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Optical Simulation Study on Indoor Organic Photovoltaics with Textured Electrodes towards Self-powered Photodetector

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Abstract

In this work, we performed an optical simulation study on the performance of a PMDPP3T:PCBM based on an organic photovoltaic (PV) device. The virtual PV device was developed in Lumerical, finite-difference time-domain (FDTD) solutions. Different layers of the PV cell have been defined through the incorporation of complex refractive index value of those layers' constituent materials. During the simulation study, the effect of the variation active layer thickness on an ideal short circuit current density ($J_{sc,\ ideal}$) of the PV cell has been, first, observed. Thereafter, we have investigated the impact of surface roughness of a transparent conducting oxide (TCO) electrode on $J_{sc,ideal}$ of the PV cells. From this simulation, it has been observed that the $J_{sc,ideal}$ value of the PV cell is strongly dependent on the thickness of its active layer and the photon absorption of the PV cell has gradually decreased with the increment of the TCO's surface roughness. As a result, the capability of the PV device has been reduced with the increment of the surface roughness of the TCO.

Keywords: Organic PV cell, Active layer thickness, Transparent conductive oxide (TCO), Surface roughness, FDTD, Optical modelin

1. INTRODUCTION

Nowadays, organic material based PV cell has tremendously attracted the attention of researches in the field of light energy harvesting technology due to its good mechanical flexibility, large coverage area, low cost and easy fabrication[1,2]. For the last twenty years, various organic semiconductor based photovoltaic (PV) cells have been developed and studied in order to design a superior organic photovoltaic (OPV) device with better life time, environmental stability and power conversion efficiency (PCE) [3]. From the literature survey it is found that, presently, the OPV cell has a very small market share as OPV exhibits lower PCE value than the widely used inorganic PV device for operating under 1-sun conditions [4]. Interestingly, the scenario as a whole has been changing, when the comparison is made under an indoor light condition. Recently, it has been observed that the OPVs have exhibited a better performance level than inorganic PV cells under a low intensity illumination of indoor light generated from different sources, such as light emitting diode (LED), fluorescent lamp (CFL), halogen bulbs, etc. due to their higher absorption coefficient and better spectral matching between absorption spectra of the organic active material of OPV and emission spectra of light sources [5,6]. In addition, the indoor light energy harvesting technique is gradually becoming attractive towards the researchers due to its promising application as a local power source with low power (μW) consumption of new generation indoor electronic applications [7]. Besides the good performance levels in the indoor environments, OPV have more attractive properties, such as low weight, small size and good mechanical flexibility, These are good benefits for indoor applications. For the last few years, therefore, scientists have been trying to fabricate different types of organic material based indoor photovoltaic (IPV) cells with better applicability with the development of various organic semiconductors, processing techniques, device architecture, and device fabrication techniques [8-12]. It is a well-known fact that the interaction between different layers of a PV cell plays a very crucial role during its operation; therefore, the surface properties of each layer should have significant effect on the overall performance of the PV device. Regarding this assumption, the PV device simulation study, by using standard optical modeling techniques, can be a very useful and energy saving approach to quantify the effect of different device's parameters, such as active layer thickness and different layer

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surface roughness, on the performance of the PV device [13,14].

In this work, therefore, we used Lumerical FDTD solution software to perform a systematic PV device simulation to realize the effects of the active layer thickness and surface roughness of TCO electrode on the overall performance of a PMDPP3T:PCBM based OPV [13] device in an indoor environment.

2. EXPERIMENTAL

2.1 Device Configuration

For the simulation study, we constructed a virtual PV device (Fig. 1) in TCDA platform of the Lumerical, FDTD software. In the device, TCO has been used as the top electrode (100 nm thickness). We have also considered a hole transport layer (HTL) of approximately 10 nm thickness around 10 nm, formed by poly (3, 4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT: PSS). The active layer of the PV cell is made of poly[[2,5-bis(2-hexyldecyl)-2,3,5,6-tetrahydro-3,6dioxopyrrolo[3,4c] pyrrole-1,4-diyl]-alt-[3′,3″-dimethyl2,2′:5′,2″terthiophene]-5,5″-diyl] (PMDPP3T:PCBM). To study the variation of the PV device's performance with the active layer thickness, we have used various values of thickness of the active layer ranging from 20 nm to 400 nm. In this work, we tried to identify the effect of the surface roughness of the TCO electrode on the overall performance of the PV cell.

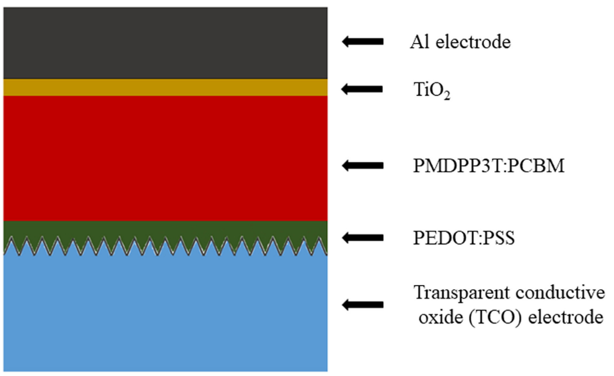

Fig. 1. Schematic diagram of the PV cell constructed for the simulation study.

For this purpose, we have considered that the electrode contained triangle ridges in which the size of the base was 20 nm. Furthermore, we have varied the height of those ridges to generate variable surface roughness in the electrode. The root mean square (RMS) value of the TCO electrode's surface roughness has been estimated through the following relation [15]:

$$R_{RMS} = \sqrt{\frac{\Sigma(z_i - z_{avg})^2}{n}} \tag{1}$$

where z_i, is the height of individual triangle ridge, z_{avg} is the average value of the all ridges and n is the number of the ridges. In this work, we have considered 10 different heights of the triangular ridge: 2, 5, 7, 10, 12, 15, 17, 20, 22, and 25 nm, and the calculated RMS values were 0.57764, 1.44, 2.021, 2.88, 3.465, 4.33, 4.9, 5.776, 6.35 and 7.22 nm, respectively.

2.2 Simulation Procedure

The 2-dimensional optical simulation study on the PV device was performed through the Lumerical, FDTD software. The different layers of the device have been defined by their complex refractive index value, which had been collected from previous studies [13]. Furthermore, we have meshed the device structure at a minimum mesh density value, above which no effect on the simulation results was observed. Through this simulation technique, the distribution of the photo generated electric field due to the light absorption within the PV structure has been estimated. This estimation was further employed to estimate the photo-generated ideal short-circuit current density ($J_{sc,ideal}$) value of the PV device. It has been assumed that the internal quantum efficiency (IQE) of the device is 100 % [16]. Furthermore, the light travelling through the PV device at 90° to the TCO electrode has also been considered. We have also set periodic boundaries along the x-axis. In this work, the device simulation was performed for two different light sources, one is an AM1.5G, i.e., 1-sun condition and the other is a 1000 lx white LED.

3. RESULTS AND DISCUSSION

In our previous work [17], we have observed that the $J_{sc,ideal}$ value of an organic PV cell (P3HT:ICBA based) is strongly dependent to the active layer thickness. In this work, therefore, we have, first, performed a simulation study on the PV device of different active layer thickness. Afterwards, we have repeated the same procedure for different surface roughness values of TCO.

The simulated $J_{sc,ideal}$ value of our PMDPP3T:PCBM based PV device (operating under the illumination of a 1000 lx white LED) had different active layer thickness and TCO electrode surface roughness, which are depicted in the Fig. 2. Here, it is noted that the simulated $J_{sc,ideal}$ of the PV cell, for a particular amount of roughness in TCO surface is gradually increasing with the active

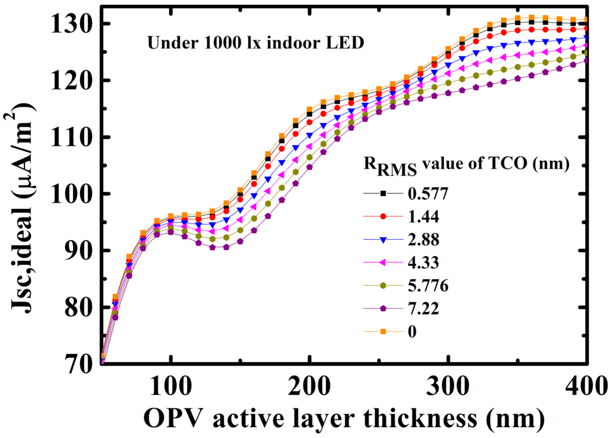

Fig. 2. Variation of simulated $J_{sc,ideal}$ value of the PV device, with active layer thickness and TCO electrode surface roughness, operated under the illumination of 1000 Lux white LED

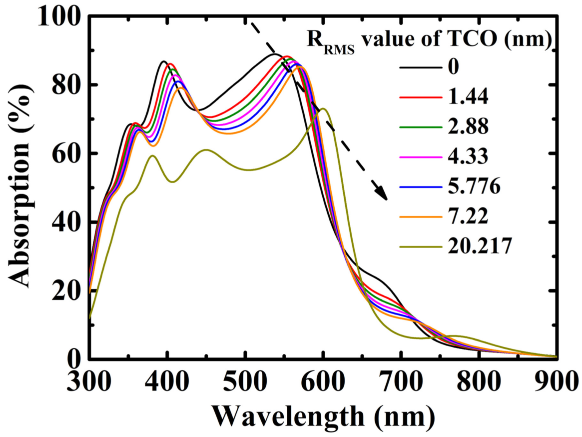

Fig. 4. Variation of simulated absorption ability of the active layer, with the surface roughness of the TCO electrode.

layer's thickness and the trend of variation is same for all TCO surface roughness values. The thicker active layer was able to absorb more photon than the thinner one, therefore, the $J_{sc,ideal}$ of the PV cell indicates a growing trend with active layer thickness.

For further investigation, we have compared the simulated $J_{sc,ideal}$ value of the PV cell, having an active layer of fixed thickness (400 nm) for different R_{RMS} of TCO electrode (Fig. 3). Here we have performed the simulation study for two different light sources (1-sun and 1000 lx white LED). From Fig. 3 it can be observed that, $J_{sc,ideal}$ of the PV cell is gradually decreasing with R_{RMS} of TCO and the trend is independent from the nature of light source. To identify the reason behind this phenomenon, we have further simulated the absorption value of the active layer (400 nm) in the wavelength range of 300 nm to 900 nm for different R_{RMS} of TCO (Fig.4). In Fig. 4, it is observed that the photon absorption capability of the PV cell's active layer is gradually decreasing with the surface roughness of the TCO electrode.

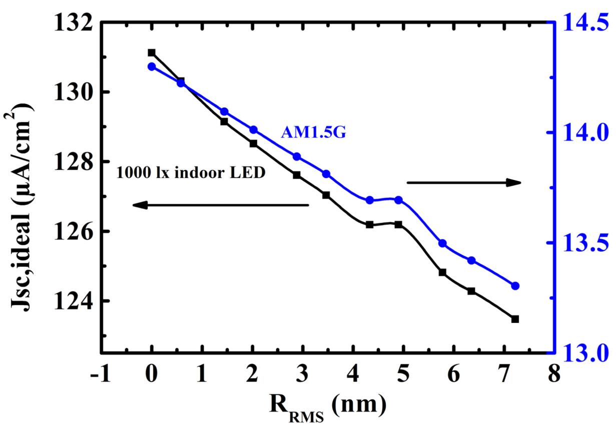

Fig. 3. Variation of simulated $J_{sc,ideal}$ value of PV device with the surface roughness of the TCO electrode.

This may be attributed to the decrement of photon induced $J_{sc,ideal}$ value of the PV cell with the increase of surface roughness of its TCO electrode.

In addition, it is observed in Fig. 4 that, the absorption edge of the PV device is gradually shifted towards the infrared region with the increase of TCO surface roughness. From this result, it is clear that the position of the absorption edge of a PV device can be controlled by varying the surface roughness of the TCO electrode. Therefore, If we can, design a PV device with an organic active material that have an absorption edge near the infrared region (have lower band gap), we may control the position of the absorption edge of the PV device by changing its TCO electrode surface roughness. Although the device would have lower power conversion efficiency due to a lower $J_{sc,ideal}$, it could be utilized as an infrared photo sensor device.

4. CONCLUSIONS

In this work the overall performance level of a PMDPP3T: PCBM based single celled organic photovoltaic (OPV) device has been realized through an optical simulation study. The effects of active layer thickness and TCO electrode surface roughness on the indoor light harvesting ability of a PV device have been examined. From this systematic study, it was observed that the ideal short circuit current density of the OPV is gradually increasing with the active layer thickness. Furthermore, surface roughness of the OPV's TCO electrode has a strong correlation with its photon absorption capability, in which a greater TCO electrode surface roughness results in lower photo absorption ability. Lastly, it was also observed that the absorption edge of the PV device is gradually shifted towards infrared region with the increase of TCO surface roughness. This phenomenon may be further utilized for self-powered infrared photo detector.

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