Optical Simulation of Organic Photovoltaic Device

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***Abstract* - The bulk heterojunction organic photovoltaic device (solar cell) has been optically simulated by OPVDM software at different active layer thickness. Organic bulk heterojunction photovoltaic device consists of mixture of P3HT and PCBM as active layer materials, ITO is a transparent electrode, PEDOT:PSS is electron blocking layer and Al is a back electrode. In this study the optical simulation has been done (wavelength 150-750 nm) at different active layer thickness 160 nm, 180 nm, 200 nm, 220 nm, and 240 nm respectively. We observed that absorption is affected by the thickness of active layer and the best absorption is obtained at the thickness of 180nm and 200 nm.**

Keywords: Organic photovoltaic device, Optical simulation, Bulk heterojunction, Organic Photovoltaic device model software.

I. INTRODUCTION:

Organic photovoltaic (OPV) devices attract more and more interest in last few years. OPV 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 established silicon photovoltaic devices which has efficiency above 20%. But OPV devices have several advantages like, flexible substrates, the possibility of low cost production [3], room temperature processing and thin film structure. OPV's can be classified into the planar heterojunction devices, where donor and acceptor materials are deposited one after the other and bulk heterojunction (BHJ) devices where two organic materials are diluted in the same solvent and spin coated as one layer. Organic photovoltaic's based on bulk heterojunction (BHJ) composites of conjugate polymers P3HT: PCBM have shown rapid improvement in the past few years [4-5]. The main advantage of the BHJ structure is that most of the generated excitons reach a nearby donor acceptor interface where they are dissociated into electrons and holes. This efficient exciton harvesting gives higher power conversion efficiencies for BHJ devices. The dark J-V characteristics of heterojunction solar cell are affected by active layer thickness [6].

Numerical models for organic bulk heterojunction (BHJ) devices allow for device structure optimization. Simulation of OPV devices can be divided into two parts, firstly there is a coupling of light into a multilayer structure which needs optical model and secondly the extraction of charges which needs an electrical model. The absorption of light within the multilayer structure is crucial process and thus one main area is numerical simulation. Optical modeling has also been performed on classical solid state semiconductor solar cells and modules where angular dependent light trapping by multiple internal reflections through surface texturing has to be taken into account [7-14]. Lacic et al. [15] uses analytical models and compares them to measured photocurrent spectra. Transfer matrix formalism has been used by Kotlarski et al. [16], to calculate the absorbed optical energy within the multilayer structure. This formalism is widely used to optimize layer structure for single junction [17] as well as tandem cells [18]. Here we operated optical simulation of bulk heterojunction (BHJ) solar cell using OPVDM (Organic photovoltaic device model) software at different active layer thickness.

II. BULK HETEROJUNCTION STRUCTURE

Bulk heterojunction is a mixture of interpenetrating mixture of electron donor and electron acceptor conjugated polymers that allows absorption of light, the generation of excitons, splitting of excitons at donor-acceptor interface, and transport of positive and negative charges to opposite electrodes.

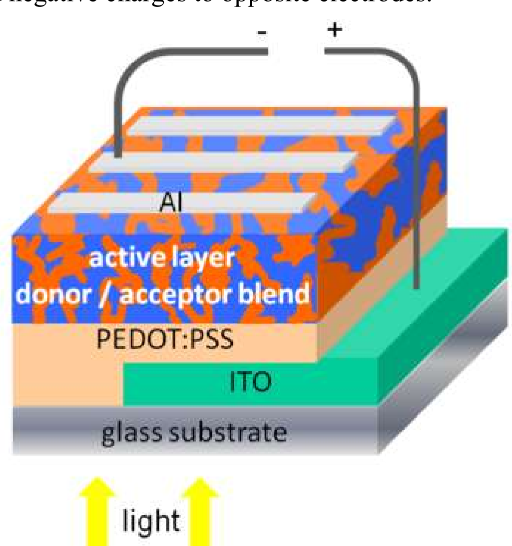

Figure 1. Bulk Heterojunction solar cell

Bulk heterojunction (BHJ) are mostly created by forming a containing 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 [19]. The structure of bulk heterojunction solar cell is shown in figure 1. After the capture of a photon, electron move to the acceptor domains, then 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 large, it will result in poor charge transfer through the layer. In charge transfer, both donors contribute to the generation of charge carriers

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 C_{61}-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 ability of good conduction. PEDOT:PSS or poly (3,4-ethylene dioxy thio phene) poly (styrenesulfonate) is an electron blocking layer. PEDOT:PSS may be used as buffer layers between the transparent electrodes and active layer to block the electron and hole transfer in the wrong direction.

III. OPTICAL SIMULATION

Bulk heterojunction solar cell ITO/PEDOT: PSS/ P3HT: PCBM/Al is simulated by the OPVDM software at different active layer thickness. OPVDM 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, enabling both current- voltage characteristics to be simulated as well as optical properties. The optical model simulation usually includes the glass substrate, the contacts and layers such as PEDOT: PSS. The electrical simulation usually only carriers, 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. We must therefore explain the optical model, which layer in the optical simulation represents the active layer. This is done by placing a ‘yes’ in column (active layer) in the figure 2.

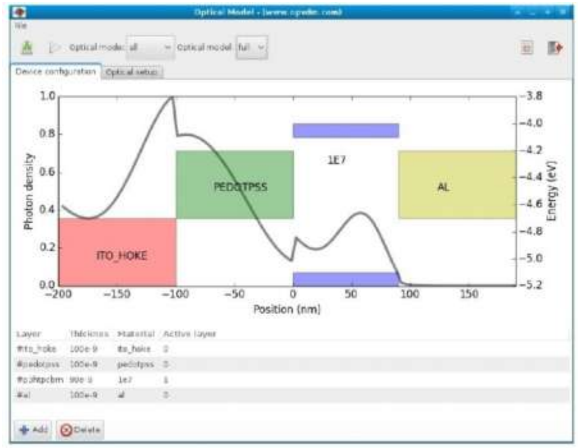

Figure 2. Optical Simulation Window

IV. RESULT AND DISCUSSION

In this paper, we have studied the optical properties of ITO/PEDOT: PSS/P3HT: PCBM/Al bulk heterojunction solar cell, which is designed by the OPVDM software. It is found from the result that 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 160nm, 180nm, 200nm, 220nm, and 240nm. The absorptions at different active layer thickness are shown in the figures 3-7.

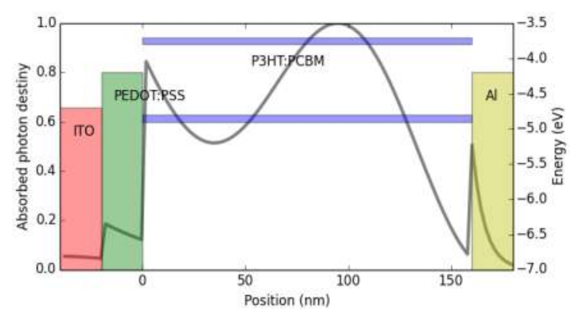

Figure 3. Active Layer Thickness 160 nm

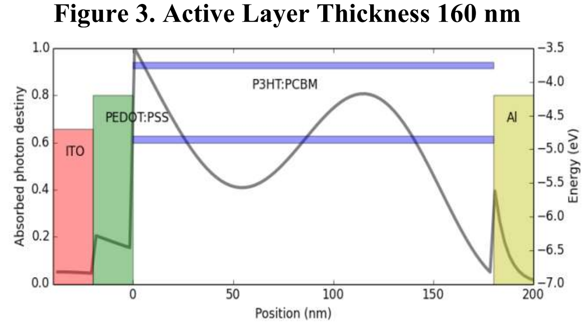

Figure 4. Active Layer Thickness 180 nm

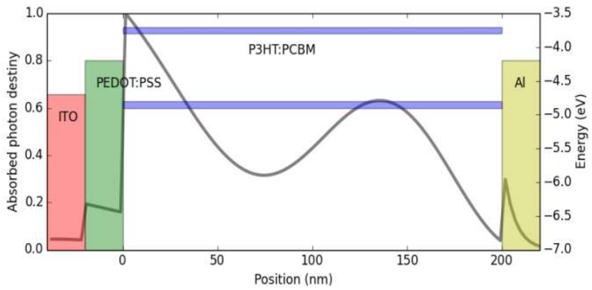

Figure 5. Active Layer Thickness 200 nm

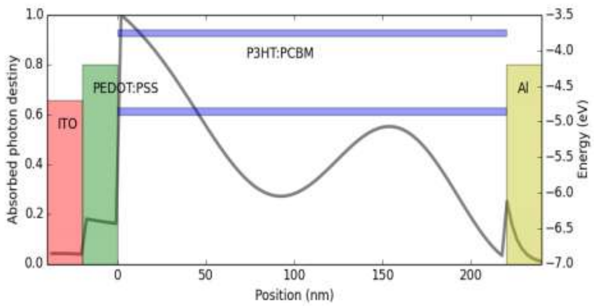

Figure 6. Active Layer Thickness 220 nm

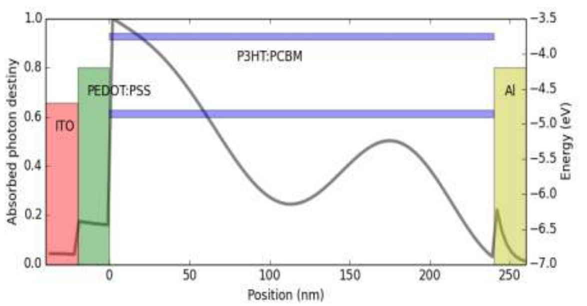

Figure 7. Active Layer Thickness 240 nm

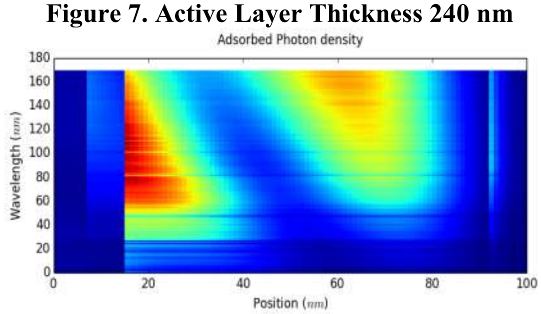

Figure 8. Absorbed Photon distribution at thickness 200 nm

The absorbed photon distribution at 200 nm is shown in figure 8. The best absorption is obtained at the thickness 180 nm and 200 nm and the absorption of photons is maximum near the electrode and the reflection is minimum near the electrode and maximum at the middle of the active layer. As we vary the thickness of active layer of bulk heterojunction solar cell. We found different absorption patterns, below 180 nm thickness; an absorption peak is obtained at the middle of the active layer. As the thickness increased the absorption peak moves towards the electrodes. At 200 nm thickness absorption peaks are obtained near the electrodes (ITO and Al). Above the 200nm thickness, the absorption peak decreases towards the Al electrode. It is concluded that at 180nm and 200nm more photons are absorbed by the active layer nearer the electrodes and more excitons are generated nearer the electrodes. Due to low mobility of the charge carriers in organic solar cell, it is difficult for the carriers dissociated from the middle of the active layer to diffuse to the electrode. Therefore, the electron-hole pairs dissociated in the active layer nearer to electrode contribute to the effective absorption. For electron-hole pairs generated in the middle of the active layer, electrons or holes must travel a long distance to reach electrodes which are mostly difficult. The photo-generated carriers' width short distance to electrodes can be collected effectively. Facilitating hole collection from donor towards device anode improves the photovoltaic response [20].

V. CONCLUSION

In this study, we have presented optical simulation of the P3HT: PCBM based bulk heterojunction solar cell. For different active layer thickness, the absorption pattern of the active layer of organic solar cell varies with thickness. At 200 nm we get absorption peaks near the electrodes. Thus by tuning the active layer thickness, the effective absorption of P3HT : PCBM based solar cells can be optimized.

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