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GPVDM Simulation of Layer Thickness Impacts on Power Conversion Efficiency, Maximum Power of P3HT: PCBM Based Tandem Solar Cell

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ABSTRACT

In this research, we utilized the GPVDM software to simulate the effects of layer thickness in an Organic Bulk Heterojunction Tandem Solar Cell based on P3HT and PCBM. We considered a double-junction Tandem solar cell and investigated the impact of layer thickness on Power Conversion Efficiency (PCE) and Maximum Power (MP). GPVDM is a versatile opto-electronic device simulation tool that can simulate various types of solar cells, including organic, perovskite, and more.

The PCE of single-junction organic solar cells has already surpassed 10%. Tandem OPV devices, which consist of two subcells connected in series, are predicted to reach or even exceed a 15% milestone (as mentioned in reference [2]). In our study, we achieved a PCE of 18.90%. Our model consisted of two bulk heterojunction organic solar cells connected in series, hence the term "Tandem solar cell".

We made advancements by carefully considering the layers in the Tandem solar cell without any defects. The results demonstrated that adjusting the thickness of the layers can significantly modify the PCE and MP. In this case, we increased the PCE to 18.90% and the MP to 189.08 Watts .

Keywords—active layers, contacts, Organic Tandem solar cell, GPVDM software, PCE, MP

I. INTRODUCTION

Solar cell is the electronic device that converts the light of the sun directly into the electricity. The electricity obtained is DC which depends directly on the intensity of light. There are various types of solar cells like crystalline- silicon, thin- film, organic & pervoskites solar cells. Crystalline- silicon comes in the category of 1st generation solar cells, thin- film comes in the category of 2nd generation solar cells while organic, and pervoskites and tandem comes in the category of 3rd generation solar cells. Third generation solar cells are in the research and building phase while 1st and 2nd generation solar cells are available in the market.

Very recently Organic Photovoltaic (OPV) devices are the main focus and subject of interest of researchers. Organic solar cells provide significant promise for use in new solar technology, because of their flexible material properties and low- cost fabrication and manufacture [1]. OPV cells are really awesome due to their ease of processing, mechanical flexibility and low cost. So far, the reported efficiencies of Organic solar cells are less as compared to 1st and 2nd generation PV technologies. The recent realization of Tandem solar cells is one of the most beneficial approaches of Organic solar cells to eliminate the important losses in the single junction OPV devices, like narrow absorption window and thermaliztion losses and may take the way towards improved performance OPV devices [2, 3].

In single- junction solar cells (OSC), the two major losses occurring are transmission loss and thermalization of hot charge carriers. One way is to tackle the both issues simultaneously is the concept of Tandem solar cell (TSC) [3]. Firstly, the detailed performance or tandem structures was studied by De Vos [3]. De Vos explained that conjoin several subcells in series can cross the theoretical efficiencies beyond the Shokley- Queisser limitation.

In Bulk heterojuction OSC, the active layer consists of P3HT and PCBM materials which are conjugate blends that allow maximum light absorption and has been considered amid most efficient smart material for researchers investigation and studies to improve their PCEs. The PCE of bulk heterojuction (BHJ) solar cell based on P3HT: PCBM blends are approximately 6% and PCE of PCDTBT: PCBM based solar cell has achieved 6.1% [4]. The pros of BHJ structure is that the active layer absorbed maximum photons and most of the generated electron- hole pairs reach a near donor- acceptor interface where they becomes separated into free charge carriers (electrons & holes) [3]. When two or more sub organic solar cells are connected in series or parallel, a structure is formed called Tandem solar cells. It has the advantage to remove the limitations of single- junction solar cells.

Solar cells are devices that directly convert sunlight into electricity. They come in different types like crystalline-silicon, thin-film, organic, and perovskite solar cells. The first and second generation solar cells are already available in the market, while the third generation solar cells are still being researched. Organic Photovoltaic (OPV) devices are gaining interest due to their flexibility and low-cost fabrication. Although their efficiencies are currently lower compared to first and second generation technologies, the development of tandem solar cells shows promise in improving performance. Tandem solar cells combine multiple subcells in series to surpass theoretical efficiency limits.

II. THEORATICAL APPROACH

In the P3HT: PCBM Tandem solar cell, the active layer consists of P3HT and PCBM. P3HT acts as an electron donor, while PCBM serves as an electron acceptor. Indium Tin Oxide (ITO) is used as a transparent material to allow precise transmittance of visible wavelengths and block other wavelengths. The PEDOT: PSS layer acts as an electron blocking layer.

In this tandem structure, the two subcells' active layers based on P3HT: PCBM are separated by a thin metallic gold (Au) layer. This layer is highly transparent and conductive, facilitating the transport of both electrons and holes. The interconnected layer (ICL) of gold also maintains charge neutrality by eliminating excess charge carriers from different subcells, preventing recombination of opposite charges.

The main electrical parameters of a solar cell can be analyzed through its I- V characteristic curve. The important parameters include open circuit voltage (Voc), Short circuit current (Isc), Fill Factor (FF) and Power Conversion Efficiency (PCE). Isc is the solar cell current when voltage is zero i.e. when solar cell is shorted and Voc is the voltage when current is zero i.e. when solar cell is open circuited. The FF is equal to the ratio of maximum power to the product of Voc & Isc. Emperically the FF is given by [5].

$$FF = \{\upsilon oc - \ln(\upsilon oc + 0.72)\} \div (\upsilon oc + 1)$$

Where υoc is normalized Voc and is given by

$$\upsilon oc = \frac{q}{nkT} Voc$$

The PCE is equal to the ratio of maximum generated power to the incident power. Solar cells are tested and measured under Standard Test Conditions (STC), in which the incident light spectrum is AM1.5 and irradiance of 1000w/m2 [5].

III. METHODOLOGY

The GPVDM software was used to simulate the model. It's a free simulation tool for light harvesting devices that solves Poisson's equations to calculate the internal electrostatic potential. There's a detailed software manual available for reference [7].

A. Simulation parameters

The parameters used here are GPVDM built- in default parameters.

- 1^{st} / top P3HT: PCBM active layer parameters are shown in table 1.

TABLE 1

DEFAULT TOP P3HT: PCBM LAYER PARAMETERS

Parameters	**Values**
Electron trap density	1e24m-3eV-1
Hole trap density	1e24m-3eV-1
Electron tail slope	40e-3eV
Hole tail slope	40e-3eV
Electron mobility	2e-7m2V-1s-1
Hole mobility	2e-7m2V-1s-1
Relative permittivity	3.8au
Number of traps	20bands
Free electron to trapped electron	2e-20m-2
Trapped hole to free electron	1e-22m-2
Free hole to trapped hole	2e-20m-3
Effective density of free electron states	5e26m-3
Xi	3.8eV
Eg	1.1eV

- Interconnected layer (ICL) of metal/Au parameters are shown in table 2.

TABLE 2 ICL LAYER PARAMETERS

Parameters	**Values**
Electron trap density	1e24m-3eV-1
Hole trap density	1e24m-3eV-1
Electron tail slope	40e-3eV
Hole tail slope	40e-3eV
Electron mobility	2e-2m2V-1s-1

Hole mobility	2e-2m2V-1s-1
Relative permittivity	3au
Number of traps	5bands
Free electron to trapped electron	2e-20m-2
Trapped hole to free electron	1e-22m-2
Free hole to trapped hole	1e-22m-3
Effective density of free electron states	5e26m-3
Xi	4.2eV
Eg	1.1eV

- 2nd / bottom P3HT: PCBM active layer parameters are shown in table 3.

TABLE 3

DEFAULT BOTTOM P3HT: PCBM LAYER PARAMETERS

Parameters	**Values**
Electron trap density	1e24m-3eV-1
Hole trap density	1e24m-3eV-1
Electron tail slope	7.763936e-2eV
Hole tail slope	1.046922e-1eV
Electron mobility	2e-7m2V-1s-1
Hole mobility	2e-7m2V-1s-1
Relative permittivity	3au
Number of traps	5bands
Free electron to trapped electron	2e-20m-2
Trapped hole to free electron	1e-22m-2
Free hole to trapped hole	2e-20m-3
Effective density of free electron states	5e26m-3
Xi	3.8eV
Eg	1.1eV

B. Device Structure

In Figure 1, Tandem architecture is shown based on P3HT: PCBM solar cell.

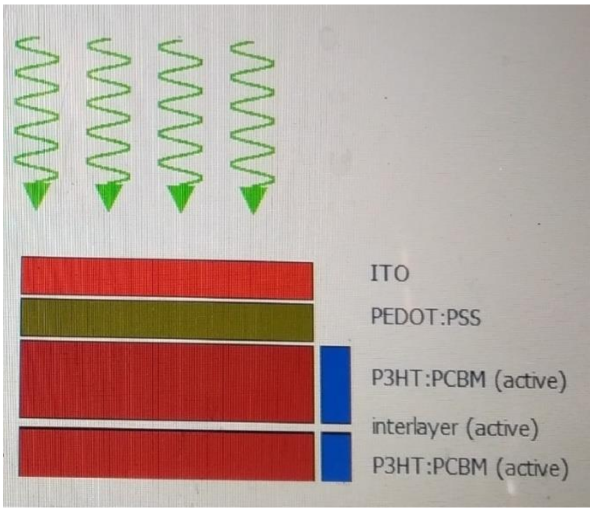

Fig. 1 Tandem structure of the studied solar cell

IV. SIMULATION

The simulation is based on study of effects of different layer thickness on Fill Factor (FF), Power Conversion Efficiency (PCE) and Maximum Power (MP). Initial default built- in layer thickness are given in table yields the J-V characteristic curve shown in Figure 2, in which FF is 0.64au, PCE is 11.34% and MP is 113.43watt.

TABLE 4

INITIAL VALUES OF LAYERS THICKNESS

Layer name	**Thickness value**
ITO	1e-7
PEDOT: PSS	1e-7
P3HT: PCBM	4e-7
Inerlayer (Au)/metal	5e-9
P3HT: PCBM	2e-7
Al/ metal	1e-7

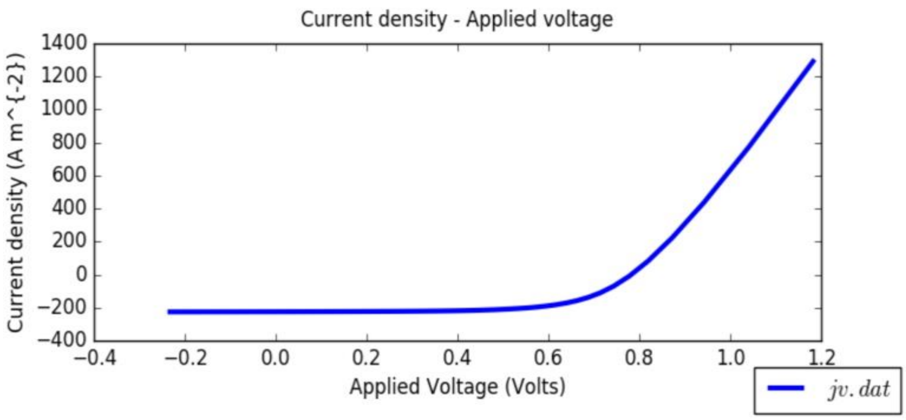

Fig. 2 J-V characteristic curves for initial thickness values

V. RESULTS AND DISCUSSIONS

The impacts of adjustments in active layers thickness based on P3HT: PCBM both top and bottom on PCE, FF & MP are shown in table 5.

TABLE 5

P3HT: PCBM LAYERS THICKNESS EFFECTS ON PCE, FF & MP

Top layer	Bottom layer	PCE (%)	FF (au)	MP (watt)
4.5e-7	1.5e-7	12.41	0.678	124.19
5e-7	1e-7	13.72	0.722	137.20
5.3e-7	8.8e-8	13.30	0.722	132.04
5.5e-7	8.6e-8	13.39	0.719	133.91
5.9e-7	8.2e-8	13.88	0.740	138.88
6.1e-7	8e-8	14.07	0.735	140.71
6.5e-7	7.6e-8	13.80	0.734	138.04
7.9e-7	6.1e-8	14.55	0.765	145.59
8e-7	4e-9	15.78	0.785	157.81

Next fix the both top & bottom active layers thickness on 8e-7 & 4e-9 respectively, and change the PEDOT: PSS layer thickness and obtain curves are shown in figures 3, 4 and 5.

TABLE 6

PEDOT: PSS LAYER THIKNESS EFFECTS

Layer thickness	**PCE (%)**	**FF (au)**	**MP (watt)**
1e-8	17.11	0.778	171.19
1.8e-8	17.07	o.778	170.78
2.6e-8	17	0.778	170.05
3.4e-8	16.36	0.782	163.77
8e-9	17.28	0.777	172.87
3e-9	17.70	0.775	177.08
8e-10	17.89	0.774	178.95

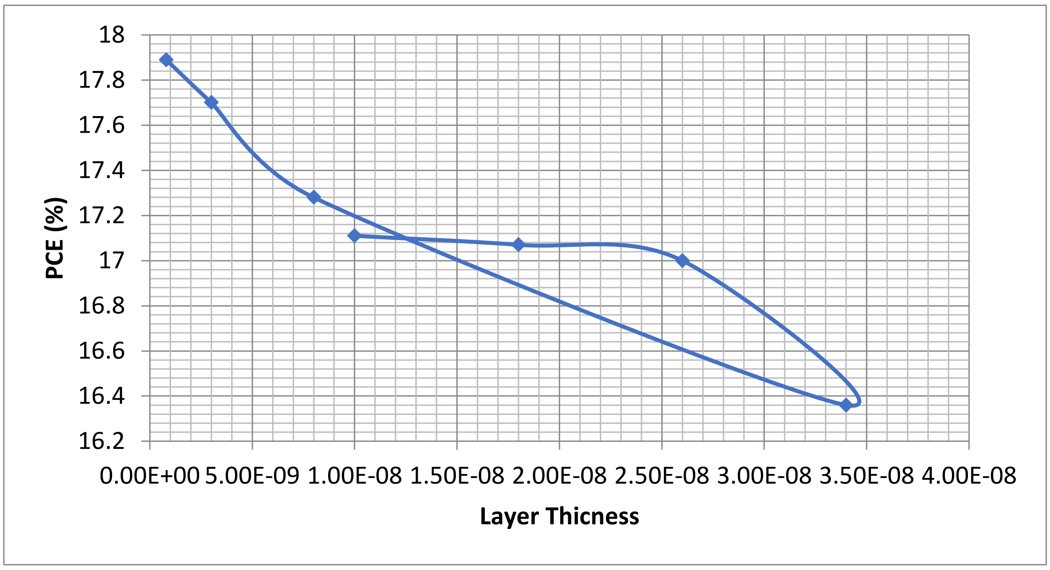

Fig. 3 Plot of PCE with respect to Layer thickness

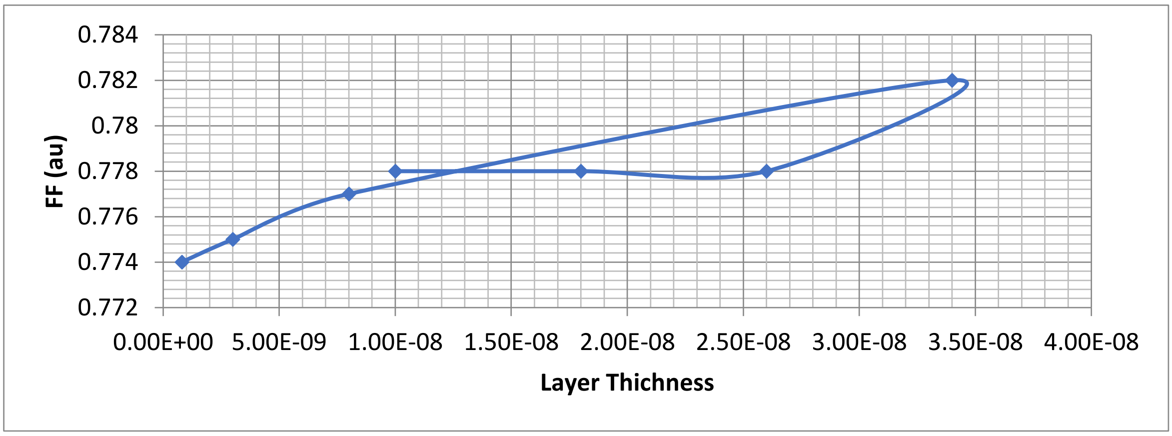

Fig. 4 Graphic variations of FF with respect to layer thickness

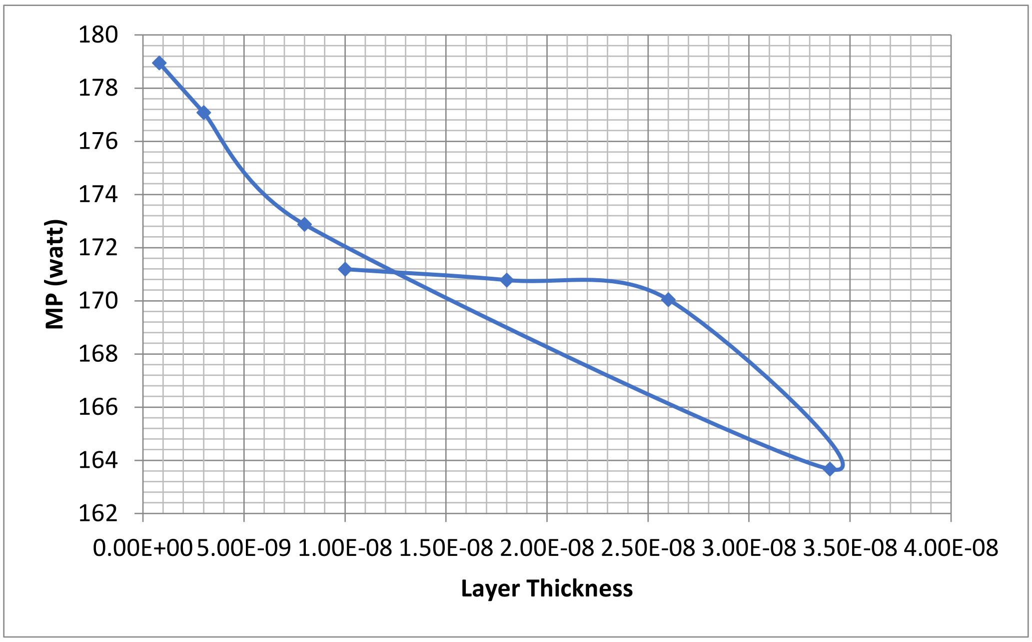

Fig.5 Graph represents variations in MP with respect to layer thickness

Fix the PDOT: PSS layer thickness on 8e-10, effects of ITO based layer thickness variations on PCE, FF and MP are shown in table 7.

TABLE 7

Effects of ITO based layer thickness

Layer thickness	**PCE (%)**	**FF (au)**	**MP (watt)**
8e-9	18.90	0.770	189.08
9e-9	18.80	0.770	188.06
1e-8	18.70	0.771	187.03

The result is presented different layer thickness impacts on PCE, FF & MP for a P3HT: PCBM based tandem solar cell where we saw that PCE had been increased from 11.34% of initial parameters to 18.90% with optimized parameters.

The J-V characteristic curve for optimized layers thickness parameter is shown in Figure 6.

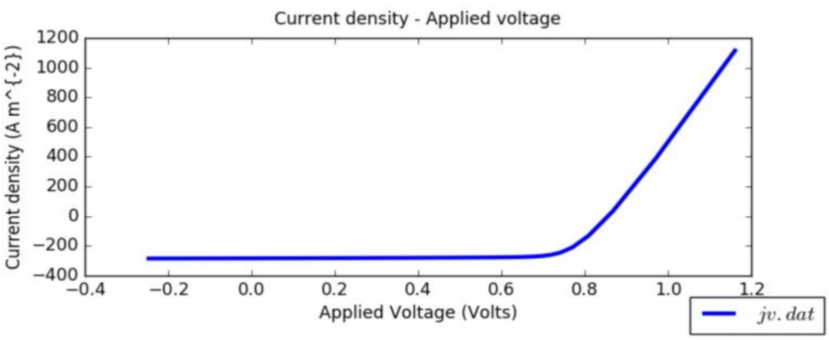

Fig.6 J-V characteristics curve for optimized layer thickness

VI. CONCLUSIONS

The GPVDM simulation software was used to analyze the Tandem solar cell's PCE, FF, and MP. The results showed that adjusting the thickness of different layers in a well-coordinated manner led to a significant increase in PCE and MP. By adjusting the thickness of the P3HT: PBCM-based layers, the PCE reached an impressive 15.78%. By maintaining the optimal thickness of both the P3HT: PCBM-based layers and the ITO & PEDOT: PSS-based layers, the Tandem solar cell achieved its maximum PCE milestone. To further enhance the PCE, it is possible to set and optimize the band gaps (Eg) of the P3HT: PCBM-based active layers. For example, by setting the top P3HT: PCBM-based active layer's Eg to 1.5, while keeping the other parameters at their default values and the layer thicknesses at their optimal levels, the Tandem solar cell achieved an impressive PCE milestone of 28.49% with an FF less than 1. This achievement represents the highest PCE ever reported in reference [2].

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