

OPTO-ELECTRO SIMULATION OF ORGANIC SOLAR CELL AT DIFFERENT ACTIVE LAYER THICKNESS AND CHARGE CARRIERS MOBILITY BASED ON P3HT: PCBM MATERIALS

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Abstract: *In this research work, bulk heterojunction organic solar cell is simulated optically and electrically at different active layer thickness and different hole mobility by GPVDM software. Organic bulk heterojunction solar cell consists of mixture of P3HT and PCBM as active layer material, ITO is a transparent electrode, PEDOT: PSS is an electron blocking layer and Al a back electrode. In this study, the optical simulation has been done at different active layer thickness i.e. 180 nm, 200 nm and 220 nm, and electrical simulation at different hole mobility $1 \times 10^{-4} \text{cm}^2/\text{Vs}$, $1 \times 10^{-5} \text{cm}^2/\text{Vs}$, $1 \times 10^{-6} \text{cm}^2/\text{Vs}$ and $1 \times 10^{-7} \text{cm}^2/\text{Vs}$ respectively. It is observed that current-voltage (j-v) characteristics are affected by the hole mobility. The best current-voltage (j-v) characteristic is obtained at $1 \times 10^{-6} \text{cm}^2/\text{Vs}$ mobility and the best absorption at 200 nm. It is concluded that in the organic BHJ solar cell the efficiency increases, when mobility decreases (from 10^{-4} to 10^{-6}) where as above 10^{-7} mobility, the efficiency further decreases. If the mobility is increased from $1 \times 10^{-5} \text{cm}^2/\text{Vs}$ the dissociation probability is increased and will be maximum at $1 \times 10^{-6} \text{cm}^2/\text{Vs}$, and again increase the mobility the dissociation will not further increase and efficiency is decrease.*

Key words: GPVDM software, carrier mobility, bulk heterojunction, organic solar cell

1. INTRODUCTION

Solar cell or photovoltaic cell is the optical device that converts sun radiation to electricity. The green plant does some similar work, the convert sun light to chemical energy so a group of solar cells so called organic solar cells. The sun supplies us a clean and unlimited resource of energy and help us relieve the energy crises and world pollution. Organic solar cells based on conjugate polymers are much promising for a cheap and flexible alternative to inorganic solar cells. Today several solar cell technologies exist in which organic solar cells are one of the newer classes of technologies.

Organic solar cell (OSC) devices attract more and more interest in last few years.

These devices yield an energy conversion efficiency of around 6% to 7% for single junction cell [1] as well as tandem cells [2]. This is much less compared to already accepted silicon photovoltaic devices, which has efficiency above 20%. But organic photovoltaic (OPV) devices have several advantages like, flexible substrates, the possibility of low cost production [3], room temperature processing and thin film structure. Organic solar cells consist of a mixture of polymer P3HT (donor) and PCBM (acceptor) as the photoactive layer. In bulk-heterojunction (BHJ) organic solar cells, the absorbed incident photons generate tightly bound electron-hole pairs, which can dissociate into (charge carrier) electrons and holes at the nearby donor/acceptor interface. The electrons and holes are then transported to their respective electrodes [4-6]. Research efforts in the last decade have significantly improved organic solar cell performance [7-12] and power conversion efficiency (PCE) values better than 10% have recently been achieved [13-14]. Over the years, significant research efforts have been performed at developing low band gap polymers to extends absorption and harvest more solar energy for which the more short circuit current can be produced.

In ITO/PEDOT: PSS/P3HT: PCBM/Al organic bulk heterojunction solar cells, P3HT (3-hexyl thiophene) is an electron donor material that effectively transports positive holes, PCBM ([6, 6]-phenyl C₆₁-butyric acid methyl ester) is an electron acceptor materials. It effectively transports electrons from molecule to molecule. The ITO (Indium Tin Oxide) film is used as a transparent electrode. Since, it has high transmittance in visible region and capacity of good conduction. PEDOT: PSS or poly (3, 4-ethylenedioxythiophene) poly (styrene sulfonate) is an hole transportation layer. PEDOT: PSS may be used as buffer layers between the transparent electrodes and active layer of materials to block the electron and hole transfer in the wrong direction. In this study we present optical and electrical stimulation of bulk heterojunction (BHJ) solar cell using GPVDM software at different active layer thickness. The main advantage of the bulk heterojunction solar cell is that most of generated excitons reach a nearby donor-acceptor interface, where they associated into free charge carriers [24].

These efficient Excitons harvesting lead to higher power conversion efficiencies for BHJ solar cell. The organic solar cell has two competing process, extraction and recombination of the charge carriers, both process are conducted by the mobility of charge carrier. As increase charge carrier mobility would a positive effect on transport, facilitating extraction, but on other hand it increase the recombination.

1.1 Bulk Heterojunction Structure and Charge Carriers Generation

Bulk heterojunction is a mixture of interpenetrating mixture of electron donor and

electron acceptor conjugated organic materials that allows absorption of light, the generation of charge carriers (excitons), splitting of excitons at donor-acceptor interface, and transport of positive and negative charges to opposite electrodes. Bulk heterojunction (BHJ) are mostly generated by forming the two conjugate polymers, casting and then allowing separating the two phases, usually with the help of annealing process. The two conjugate polymers will self-assembled into an interpenetrating network connecting the two electrodes [15]. The structure of bulk heterojunction solar cell is shown in fig.1.

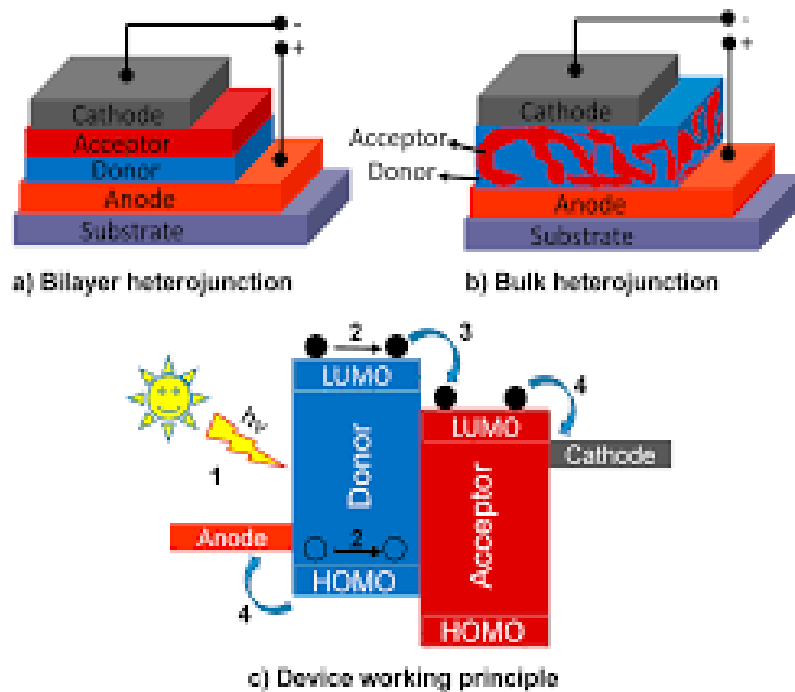


Fig.1 Bulk Heterojunction solar cell

After the capture of a photon, electron move to the acceptor domains, then are carried through the device and collected by the one electrode and holes moves in opposite direction and collected at other side. If the dispersion of the two materials is very much larger, it will result in poor charge transfer through the active layer. In charge transfer, both donors and acceptor contribute to the generation of charge carriers.

Organic solar cells produce natural mobile excitons after absorption of light. In order to separate the excitons into free charge carriers a donor- acceptor system must be employed [16]. When the excitons reaches the donor/ acceptor interface the electron will transfer to the material with lager electron affinity and the hole will be accepted by the material with the lower ionization potential. Due to the lower excitons diffusion lengths to 1-10 nm in polymeric materials [17-18] a simple bilayer structure will result in low efficiencies, since only photons absorbed within this distance from D/A interface

will contribute to the device current[19]. An increase in the generated photo current can be achieved by employing an interpenetrating network of donor and acceptor materials [20-21]. Ideally in bulk-heterojunction (BHJ), all absorbed photons will be in the vicinity of donor acceptor interface and these can be contributing to the generated photocurrent.

2. SIMULATIONS

2.1 Electrical Simulation

Bulk heterojunction solar cell ITO/PEDOT: PSS/P3HT: PCBM/Al is simulated by the GPVDM software at different series resistance of the device. GPVDM software is specifically designed to simulate bulk heterojunction organic solar cells, such as those based on the P3HT: PCBM materials. The model contains both an electrical and optical

properties, enabling both current- voltage characteristics to be simulated as well as optical properties [22-23]. The electrical model only covers the active layer of the device. In this model, there are two type's of charge carrier electrons (holes), free electrons (holes) and trapped electrons (holes). Free electrons (holes) have a finite mobility of $\mu_e^o(\mu_h^o)$ and trapped electrons (holes) cannot move at all and have a mobility of zero. To evaluate the average mobility we take the ratio of free to trapped carriers and multiply it by the free carrier mobility.

$$\mu_e(n) = \frac{\mu_e^o n_{free}}{n_{free} + n_{trap}} \quad (1)$$

Thus if all carriers were free the average mobility would be μ_e^o and if all carriers were trapped the average mobility would be zero. It should be noted that only $\mu_e^o(\mu_h^o)$ are used in the model for computation and using $\mu_e(n)$ is an output parameter. The electrical simulation window is shown in fig 2.

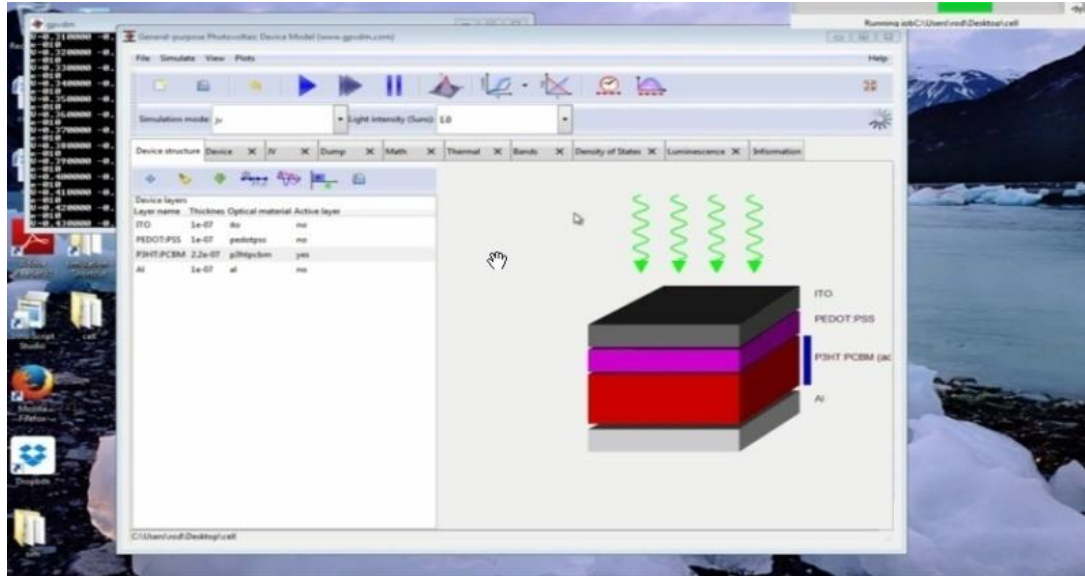


Fig.2. Electrical simulation window

2.2 Optical simulation

Bulk heterojunction solar cell ITO/PEDOT: PSS/P3HT: PCBM/Al is simulated by the GPVDM software at different active layer thickness. GPVDM software is specifically designed to simulate bulk heterojunction organic solar cells, such as those based on the P3HT: PCBM material. The model contains both an electrical and optical properties of the solar cell; accredit both current-voltage characteristics to be simulated as well as optical properties.

GPVDM is consisting of both an electrical and optical model. The optical model simulation usually includes the glass substrate, the contacts and layers such as PEDOT: PSS. The electrical simulation usually only cover, the active layer of the device, thus a typically optical simulation is much bigger than electrical simulation window. The optical model feeds the calculated optical profile of the light into the electrical simulation. Therefore, it described the optical model which can process the optical simulation and it also represents the active layer. This is done by placing a 'yes' in column (active layer) in the figure 3.

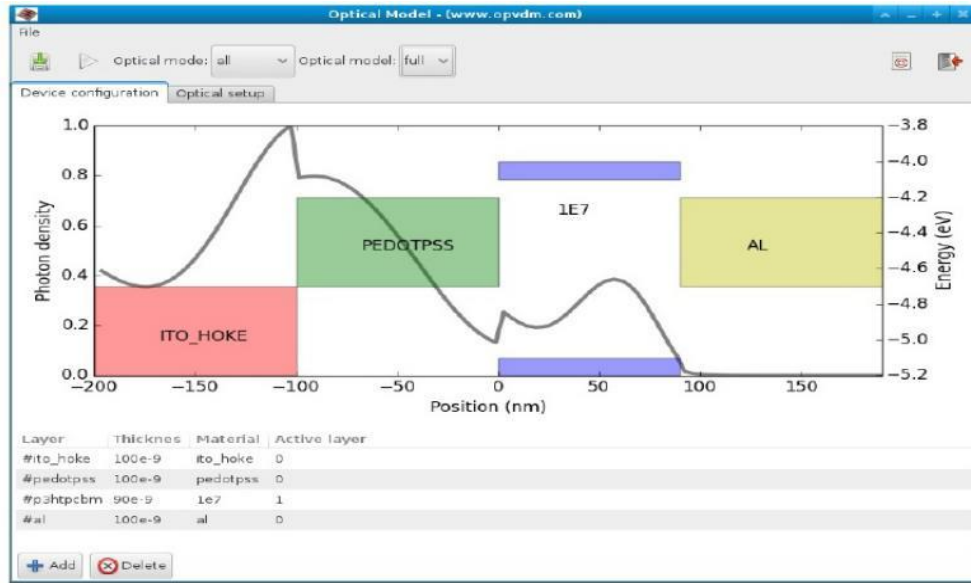


Fig.3: Optical Simulation Window

3. RESULT AND DISCUSSION

In this paper ITO/PEDOT: PSS/P3HT: PCBM/Al bulk heterojunction solar cells are designed by the GPVDM software to study the optical properties. The absorption of P3HT: PCBM active layer are more effective for the wavelength from 350nm to 750nm. The optical simulation (wavelength 150-750

nm) is made at different active layer thickness, ITO thickness 20nm, PEDOT: PSS thickness 20 nm, Al thickness 20nm and the active layer thickness are 180nm, 200nm, 220nm, and the absorptions at different active layer thickness are shown in the figures 4 a, b and c.

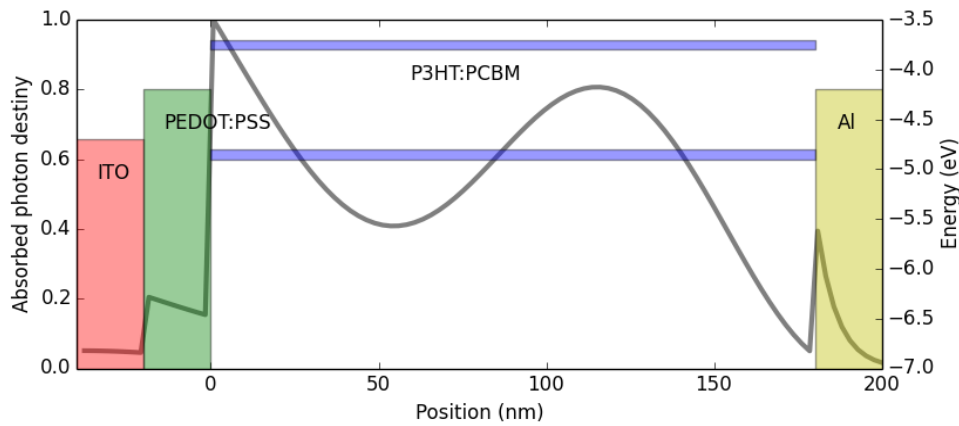


Fig. 4a. Active layer thickness 180 nm

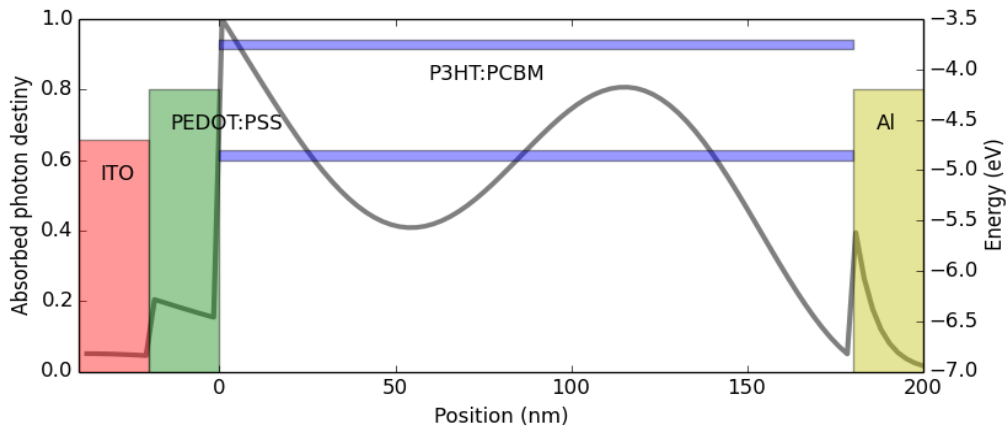


Fig. 4b. Active layer thickness 200 nm

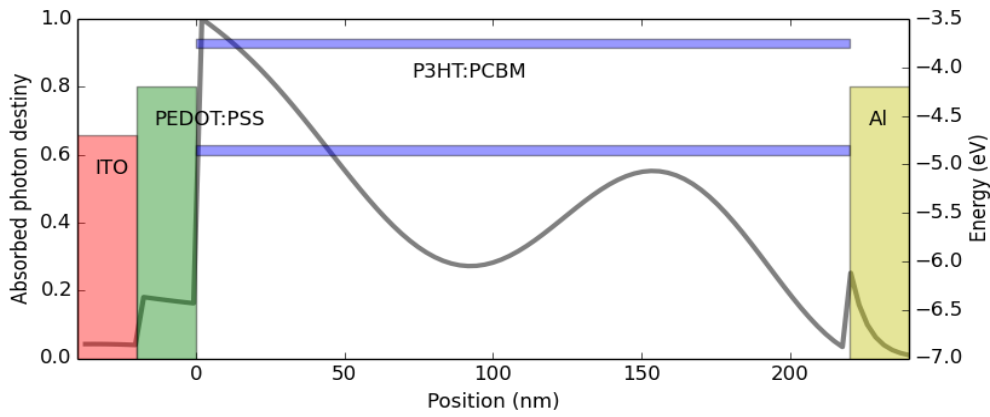


Fig. 4c. Active layer thickness 220 nm

Illumination current-voltage characteristics are simulated at different hole mobility, $1 \times 10^{-4} \text{cm}^2/\text{Vs}$, $1 \times 10^{-5} \text{cm}^2/\text{Vs}$, $1 \times 10^{-6} \text{cm}^2/\text{Vs}$ and $1 \times 10^{-7} \text{cm}^2/\text{Vs}$, which is shown in figure 5. It is clear from the

current-voltage characteristic curves that the short current density is maximum at $1 \times 10^{-6} \text{cm}^2/\text{Vs}$ and minimum at $1 \times 10^{-4} \text{cm}^2/\text{Vs}$.

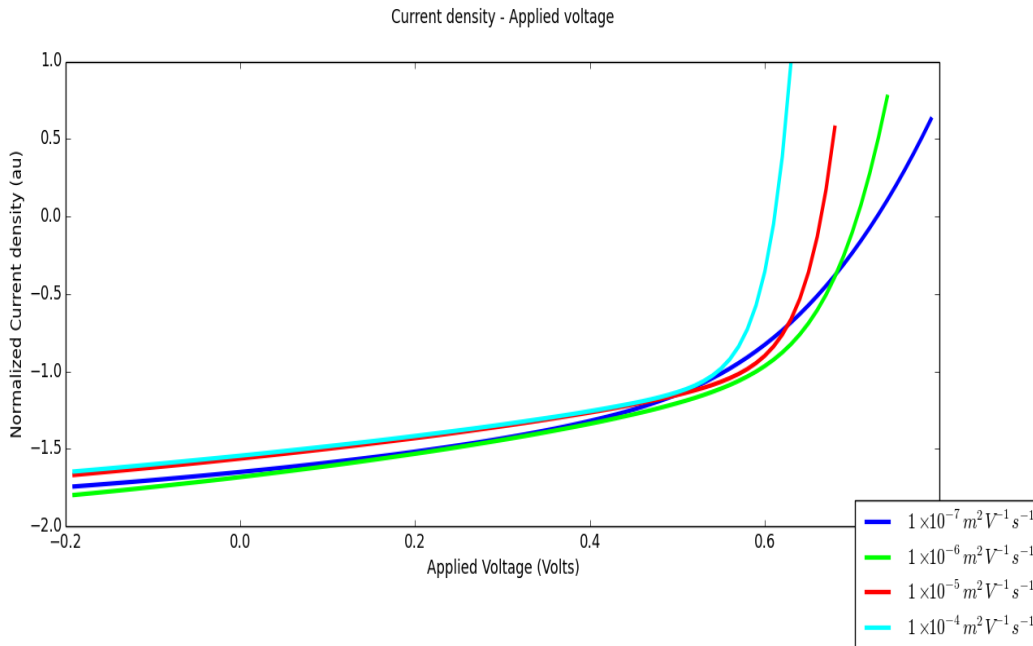


Fig. 5. Current Voltage characteristics at different hole mobility

It is clear from the curves that in organic BHJ solar cell the efficiency increases when mobility decreases (from 10^{-4} to 10^{-6}). Above 10^{-7} , the efficiency further decreases. The increased recombination of electron-hole pair and reduce dissociation efficiency, decrease efficiency whereas the loss in open circuit voltage at higher carrier mobility is responsible for the decrease of efficiency. If the mobility is increased from $1 \times 10^{-5} \text{cm}^2/\text{Vs}$ the dissociation probability is increased and will be maximum at $1 \times 10^{-6} \text{cm}^2/\text{Vs}$, and again increase the mobility the dissociation will not further increase and efficiency is decrease. It is clear that the solar cell is more efficient at definite mobility range.

4. CONCLUSIONS

In this work, we have presented optical and electrical simulation of the P3HT: PCBM based bulk heterojunction solar cell for different active layer thickness. The absorption pattern of the active layer

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of organic solar cell varies with thickness. At thickness 200 nm we get absorption peaks near the electrodes at which the maximum absorption take place. The short circuit current is affected by the electron and hole mobility and maximum short circuit current obtained at $1 \times 10^{-6} \text{cm}^2/\text{Vs}$. Thus by changing the active layer thickness and mobility the effective absorption and efficiency of P3HT: PCBM based solar cells can be optimized.

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