COLLATION OF BILAYER AND BULK HETEROJUNCTION ORGANIC SOLAR CELL SIMULATION CHARACTERISTICS FOR DISTINCT ACTIVE LAYER THICKNESS

[1]Abdul Aziz Khan J, [2]Shanmugaraja P
[1]Department of Electronics & Communication Engineering, Research Scholar, Annamalai University, Annamalainagar-608 002, Tamilnadu, India
[2]Department of Electronics and Instrumentation Engineering, Associate Professor, Annamalai University, Annamalainagar-608 002, Tamilnadu, India

Abstract: Organic solar cells (OSC) show great potential as a low-cost energy source. In addition, their mechanical flexibility allows the added advantage of use on a wide variety of surfaces. In recent years, progress in experimental strategies and modeling approaches has enabled enhancing the power conversion efficiencies of OSC. And the performance characteristics of organic solar cells based on bulk heterojunction structure has extremely improved. This article based on analyzing the 3 cases by comparing the bilayer and BHJ organic solar cell by various parameters. The active layer based on poly (3-hexylthiophene) (P3HT) and Phenyl-C70-butyric acid methyl ester (PCBM) is made, evaluating the distinct on active layer thickness (10 to 100nm) on the both Bilayer and BHJ organic solar cell The results are obtained and collation for all the three cases with I-V, J-V characteristics, active layer thickness versus efficiency.

Index Terms **- Organic solar cell, Bilayer solar cell, Bulk heterojunction (BHJ) solar cell, P3HT:PCBM**

I. INTRODUCTION

Organic solar cells allow the use of low-temperature roll-to-roll, and hence low-cost manufacturing [1]. Mechanical flexibility is the other major advantage of these devices which makes them so attractive. Huge progress has been made in the last few years towards improving the problem of low efficiencies associated with organic solar cells. This advancement (highest reported value under laboratory conditions is 9% [2]) is made possible by experimental and numerical investigations of the operating mechanisms and device structure optimization [3].

In this paper, the collation of bilayer and bulk heterojunction is simulated by varying the active layer thickness P3HT:PCBM the characteristics of current-Voltage, current density-Voltage, efficiency-active layer thickness is discussed by different 3 cases. In case one bilayer organic solar (OSC) P3HT:PC70BM is used in layer 1 and layer, case two bilayer OSC PC70BM:P3HT is used in layer 1 and layer 2 and in case three Bulk heterojunction OSC P3HT:PCBM is formed as bend at the active layer upto 100nm thickness. The electrical parameters are compared for all the three cases and discussed.

II. WORKING PRINCIPLE OF ORGANIC SOLAR CELL (OSC)

The operating working principle of organic solar cells are one of the most researched and debated fields. Generation of electro statistically bound electron-hole pair in organic solar cells instead of free charges makes its working mechanism different from that of inorganic solar cells. The mechanism includes the four basic steps: (i) absorption of light and exciton generation, (ii) exciton diffusion, (iii) exciton dissociation, and (iii) charge transport [4]. Fig.1 illustrates the basic steps of the working principle of an organic solar cell [22].

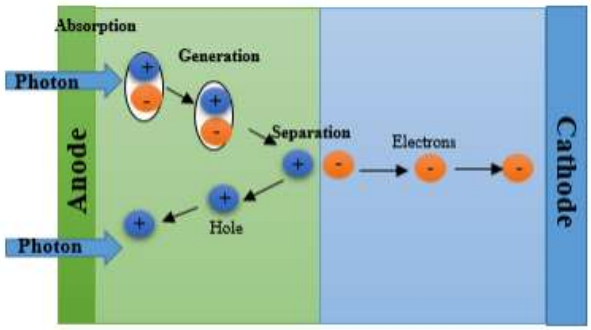

Fig 1: A schematic representing working mechanism of an organic solar cell [5]

When light (photon) get incident on photoactive layer through transparent electrode (anode), electrons get excited i.e, upon absorption of the light, material get energized and excitons (coulomb bound electron-hole pair) are formed. After absorption and exciton formation, excitons undergo through diffusion followed by dissociation. Dissociation do occur due to different work function of acceptor and donor. Excitons dissociates at LUMO level of acceptor and HOMO level of the donor [6]. Dissociation is then followed by charge separation. It occurs at organic semiconductor/metal interfaces. After getting separated, charge transportation occur and they get collected by respective electrodes.

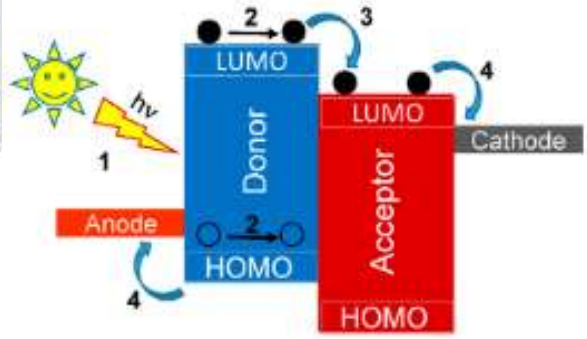

Fig 2: Operation schematic of the organic solar cell demonstrating energy levels [7]

III. ARCHITECTURE OF BILAYER AND BULKHETEROJUNCTION (BHK) ORGANIC SOLAR CELL

A. Bilayer OSC

In a bilayer device the p-n type semiconductors are stacked on top of each other. The bilayer device was discovered by using many different materials combinations of organic semiconductor. The active region of an organic solar cell consists of two materials have a differences in electron affinity and ionization energy; therefore the electrostatic forces are generated at the interfaces between the two layers. The materials are chosen properly to make the differences large enough, so these local electric fields are strong, which may break up the excitons much more efficiency than the single layer photovoltaic cells do.

However, the bilayer OSC device Power conversion Efficiency (PCE) is still reported to be lower compared with the inorganic devices. This happens because of the shortage of intrinsic exciton diffusion length in organic semiconductors, which is between 10-20 nm, however, researchers attempted to overcome this limitation in the bilayer OSC device by using buck minster fullerene, C60 in which the exciton diffusion length is around 20 nm [8, 9]. P.Peumans et al. replaced perylene tetracarboxylic derivative with C60 as an acceptor in the device structure and the device produced a PCE of 3.5% [8, 10]. Therefore, this improved PCE is caused by the longer distance travelled by excitons in the triplet state of C60. The thickness of the acceptor and donor layers ranges between 40-60 nm, which is why the absorbed large amount of photon energy is not converted to free carriers and dissipated by recombination. Therefore, this indicates that photo-generated excitons are dissociated near the interface between donor and acceptor species [8].

B. Bulkheterojunction OSC

Traditional structures were made using the model of silicon solar cells in which the photons were going through the anode before being converted to exciton in the bulk heterojunction. However it has been shown that an inverted structure behaves much

better and was more stable. The working principle of these cells is very easy: in the Bulk heterojunction, incident photons are absorbed, that leads to the creation of an exciton. These excitons can diffuse within the material, before being separated as a hole-electron pair.

Each carrier is transported to a transport layer toward its respective electrode. The bulk heterojunction is composed of a donor polymer, P3HT for example and an acceptor organic material. Owing to their strong electron negativity and high electron mobility, C_{60} derivatives like PCBM have become standard acceptor molecules in OPV devices. Today, the inverted structure with fullerene derivatives has become a standard in organic solar cells [11].

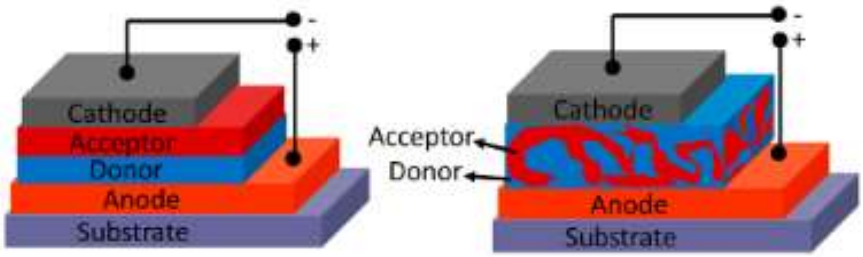

Fig (a) **Fig (b)**

Fig 3: Device structures of (a) bilayer heterojunction, (b) bulk heterojunction [7]

IV. Donor and Acceptor Materials

The fullerene derivates shows great potential being effective electron acceptor. A combination of narrow-band donor and fullerene derivate is a possible approach to efficient organic cells, including the most efficient organic cell P3HT:PCBM The P3HT:PCBM has reported an efficiency as high as 5%, which is unusual in the organic cell material. Their structures are as shown (Fig 4). PCBM is a fullerene derivative. Because of high hole mobility, it plays the role of electron acceptor in many organic cells. P3HT is among the Polythiophene family, which is a kind of conducting polymer. It is the excitation of the π-orbit electron in P3HT that gives the photovoltaic effect in the blend [12,13].

An active material can work properly if the donor and acceptor have a proper HOMO (High Occupied Molecular Orbital) and LUMO (Lowest Unoccupied molecular Orbital) [6]. P3HT (Poly(3-hexylthiophene) and PCBM (Phenyl-C61-Butyric Acid Methyl Ester) polymer has HOMO 3 eV and 4 eV respectively, facilitating electron transfer from P3HT to PCBM [7]. Poly (3-hexylthiophene) or P3HT polymeric semiconductor has matching criteria as donor material and acts as a p-type. Poly (3-hexylthiophene) has a molecular weight of 65.5 g/mol and a high hole mobility of 3.8~3.9x10-4 cm2 /Vs [8]. PCBM or C61-ButyricAcid PhenylMethyl Ester is derived from fullerenes. PCBM is typically used as a good acceptor material in organic solar cells. This causes the PCBM be a material uses in solar cell active ingredient compared to other fullerene-derived material.[14,15]

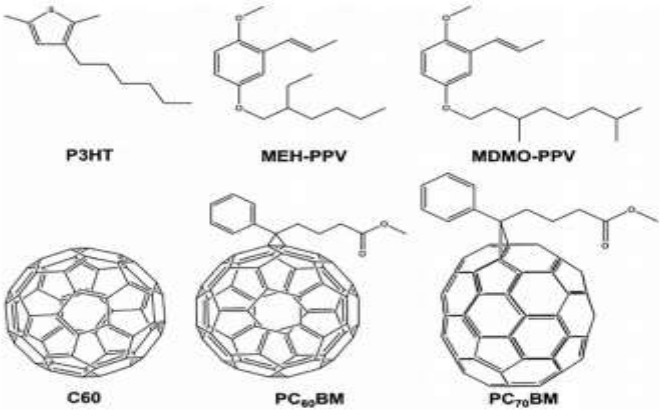

Fig 4: Molecular structures of various donor (top row) and acceptor (bottom row) materials used in PSCs

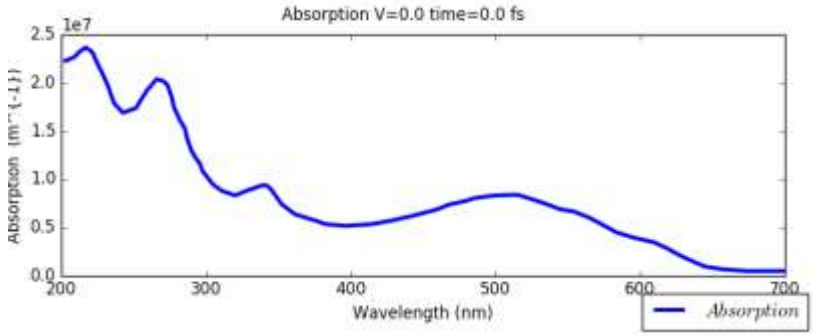

Fig (a)

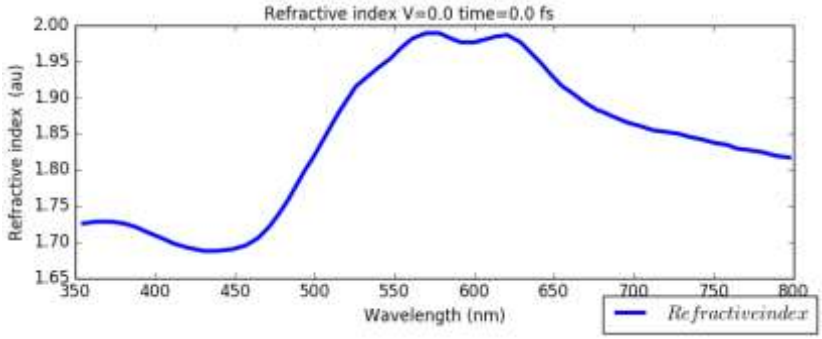

Fig (b)

Fig 5: Wavelength for (a) Absorption of P3HT:PCBM, (b) Refractive Index of PCHT:PCBM

V. I-V CURVES

The key characteristic of a solar cell is its ability to convert light into electricity. This is known as the power conversion efficiency (PCE) and is the ratio of incident light power to output electrical power. To determine the PCE, and other useful metrics, current-voltage (IV) measurements are performed [16].

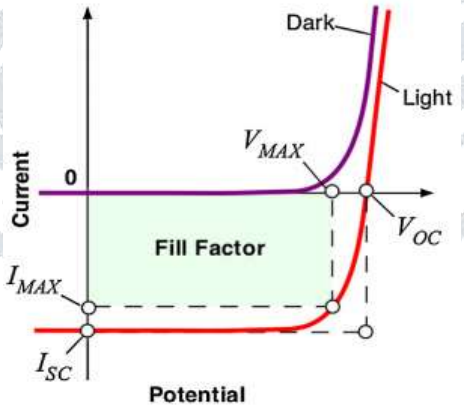

Fig 6: Typical I-V curve of a organic solar cell in Dark and under illumination [17]

The properties highlighted in the figure are:
J_{MP} – Current density at maximum power
V_{MP} – Voltage at maximum power
P_{Max} – The maximum output power (also known as maximum power point)
J_{sc} – Short-circuit current density
V_{oc} – Open-circuit voltage

ISC (Short circuit current): Short-circuit current is the current through the OSC when the voltage across the OSC is zero [18].

$$I_{SC} = I_{max} = I(E = 0) \quad (1)$$

VOC (open-circuit voltage): The open-circuit voltage is the maximum voltage available from a solar cell, where current is zero [19].

$$V_{OC} = \frac{nkT}{q} \ln\left(\frac{I_L}{Io} + 1\right) \quad (2)$$

Fill Factor (FF): Fill Factor is another important performance parameter in the measurement of solar cells, which is given by the formula below: IMP and VMP are the maximum current and voltage respectively from the solar cell [20].

$$FF = \frac{I_{MP} V_{MP}}{V_{OC} I_{SC}} \quad (3)$$

Ideally, FF is unity (1) and usually it is represented in a percentage (%) value.

Power Conversion Efficiency (PCE): PCE is defined as the ratio of power output from the solar cell to the power of input radiation energy of sun or the solar simulator lamp.

$$PCE = \frac{(V_{oc}\ I_{SC}\ FF)}{P_{in}} \quad (4)$$

Where Pin is the input power of the radiation source. PCE is expressed in percentage (%) value.

$$P_{max} = V_{OC} I_{SC} \mathrm{FF} \quad (5)$$

A solar cell is a diode, and therefore the electrical behaviour of an ideal device can be modelled using the Shockley diode equation[21]:

$$J(V) = J_{ph} - J_D = J_{ph} - J_0 \left[\exp\left(\frac{eV}{k_B T}\right) - 1\right] \quad (6)$$

Here, J_{ph} is the photo generated current density, J_D is the diode current density, J_0 is the dark saturation current density (current density flowing through the diode under reverse bias in the dark), V is the voltage, and T is the temperature. The final 2 symbols, e and k_B, are the elementary charge (1.6×10^{-19} C) and the Boltzmann constant (1.38×10^{-23} $m^2.kg.s^{-2}.K^{-1}$) respectively. However, in reality, no device is ideal and so the equation must be modified to account for potential losses that may arise:

$$J(V) = J_{ph} - J_0 \left[\exp\left(\frac{e(V + JR_s)}{nk_B T}\right) - 1\right] - \frac{V + JR_s}{R_{sh}} \quad (7)$$

Here, n is the diode ideality factor and all other symbols have their previous meanings. Using this equation, a solar cell can be modelled using an equivalent circuit diagram, which is shown below:

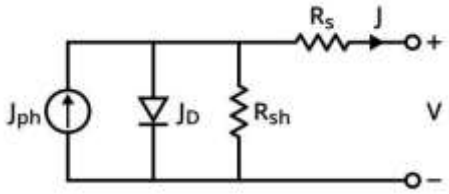

Fig 7: The equivalent circuit of a solar cell and it is modified Shockley diode equation [21].

VI. RESULTS AND DISCUSSION

Case 1: Bilayer (P3HT:PCBM)

By keeping ITO to 50nm,PEDOT:PSS to 10nm and Al to 10nm as constant the Layer 1 & 2 (below Fig. a & b) varied simultanously from 10 to 100nm.we can see the current is constant upto 0.5, it reaches the cut in voltage 0.6 the current and current density increased suddenly.The Efficiency (below fig. c)can be varied with respect to active layer thickness from 10 to 100nm the efficiency can be improved up to 12.43% in bilayer using P3HT:PCBM.

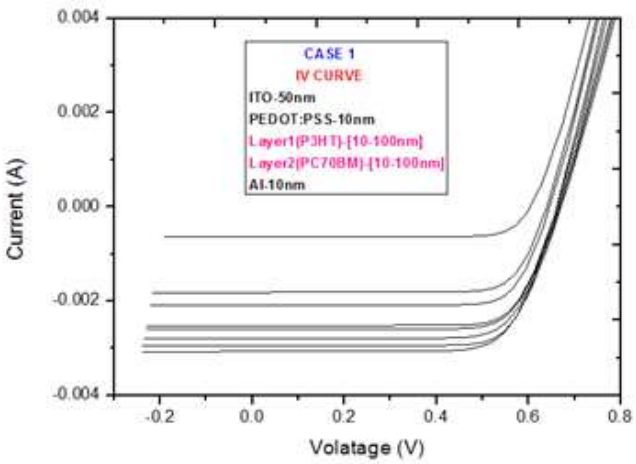

Fig. a

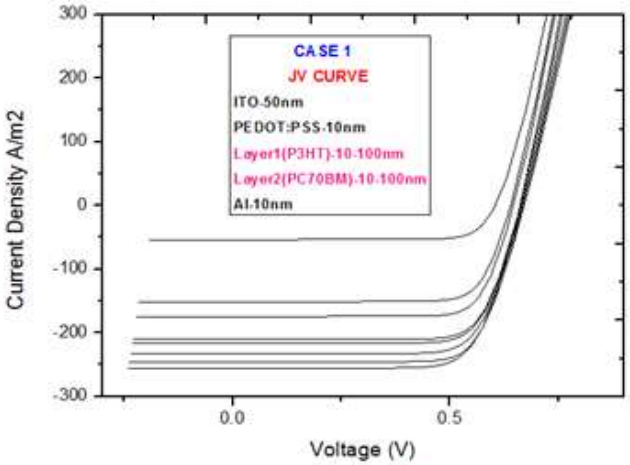

Fig. b

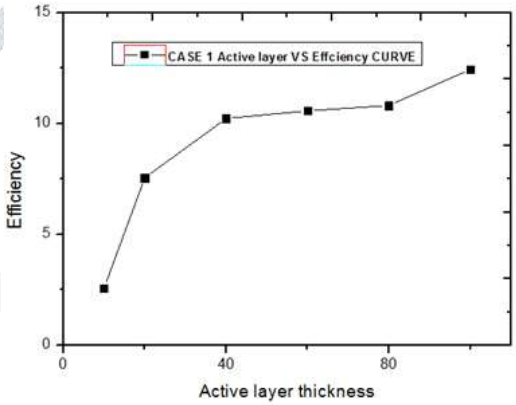

Fig. c

Fig 7: Characteristics of (a) Current-Voltage curve, (b)Current density –voltage Curve, (c) Efficiency Vs active layer thickness

Case 2: Bilayer (PCBM-P3HT)

As we discussed in case 1 here in case 2 the layer material is changed we cant see any major change in their IV and JV charactersistics.Same procedure to be followed by keeping ITO,PEDOT:PSS and Al as constant the Layer 1 & 2 varied simultanously from 10 to 100nm.we can see the current is constant upto 0.5, it reaches the cut in voltage 0.6 the current and current density get incresed suddenly.

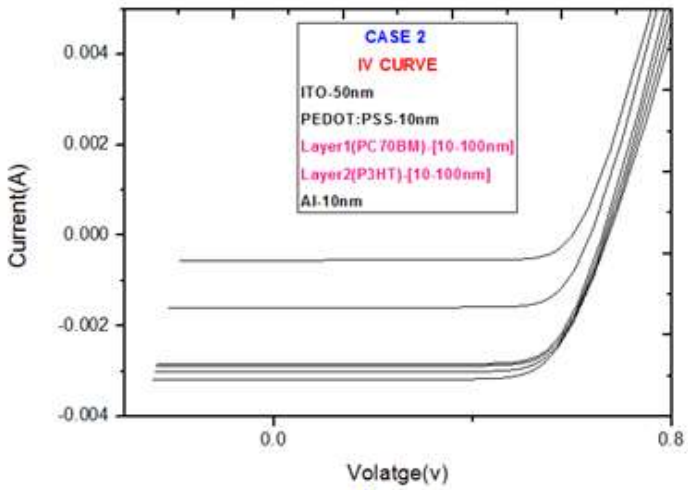

Fig. a

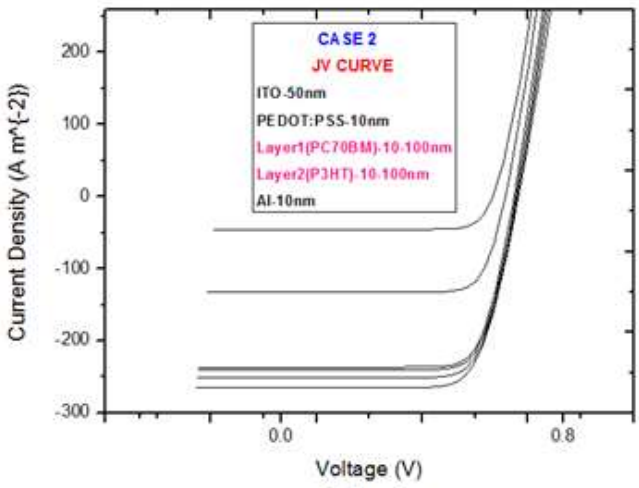

Fig. b

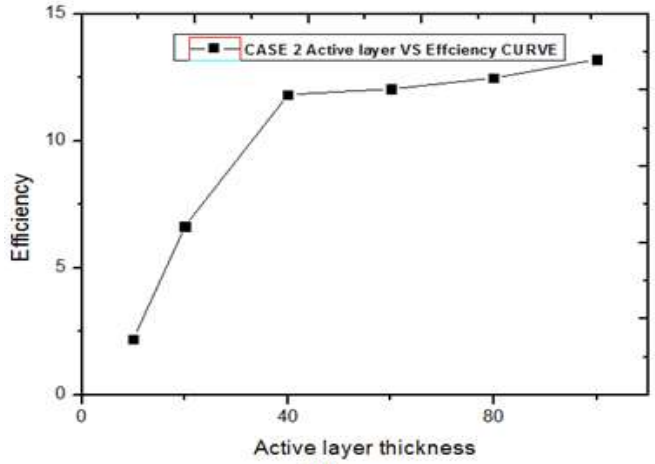

Fig. c

Fig 8: Characteristics of (a) Current-Voltage curve, (b)Current density –voltage Curve, (c) Efficiency Vs active layer thickness

Case 3: BHJ BLEND(P3HTPCBM)

In Case 3 the two materials get blended together the current and current density value gets reduced at the starting point of 10nm and the efficiency curve also gets equally increased with respect to active layer thickness.Efficiency is more improved when compared to bilayr solar cell.By keeping ITO,PEDOT:PSS and Al as constant the Blend material varied simultanously from 10 to 100nm.we can see the current is constant upto 0.5, it reaches the cut in voltage 0.6 the current and current density get incresed suddenly.

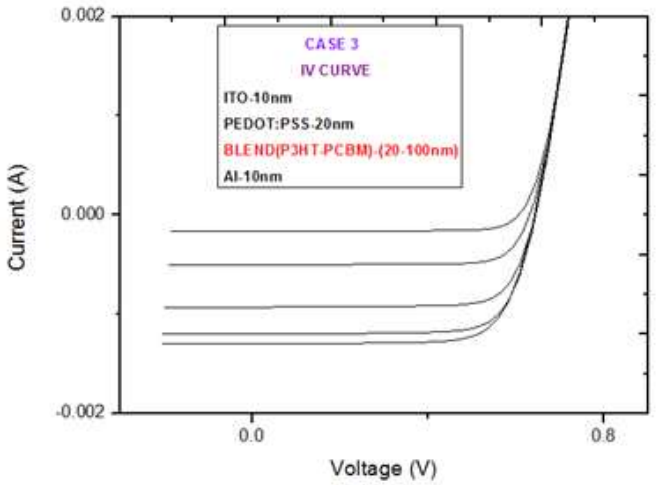

Fig. a

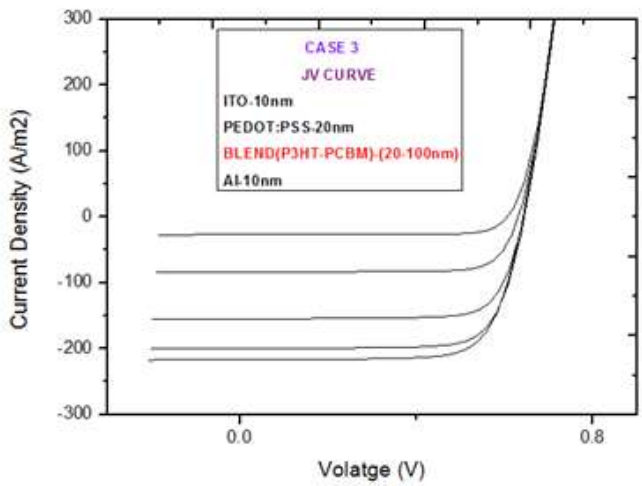

Fig. b

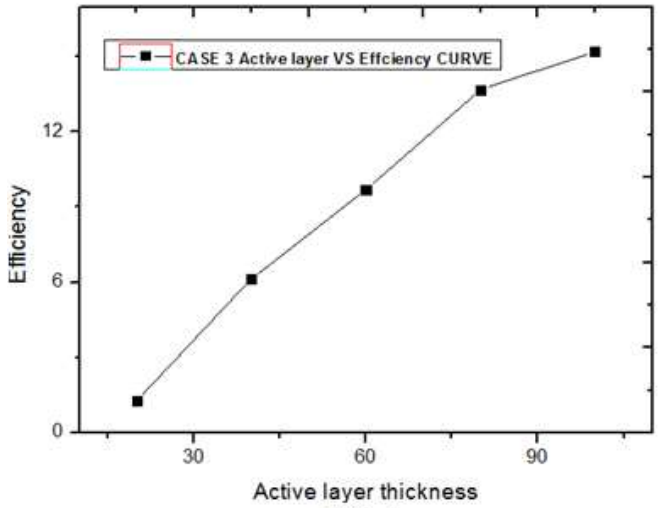

Fig. c

Fig 9: Characteristics of (a) Current-Voltage curve, (b)Current density –voltage Curve, (c) Efficiency Vs active layer thickness

OSC	Active layer Thickness	Jsc(A/m^2)	Voc(V)	FF	Efficiency (%)	Pmax(W/m^2)
	10nm	-53.450351	0.603591	79.87	2.57	25.767985
CASE1	20nm	-151.281011	0.640211	77.88	7.54	75.433932
BILAYER 1	40nm	-245.611180	0.661424	75.32	**10.23**	122.360684
Layer 1-P3HT	60nm	-210.201443	0.661901	76.00	10.57	105.753371
Layer 2-PC70BM	80nm	-216.656963	0.664740	75.06	10.81	108.112246
	100nm	-255.735479	0.670367	72.55	12.43	124.393014
	10nm	-45.925399	0.600674	80.05	2.20	22.083187
CASE 2	20nm	-132.821247	0.635928	78.57	6.63	66.372164
BILAYER 2	40nm	-236.676529	0.660826	75.62	11.82	118.274536
Layer 1- PC70BM	60nm	-240.675651	0.665245	75.19	12.04	120.400274
Layer 2-P3HT	80nm	-251.378421	0.669356	74.15	12.47	124.766882
	100nm	-265.446097	0.672954	72.61	13.20	129.720329
	20nm	-27.066363	0.605777	78.50	1.28	12.871606
CASE 3	40nm	-83.889395	0.630798	75.30	6.14	41.438607
BHJ OSC	60nm	-199.854868	0.644677	72.21	9.69	96.911415
BLEND-	80nm	-208.862214	0.645856	67.13	13.68	128.354436
P3HTPCBM	100nm	-218.449691	0.642609	61.03	14.21	135.924913

Table 1: Comparison table for Bilayer and BHJ solar cell:

As per the above table Bilayer and BHJ solar cell is compared and studied. The overall Efficiency, FF, Pmax can be much improved when compared to bilayer solar cell

VII. CONCLUSION:

The better understanding of comparing bilayer and Bulkheterojunction organic solar cell with I-V,J-V Characteristics,active layer thickness is simulated and the results are recorded by using gpvdm software.It is concluded that the variation in active layer thickness can improve the current and current density, and aslo we can improve the Efficiency and Fill factor when compare to bilayer solar cell.

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