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High performance and efficiency enhancement for organic solar cell : layers thickness optimization

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Abstract

A mathematical modeling for performance and efficiency for organic solar cell is presented, bulk hetero-junction photovoltaic of ITO layer (indium tin oxide), P3HT (Poly3-Hexylthiophene) PCBM (phenyl C₆₁-butyric acid methyl ester) was investigated, the results show main effect of all layers thickness and a major effect for the active layer thickness of the electrical energy obtained for this OPV solar cell due to open circuit voltage, fill factor and short circuit current for the OPV solar cell.

The efficiency investigation was done according to J-V curves obtained from GVPDM (General photovoltaic purpose device model) which built according to optical treatment and drift diffusion model based on the poisson's equation solution, we started from 1e-5 to 1e-9 meter thickness for each layer, then by taking optimum thickness for each layer which are about 1e-7 meter we investigate the efficiency for active layer thickness between (1e-7 to 9e-7), the efficiency obtained was about 3.7 to 2.7 respectively.

Key word: Organic solar cell, solar energy, OPV, GVPDM simulation program, solar efficiency.

1- Introduction

In past few decades a lot of interest has been done for various forms of renewable energy sources because of the significant increase for clean energy sources, dispensing strict reliance on oil and other fossil fuel.

The most popular clean energy among the distributed energy resources in environment are photovoltaic solar cells, this is mainly because solar energy is sustainable energy and is widely available everywhere in the world and under any climatic conditions. Solar energy is a much more rich resource than what is needed to supply all the energy world needs. With a simple mathematical process, we can conclude that the amount of energy received within one hour of the Earth from the sun is equivalent to consuming energy in one year. Unlike fossil fuels in oil and gas, and unlike oil and gas, this energy has few environmental impacts and pollutants [1-3].

By considering this, we can search for low-cost photoelectric cells, enabling us to obtain good energy, and therefore organic materials that work as potential candidates have been resorted to. The discovery of organic matter with exciting properties has given rise to exciting new possibilities. The main advantage of organic matter is the ability to produce photovoltaic devices with different technologies that are very inexpensive, and highly productive. These advantages give a several promising products like thin film structure, flexible substrate at room temperature processing, light weight devices[4].

2- Organic solar cell

From previous advantages mentioned and taking into consideration semi-transparency and could be easily integrated into other products to give innovative applications like combined to another parallel-connected



multi-junction devices[5], organic solar cell received much attention in researches and manufactured devices.

The organic photovoltaic cell (OPVs) consists of organic materials as thin layer which gives the basic steps in photoelectric energy harvesting from solar radiance by absorption sun light and the charge carrier will transport and extracted throw the junction or will be injected throw contacts [1].

The basic concept of this type of solar cell can be considered as absorbing photons, release electrons then drive these electrons between the polymer layers material that have different work function, this kind of polymer materials improve the main purpose of solar cell like conductivity, charge carriers to generate electric power as figure(1,2) shows that [3,1].

The single layer photovoltaic device consists of two electrodes one of them is transparent the other one photosensitive electrode while the bilayer organic structure includes an addition transporting layer, the advantage of adding is to increase exciton dissociation efficiency otherwise, intrinsically low quantum efficiency which resulting from the low mobility of charge carrier throw the organic semiconductor because it required more time to be collected from cell electrode.

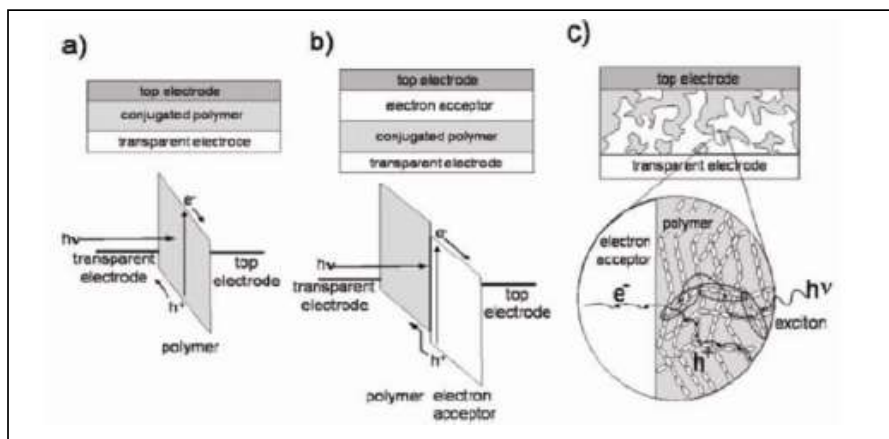


Figure (1): Organic solar diagram a)single layer device, b)multi layers device, c)bulk hetero-junction organic solar cell [3].

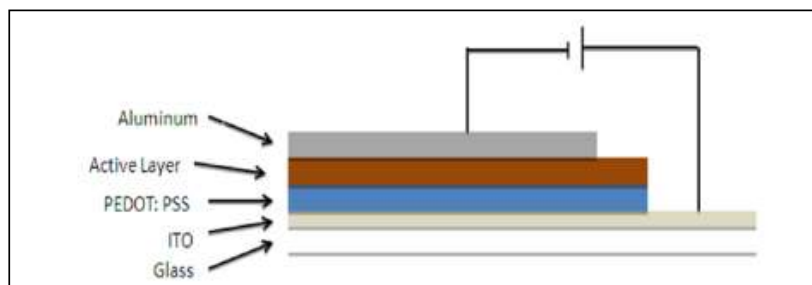


Figure (2): Basic 2-d Organic solar diagram [1].

There are many roles or causatives decreasing the efficiency of OPV cell: slow charge transport and exciton formation while there is an increasing of recombination probability of charge in device due to first role,

To overcome those problems that causes small collected amount of free exciton created in the region near donor and acceptor interface, the use of organic bulk heterojunction take a promising advantage due to a large interface between donor and acceptor[5,6].

3- Materials used in simulation

The basic structure material used in this paper consists of (ITO) layer (indium tin oxide) having a high work function while the lower work function is kept in normally a layer of aluminum (AL) as a conductive electrodes to insure easy collection of electrons, two sandwich layers among them are placing to generate electrostatic force at the interface region due to the different affinity electron which also called planer donor-acceptor hetero-junction, the first on acts as a buffer layer and the second on acts as active layer as shown in figure(3)[8].

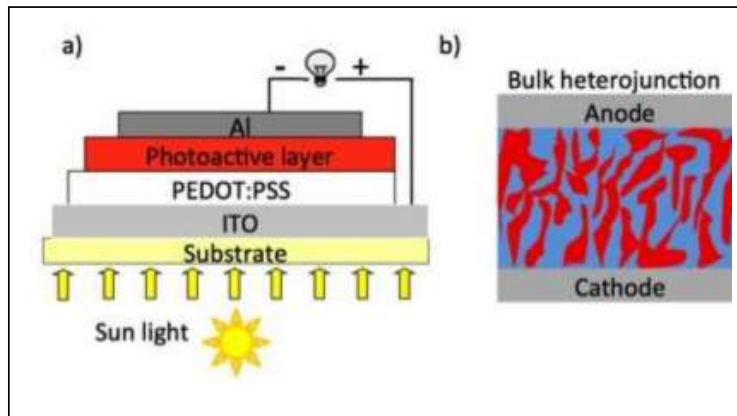


Figure 3: Bulk structure hetero-junction OPV solar cell [8].

The ITO front electrode layer used as transparent film, as well as the buffer layer having an ability of transmitted the visible light and conducting, the active layer consists mainly of donor-acceptor thin blends which allow light to be absorbed and generate excitons[9].

The donor blend here having a good electron mobility is P3HT (see figure 4) with the combination of (Poly3-Hexylphosphene) which effectively transport electrons, the other blend which must be the acceptor is PCBM with the combination of (phenyl C₆₁-butyric acid methyl ester), this layer transport electrons between molecules, the efficiency has improved very well by adding ITO layer for the OPV solar cell [10].

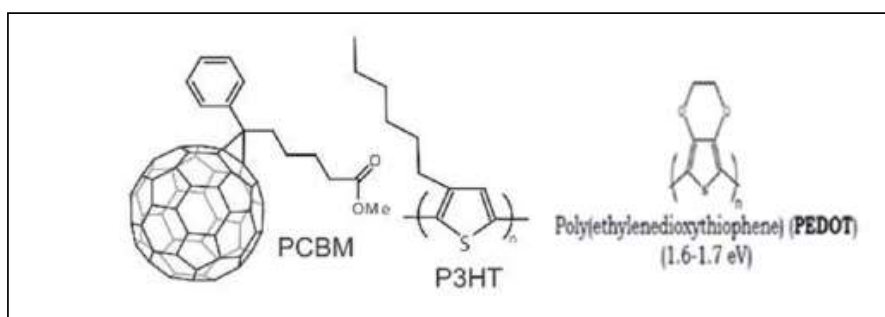


Figure 4: Chemical structure for the hetero-junction OPV solar cell [2].

The benefit of the installation referred to above when an organic active material located between two metal electrodes will be able to introduce two schottky junctions, these two metals electrodes having two different work functions will produce a Fermi level alignment having internal electric field called built in electronic field while its corresponding electric voltage at the electrodes called built voltage. In organic solar cell experimental built in voltage is mainly about 1.3 volt [11,12].

4- Controlled parameters

Harvesting electrical energy from OPV solar cell suffers from a lot of influences parameters, with its low power conversion efficiency but it have a lot of promising alternative for giving clean energy from sun ray, to increase the conversion efficiency a major strides must be done one of the approaches is by increasing the surface area as well as increasing of the number of absorbed electrons, increased optical thickness, decreased diffusion length, reduced optical reflection and enhanced absorption for incident solar cell. These processes are influenced by the production and manufacture of the organic solar cell, the physical description for approved effects are[13]:

Total efficiency =[light absorption efficiency+ exciton dissociation efficiency + charge transport efficiency + charge collection efficiency]

Theses parameters was directly modeled by GVPDM with two simulation methods the first one is the optical model for OPV solar cell based on transfer matrix formulation which describe the exciton generation rate per unit volume, the second one is the poisson's equation solution based on the drift diffusion model for the electrostatic potential Ψ which describe the self-consistent equations densities of electron, holes and excitons taking into account the flux due to drift and diffusion, generation rate for excitons and its dissociation recombination rates.

The first simulation step is to built in potential for device after knowing the carrier concentrations, effective densities of states and energy gab as below[14]:

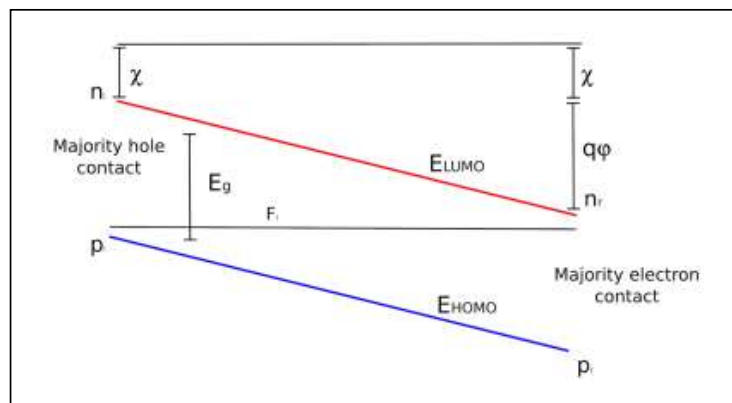


Figure 5: The band structure in equilibrium [14].

Here we can write the energy for LOMO and HOMO by [13,14]:

$$E_{LOMO} = -\chi, \quad E_{HOMO} = -\chi - E_g \dots \dots [1]$$

Maxwell Boltzmann statistics can be use to calculate the equilibrium Fermi level as:

$$P_l = N_v \exp \frac{E_{HOMO} - F_p}{KT} \dots \dots [2]$$

$$n_l = N_c \exp \frac{F_n - E_{LOMO}}{KT} \dots \dots [3]$$

Now for the case of charge carrier transports one use:

$$J_n = q\mu_e n_f \frac{\partial E_{LOMO}}{\partial x} + qD_n \frac{\partial n_f}{\partial x} \dots \dots [4]$$

$$J_p = q\mu_h p_f \frac{\partial E_{HOMO}}{\partial x} - qD_p \frac{\partial p_f}{\partial x} \dots \dots [5]$$

For both electrons the solution will be:

$$\frac{\partial J_n}{\partial x} = q(R - G) \dots \dots [6]$$

$$\frac{\partial J_p}{\partial x} = -q(R - G) \dots \dots [7]$$

Where G,R are generation rate per unit volume and net combination respectively.

The internal potential distribution for the OPV device can be obtained from poisson's equation solved in the form[15]:

$$\frac{d}{dx} \cdot \epsilon_o \epsilon_r \frac{d\psi}{dx} = q(n_f + n_t - p_f - p_t - N_{ad}) \dots \dots [8]$$

Where n_f, n_t are carrier densities of free, trapped electrons, p_f, p_t are carrier densities of free, trapped holes while N_{ad} is doping density.

After knowing solar cell parameters we can calculate power efficiency from the JV plots obtained from simulation program for each case studied as this figure shows that[13].

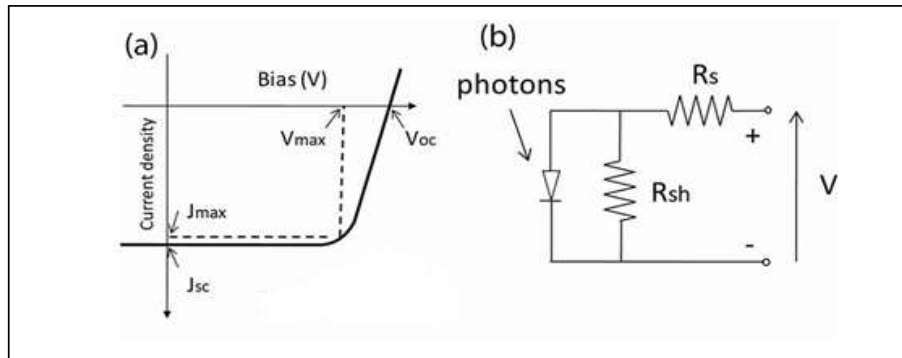


Figure 6: calculating efficiency from

JV curves [13].

From the previous figure now we are able to evaluate the conversion efficiency for OPV solar cell as [16]:

$$\eta_{max} = \frac{P_{max}}{P_{in}} = \frac{V_{max}J_{max}}{P_{in}} \dots \dots [9]$$

While the fill factor is given by:

$$FF = \frac{V_{max}J_{max}}{V_{op}J_{sc}} \dots \dots [10]$$

$$\eta_{max} = \frac{FFJ_{sc}V_{op}}{P_{in}} \dots \dots [11]$$

Where η_{max} , FF , J_{sc} , V_{op} , P_{in} , P_{max} are the total efficiency, fill factor, short circuit current, open circuit voltage, input power and maximum power.

Finally enhanced carrier collection efficiency these parameters affected by a lot of cell parameters taken in our simulation as shown in table (1):

Table 1: OPV solar cell parameters for active layers

Layer type	P3HT	PCBM
Thickness m	1e-5~1e-9	1e-5~1e-9
Dielectric constant	3.4	3.0
Electron mobility Cm ² /V/s	1e-4	1e-3
Hole mobility Cm ² /V/s	1e-3	1e-4
Conduction band effective density of state Cm ³	1e+22	1e+22
Valence band effective density of state Cm ³	1e+22	1e+22
Number of acceptor /Cm ³	-----	3.17e13
Number of donors /Cm ³	3.17e13	-----
Energy band gap eV	1.85	2.1
Electron Affinity eV	3.1	3.7

5- Results and discussion

Analysis of organic solar cell based on different photovoltaic layer thickness have been presented, simulation done with GVPDM electric simulation to evaluate and plot the relation of I-V, J-V figures, efficiency investigation have been done using the open circuit voltage, short circuit voltage and fill factor using equations (9-11) with assistant of figure[6].

An ITO layer (indium tin oxide), P3HT (Poly3-Hexylphosphene) PCBM (phenyl C₆₁-butyric acid methyl ester) bulk hetero-junction solar cell was investigated theoretically after giving the values for the physical properties for each layer of organic solar cell from table1 the figures below shows the I-V curves for each layer.

Figure 7 shows that there is a main difference between the applied voltage and the current obtained for OPV solar cell due to the ITO layer thickness about 1e-5 there will be a small amount of the solar radiation inters to the active layers while it will be a good optimize for thickness about 1e-7 to 1e-8 meter.

In a same way we can see that the 2nd layer thickness PDOT will have converging values for current voltage relation, for third layer thickness which is the active layer in our simulation we see a different values for each layer thickness with minimum and maximum I-V curves or values.

From figures (7-12) one can conclude that the active layer thickness play a main rule for current voltage harvesting form sun ray other layer thickness will absorb incident photon when layer thickness increase.

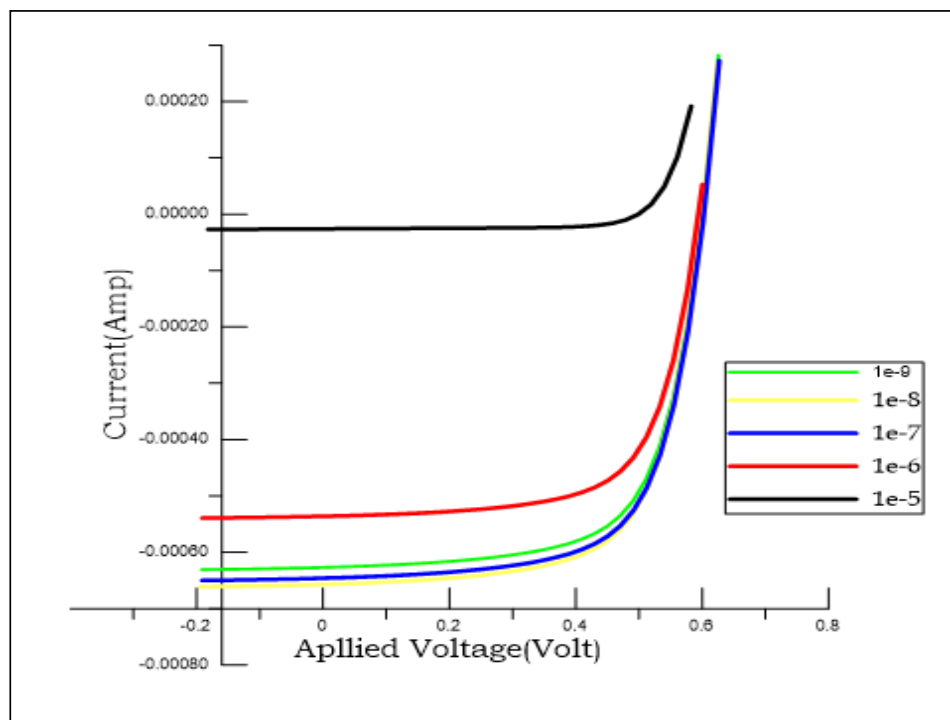


Figure 7: applied voltage vs current obtained with different ITO layer thickness.

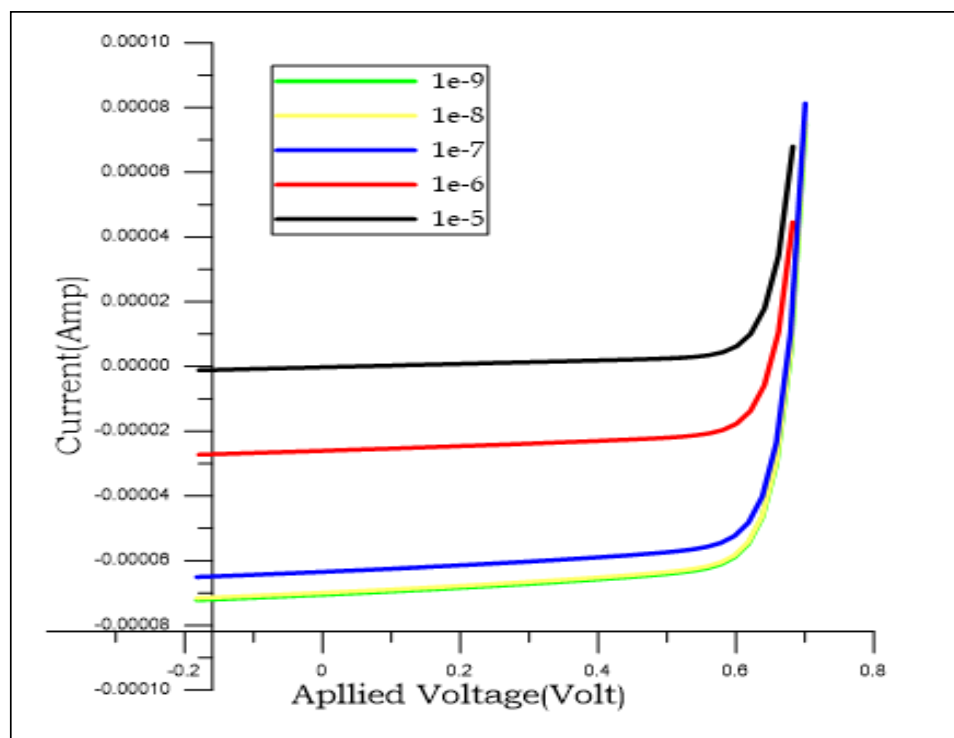


Figure 8: applied voltage vs current obtained with different PDOT layer thickness.

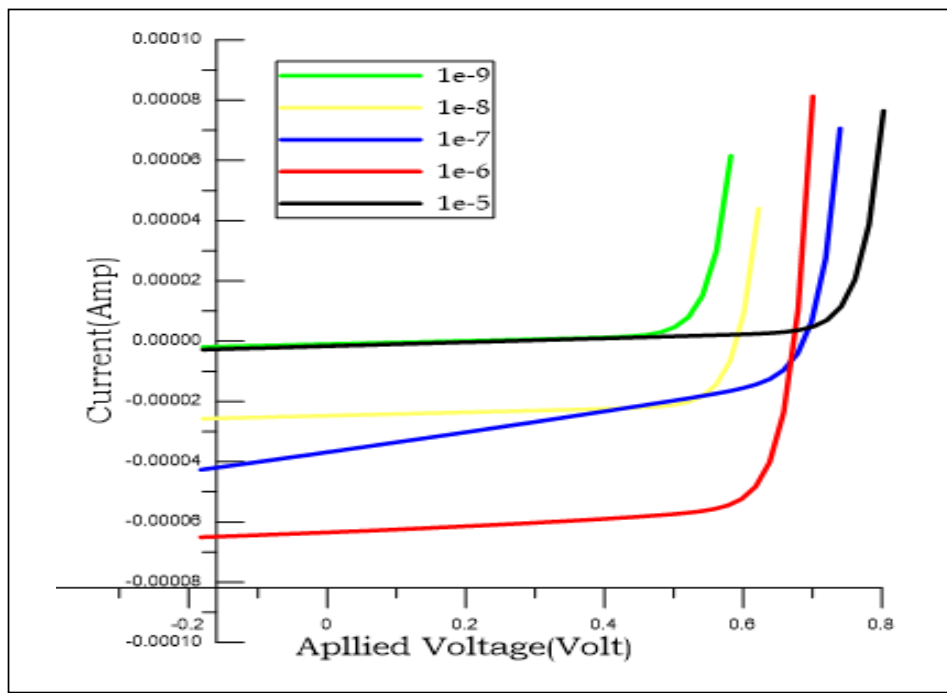


Figure 9: applied voltage vs current obtained with different P3PHT layer thickness.

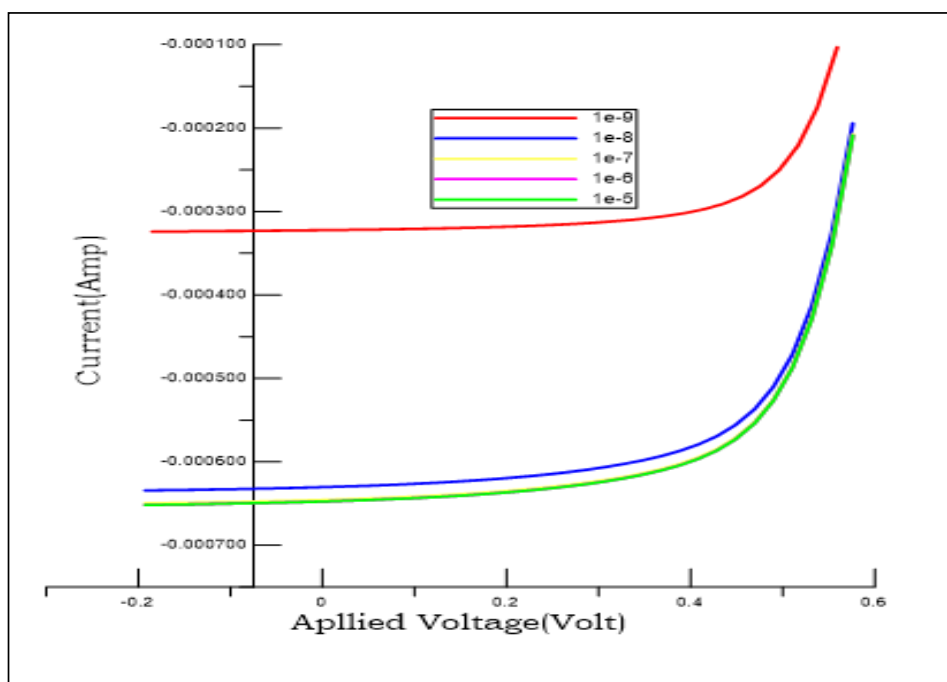


Figure 10: applied voltage vs current obtained with different AL layer thickness.

From previous figures we will chose the active layer thickness to be $1\text{e-}7$ to $9\text{e-}7$ m while other layers thickness fixed to $1\text{e-}7$ m and simulate the resulting values of J-V curves using equations (9 -11) with the figures below:

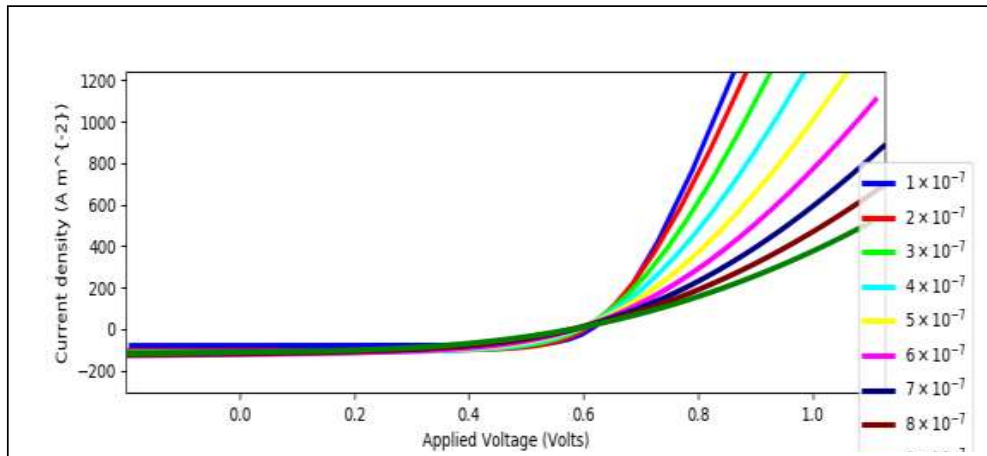


Figure 11: applied voltage vs current density with different active layer thickness.

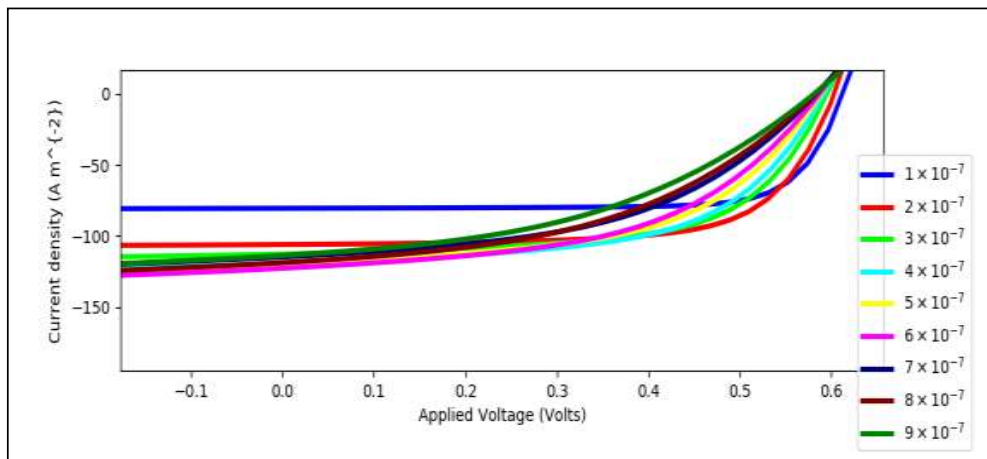


Figure 12: applied voltage vs current density with different active layer thickness.

Here we introduce table 2 counting the efficiency simulation for given active layer thickness.

Table2: efficiency of OPV solar cell for studied active layer thickness.

Thickness (m)	1e-7	2e-7	3e-7	4e-7	5e-7	6e-7	7e-7	8e-7	9e-7
Fill factor a.u.	0.76499	0.6803	0.6127	0.5680	0.5323	0.5027	0.4797	0.4499	0.4273
Pow. con. effic. %	3.7646	4.3455	4.100	3.993	3.725	3.577	3.170	3.072	2.783
Max power W/m ²	37.646	43.455	41.00	39.93	37.25	35.77	31.70	30.72	27.83
Voc volt	0.611	0.602	0.594	0.598	0.587	0.586	0.582	0.583	0.581

The efficiency will be low when the device thickness is very thin due to it cannot absorb many photons, and when the device become thicker the efficiency will decreases as the charge carrier must travel for a large

path from the generation to extraction place leading the probability of recombination to increase, there for there must be a balance in between these two opposite effects of layer thickness

6- Conclusions

There results of direct simulation are in good agreement with other researchers, and the results of our simulation leads to conclude that the electric current obtained for this kind of OPV organic solar cell highly depends on layer thickness, the active layer have a main direct impact on the amount of electrical energy harvested from sun ray due to the optical effects that took place in the structure and that the optimum domain size is smaller comparing with the exciton diffusion length.

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