of voltage. Also shown are the cells short-circuit current (I_{SC}) and open-circuit voltage (V_{OC}) points, as well as the maximum power point (V_{max} , I_{max}).

As FF is a measure of the "squareness" of the IV curve, a solar cell with a higher voltage has a larger possible FF since the "rounded" portion of the IV curve takes up less area. The maximum theoretical FF from a solar cell can be determined by differentiating the power from a solar cell with respect to voltage and finding where this is equal to zero. Hence:

$$\frac{d(IV)}{dV} = 0$$

giving:
$$V_{MP} = V_{OC} - \frac{nkT}{q} \ln \left(\frac{qV_{max}}{nkT} + 1 \right) \quad (2)$$

Equation 2 is an implicit equation, but it converges rapidly with iteration. By starting with $V_{MP} = 0.9 \times V_{OC}$ as the initial condition, there is < 1% error after one iteration and negligible (< 0.01%) after three iterations. An alternative is using Lambert functions (see below). Substituting the value of V_{MP} back into the diode equation gives I_{MP} and then FF . A more commonly used empirical expression for the FF is [25]:

$$FF = \frac{v_{oc} - \ln(v_{oc} + 0.72)}{v_{oc} + 1} \quad (3)$$

Where v_{oc} is defined as a "normalized V_{OC} ":

$$v_{oc} = \frac{q}{nkT} V_{OC} \quad (4)$$

The above equations show that a higher voltage will have a higher possible FF . However, large variations in open-circuit voltage within a given material system are relatively uncommon

2.2. Solar Cell Efficiency

The efficiency is the most commonly used parameter to compare the performance of one solar cell to another. Efficiency is defined as the ratio of energy delivered the solar cell to input energy from the sun. In addition to reflecting the performance of the solar cell itself, the efficiency depends on the spectrum and intensity of the incident sunlight and the temperature of the solar cell. Therefore, conditions under which efficiency is measured must be carefully controlled in order to compare the performance of one device to that of. Terrestrial solar cells are measured under AM1.5 conditions and at a temperature of 25°C. Solar cells intended for space use are measured under AM0 conditions. The efficiency of a solar cell is determined as the fraction of incident power which is converted to electricity and is defined as:

$$\eta = \frac{V_{OC} I_{SC} FF}{P_{in}} \quad (5)$$

Where: V_{OC} is the open-circuit voltage; I_{SC} is the short-circuit current; FF is the fill factor and η is the efficiency.

The input power for efficiency calculations is 1 kW/m² or 100 mW/cm².

2.3. Open circuit Voltage V_{OC}

V_{OC} is voltage when current equals to zero. In order to try and understand the physical mechanisms which may be responsible for the observed temperature dependence of V_{OC} in the high and low temperature ranges it is instructive to start with an analysis of the V_{OC} behavior of conventional inorganic semiconductor solar cells with a p - n junction [26].

For that situation:

$$V_{oc} = \frac{AkT}{q} \ln\left(\frac{I_{sc}}{I_0} + 1\right) \quad (6)$$

Where A is a diode quality factor of the p - n junction and I_0 is the reverse saturation current. According to the simple model of Shockley [27], I_0 is given by:

$$I_0 = qN_vN_c \exp\left(\frac{-E_g}{kT}\right) \left(\frac{L_n}{n_n\tau_n} + \frac{L_p}{p_p\tau_p}\right) \quad (7)$$

Where N_v and N_c are the effective densities of states in the valence and conduction band, respectively, E_g is the semiconductor band gap, L_n , L_p , n_n , p_p , τ_n , τ_p are the diffusion lengths, the carrier densities and the lifetimes of electrons and holes, respectively.

Since $I_{sc} \gg I_0$, we obtain:

$$V_{oc} = \frac{AE_g}{q} - \frac{AkT}{q} \ln\left(\frac{1}{I_{sc}} qN_vN_c\right) \left(\frac{L_n}{n_n\tau_n} + \frac{L_p}{p_p\tau_p}\right) \quad (8)$$

$$V_{oc} = a - bT \quad (9)$$

Where

$$a = \frac{AE_g}{q}$$

And

$$b = -\frac{d}{dT} V_{oc} = \frac{Ak}{q} \ln\left(\frac{1}{I_{sc}} qN_vN_c\right) \left(\frac{L_n}{n_n\tau_n} + \frac{L_p}{p_p\tau_p}\right)$$

in that we also observe a linear decrease of V_{oc} with T

3. METHODOLOGY

3.1. General-purpose Photovoltaic Device Model

General-purpose Photovoltaic Device Model (GPVDM) is a free general-purpose tool for simulation of light harvesting devices. The model solves both electrons and holes drift-diffusion, and carrier continuity equations in position space to describe the movement of charge within the device. The model also solves Poisson's equation to calculate the internal electrostatic potential. Recombination and carrier trapping are described within the model using Shockley-Read-Hall (SRH) formalism, the distribution of trap states can be arbitrarily defined. A more detail description of the model can be found in the software manual [28]. The software gives an output which is the (I-V) characteristic curves of the device [29].

3.2. Device Structure

Our choice is aorganic solar cell of bulk heterojunction, made up at the nanoscale level of a mixture of donor material P3HT and an acceptor material PCBM. The device structure is given in Fig -2. The thickness of the layers are ITO (100 nm) / PEDOT :PSS (100 nm) / P3HT :PCBM (150 nm)/ Al (100 nm)

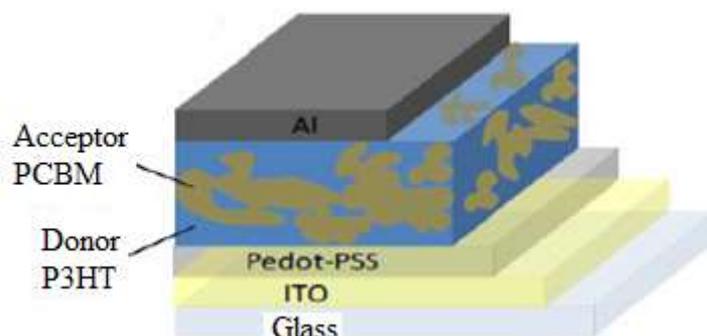


Fig -2: Schematic representations Bulk heterojunction of organic solar cell, the layer thickness are given in bracket [28].

3.3. Simulation Parameters

The structure was introduced into a GPVDM solar cell simulator because it is capable of solving the system of semi-basic equations conductive, Poisson's equation and continuity equations of electrons and holes. The active layer P3HT:PCBM parameters used for the simulation are shown in the Table 1.

Table-1: Parameters used for the simulation at 300 K

Parameters	Value
Electron mobility [$\text{m}^2\text{V}^{-1}\text{s}^{-1}$]	$3\text{e-}7$
Hole mobility [$\text{m}^2\text{V}^{-1}\text{s}^{-1}$]	$0.2\text{e-}7$
Relative permittivity [au]	3.8
Effective density of free electron states [m^{-3}]	$1.28\text{e+}27$
Effective density of free hole states [m^{-3}]	$2.86\text{e+}25$
X [eV]	3.8
E_g [eV]	1.1

3.4. The Simulation

In this work, the simulation was run twice; the first for different set P3HT: PCBM layer thickness and the second for different set of temperature. During the first simulation process, the thickness of P3HT:PCBM layer was optimized varying it from 80 to 220 nm in a step of 20 nm, i.e. the thickness that gives the highest efficiency. The optimal thickness obtained in the first simulation was used in the second simulation. Here the temperature was varied from 300 K to 350 K in a step of 10K.

4. RESULTS AND DISCUSSION

Current density-Voltage (J-V) characteristic curves obtained in the first simulation is shown in Fig-3. The short circuit current density (J_{sc}), open-circuit voltage (V_{oc}), maximum power point voltage (V_{max}), and maximum current density (J_{max}) were deduced from the Current density-Voltage characteristic curves in both simulations, and these are tabulated with fill factor, the maximum power and efficiency.

The curve J(V) is determined both in darkness and under illumination (AM1.5, $1\text{mW}/\text{cm}^2$) using GPVDM. The parameters of the variation of the current density according to the voltage of a PV cell in darkness and under illumination (Table 2) provide access to many physical parameters characteristic of the component.

Table-2: Parameters used for the simulation at 300 K and d = 150 nm

Parameters	Value	
	No illumination	Under illumination
V_{oc} [V]	-1.000000	0.760380

J_{SC} [$A.m^{-2}$]	1.754386e-02	-7.483392e+01
V_{max}	-1.000000e+00	6.516817e-01
J_{max}	-1.000000e+00	-7.109614e+01
P_{max} [$W.m^{-2}$]	-1.000000	46.332049
FF	-1.000000	0.814240
Power conversion efficiency [%]	-1.000000	4.633205

This table clearly shows that with no illumination, current density-voltage characteristic passes through the origin while the curve under illumination is offset by relative to the first of a J_{sc} value that translates current generation by light-number of physical parameters characteristic of the component.

From the values provided by the GPVDM software, we were able to draw the curves that describe the influence of the active layer thickness on the conversion efficiency (Fig-3). We will study the impact of the active layer thickness of the organic solar cell based on P3HT/PCBM on its performance. To do this we will vary the thickness of the active layer from 80 to 220 nm. The simulation results for the different thicknesses of the active layer are presented together in Table -3.

Table-3: Solar cell parameters for different active layer thickness

active layer thickness d	V_{oc}	J_{sc}	V_{max}	J_{max}	Max power P_{max}	Fill Factor FF	Power conversion efficiency η
80	0.738567	-6.149313 ^{e+01}	6.330884 ^{e-01}	-5.907269 ^{e+01}	37.398234	0.823445	3.739823
100	0.744029	-6.318080 ^{e+01}	6.530670 ^{e-01}	-5.925580 ^{e+01}	38.698005	0.823216	3.869801
120	0.749556	-6.623648 ^{e+01}	6.526912 ^{e-01}	-6.246770 ^{e+01}	40.772122	0.821225	4.077212
140	0.756368	-7.104797 ^{e+01}	6.521225 ^{e-01}	-6.732824 ^{e+01}	43.906262	0.817037	4.390626
160	0.762947	-7.925291 ^{e+01}	6.511683 ^{e-01}	-7.548415 ^{e+01}	49.152885	0.812904	4.915288
180	0.768901	-8.913806 ^{e+01}	6.702861 ^{e-01}	-8.302429 ^{e+01}	55.650024	0.811954	5.565002
200	0.774280	-9.540805 ^{e+01}	6.695319 ^{e-01}	-8.947034 ^{e+01}	59.903303	0.810901	5.990330
220	0.779249	-9.974653 ^{e+01}	6.690114 ^{e-01}	-9.391901 ^{e+01}	62.832886	0.808375	6.283289

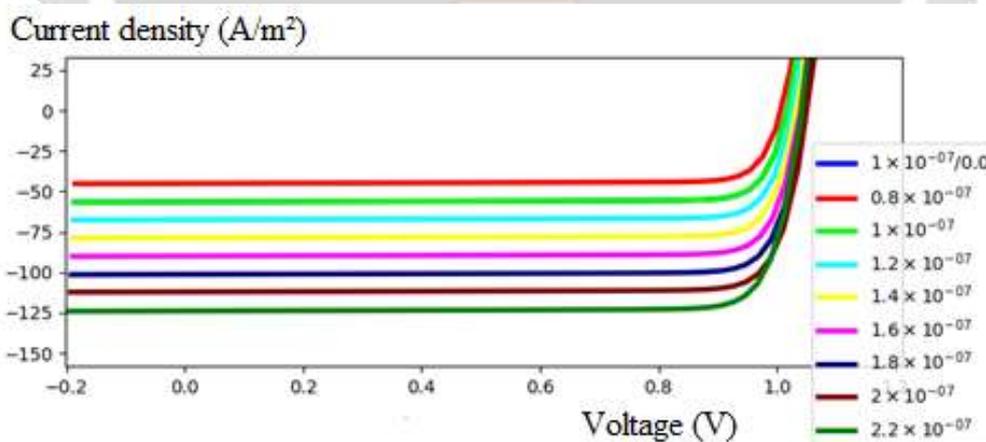


Fig -3: J(V) characteristics for different thicknesses of the active layer

We study the influence of the thickness of cell on the characteristic J(V) (Fig-3) and on the performance of cell P3HT: PCBM (Fig-4). A higher thickness means better absorption on one side and on the other side a lower internal field so that the dissociation of the polar pairs is less. This means that there is an optimal thickness for better performance of organic solar cells.

A thick cell would increase the efficiency, since more light would be absorbed; the low absorption of solar radiation is a cause of poor performance. In addition, we note that the optimal thickness moves to higher values

as mobility increases. However, the thicker cells make both a technical problem and, on the other hand, economic from the point of view of the cost of manufacturing which is not interesting.

Fig- 4(a) it shows that as the thickness is changing from 80 nm to 220 nm, the Power conversion efficiency slowly increases to about 6.28 %. The production of new charges carrier occurs due to increase in thickness which in turn increases the efficiency. The fill factor of model device decreases almost linearly as the thickness of active layer increases (Fig-4(b)), which is in agreement with reports on bulk heterojunction organic solar cells and polymer bulk heterojunction solar cells. The electric field at the maximum power point on J(V) curve is smaller than that at short-circuit condition, bringing about lower dissociation rate and a higher recombination rate. In thicker devices the electric field is smaller due to the larger distance between the electrodes. Therefore recombination of charge carriers at the maximum power point is more prominent in thicker device, resulting in a low FF.

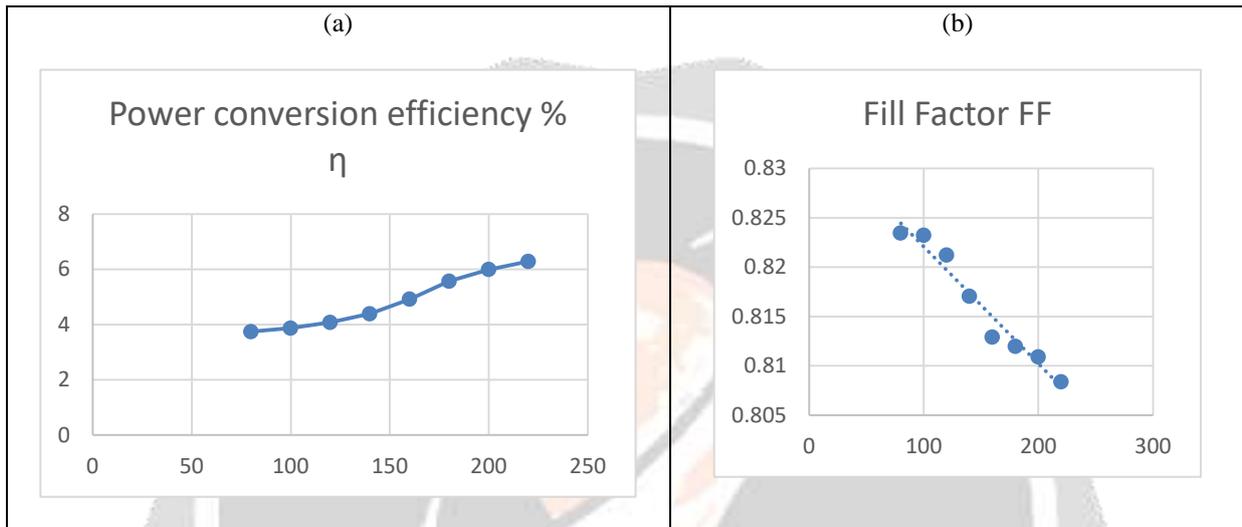


Fig -4 : Graph representing (a) the variation of power conversion efficiency (b) the variation of fill factor by varying thickness

Table-4 represent the variation of temperature the characteristic J(V) and on the performance of cell P3HT: PCBM. It can be deduced that as the temperature increases, there is a decrease in the performance of a device. The fact that FF decreases as temperature increases, is evident from the empirical equations. As the temperature increases there is increase in the series resistance which leads to the decrease in the carrier diffusion length. The recombination rate also increases due to increase in temperature. Due to these the efficiency and fill factor drops. Figs-5 (a) and (b) show that as the temperature is changing from 300 K to 350 K.

Table-4: Solar cell parameters for different device temperature

Temperature	Fill Factor FF	V _{oc}	J _{sc}	V _{mpp}	J _{mpp}	Max power P _{max}	Power conversion efficiency η
300	0.808375	0.779249	-9.974653 ^e +01	6.690114 ^e -01	-9.391901 ^e +01	62.832886	6.283289
310	0.802954	0.766352	-9.974484 ^e +01	6.489338 ^e -01	-9.458204 ^e +01	61.377482	6.137748
320	0.798347	0.755137	-9.974294 ^e +01	6.491623 ^e -01	-9.262887 ^e +01	60.131174	6.013117
330	0.792927	0.743486	-9.974082 ^e +01	6.290636 ^e -01	-9.347255 ^e +01	58.800179	5.880018
340	0.786126	0.731370	-9.973845 ^e +01	6.089827 ^e -01	-9.416446 ^e +01	57.344522	5.734452
350	0.781008	0.720746	-9.973581 ^e +01	6.092178 ^e -01	-9.215438 ^e +01	56.142095	5.614209

(a)

(b)

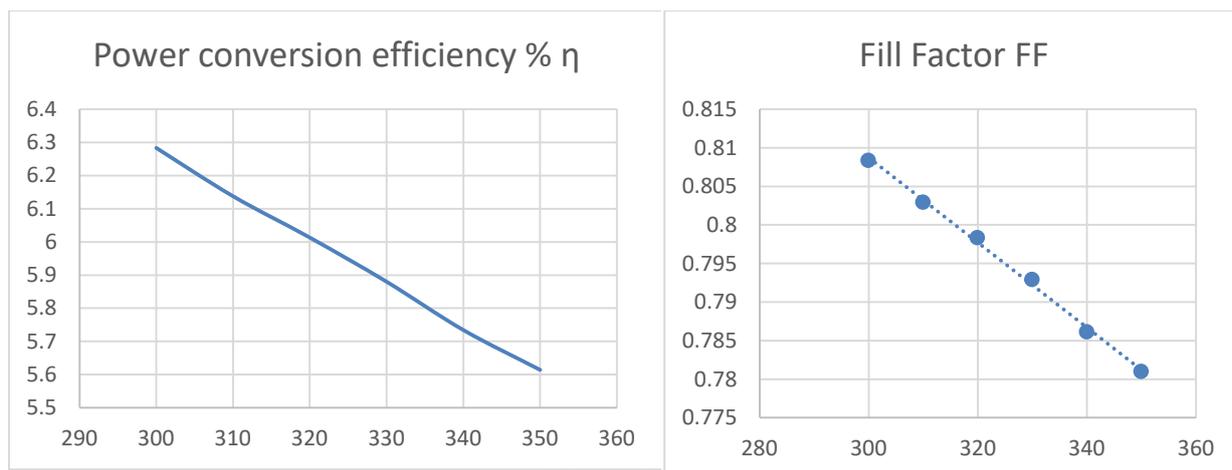


Fig -5: Graph representing (a) the variation of Conversion Efficiency, (b) the variation of fill factor by varying the temperature.

The temperature has a definite influence on the performance of the organic cell; we note a decrease in the performance of the cell (η , J_{SC} , V_{OC} , FF) with the increase of the temperature. However, the impact of temperature change on open circuit voltage V_{oc} in organic cells is significantly less than that observed in inorganic cells. It has been observed that on average the open circuit voltage decreases with the temperature increase of about 184.30544 mV per 10°K, implying a significant advantage of organic photovoltaic cells in many areas of use.

5. CONCLUSION

In this work it was observed that as the thickness of the active layer (in this case P3HT: PCBM) increases, the efficiency increases linearly by 0.363352% with increasing the thickness up to 20 nm. In this case, the devices were found to have power conversion efficiency up to 6.283289%. On other hand the FF decreases as the thickness increases. The FF is highest at active layer thickness of 80 nm. The effect of device temperature also studied and the optimal working temperature was found to be 300 K, where power conversion efficiency and FF are 6.283289% and 0.808375 respectively. The simulations carried out on organic photovoltaic cells Bulk Heterojunction based on P3HT/PCBM are in perfect harmony with the literature, and show the undeniable advantages of this cells on single layer structures and bilayer structures. In addition, these simulations allowed us to determine and study the effects of the active layer thickness, and the effects of temperature on the performance of organic cells.

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