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Proceeding Paper

Parametric Optimization of High-Dielectric Organic Thin-Film Solar Cells †

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Abstract: Organic solar cells (OSCs) have the potential to generate electricity under sunlight at a low cost. In this study, the influence of active layer thickness, defect density, temperature and the presence of reflective coating is studied for the structure ITO/PTAA/PBDB-T: ITIC-OE/PDINO/Ag, by applying PTAA as a hole transport layer (HTL), while the blend of PBDB-T: ITIC-OE is used as an active layer and PDINO is applied as electron transport layer (ETL), respectively. Solar capacitance simulator one-dimensional (SCAPS—1D) software is used to optimize different parameters, which affect the performance of OSCs. By introducing backside reflective coating, the efficiency increases by 2.5%. In the future, this study can be used for the power conversion efficiency (PCE) enhancement of OSCs.

Keywords: organic solar cell; hole transport layer; SCAPS—1D; reflective coating; thickness optimization

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1. Introduction

Organic solar cells (OSCs) have shown promising improvement in the last few years [1]. Fullerene acceptors (FAs) have morphological instabilities that are overcome by non-fullerene acceptors (NFAs), making them a promising choice for high-efficiency OSCs [2–6]. PEDOT: PSS is widely used as a hole transport layer (HTL) in conventional OSCs due to improved transparency, high work function and high conductivity [1,7]. However, PEDOT: PSS is acidic in nature and its effectiveness at collecting holes remains uncertain [8,9]. To enhance charge transport towards the respective electrode in OSC devices and minimize charge recombination, numerous alternative HTL materials have been investigated [10–12].

FAs have good characteristics, i.e., high electron mobility at room temperature such as 0.1 cm^2/Vs [13,14]; however, their stability is low and has high synthetic cost [2]. The main advantages of NFAs as compared to FAs are their low voltage losses, low production cost and high efficiency [2].

Besides practical work, simulation study is also important. Numerous simulation works have been presented using SCAPS—1D software. The authors of [14] presented a simulation work on the enhancement of the performance of NFA OSCs using several types of HTL materials. The highest efficiency is achieved for WS_2 (23.55%), MoS_2 (20.05%) and GO (15.89%). Nithya et al. [1] presented a simulation study on PBDB-T: ITIC, (NFA) OSC using copper iodide (CuI) instead of PEDOT: PSS. The simulation results demonstrated that the output performance of NFA based OSCs can be improved using CuI. The PCE of the proposed solar cell is reported as 15.68%.

Our previous work [15] was about the optimization and PCE enhancement of modified polymer solar cells using spiro OMeTAD under the 90% reflection coating and the PCE achieved was 9.40%. In this study, we modeled modified NFA-BHJ OSCs using PTAA as a hole transport layer (HTL); meanwhile, PDINO was employed as an electron transport layer (ETL) to optimize its technological parameters such as active layer thickness, defect density, and temperature, and its efficiency was increased by introducing 50% reflective coating. Modified ITIC-OE is a modified acceptor which is introduced by [16]. To our knowledge, so far, no studies have been conducted using PTAA as an HTL and by applying backside reflective coating to increase the PCE of high-dielectric OSCs.

2. Methodology Approach

SCAPS—1D Software and Simulation Parameters

Numerous software programs are available, such as SCAPS, WAMPS, COMSOL and SILVACO, to investigate solar cell performance parameters. In this study, SCAPS simulation 1D software is used to determine the output performance of proposed high-dielectric OSCs. SCAPS-1D software was developed by Ghent University Belgium, department of EISs (Electronics and Information Systems) [17]. SCAPS—1D software works based on the Poisson, continuity and transport equations.

Organic solar cells are composed of an anode, cathode, active layer, ETL and HTL. In our investigated structure, Poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b′]dithiophene))-alt-(5,5-(1′,3′-di-2-thienyl-5′,7′-bis(2-ethylhexyl)benzo[1′,2′-c:4′,5′-c′]dithiophene-4,8-dione))]:(3,9-bis (2-methylene-(3-(1,1-dicyanomethylene)-indanone)-5,5,11,11-tetraki (4-hexylphenyl)-dithieno [2,3-d:2,3-d]-s-indaceno [1,2-b:5,6-b]dithiophene)) with oligoethylene, PBDB-T: ITIC-OE is used as the active layer (an active layer is the blend of donor and acceptor materials). Poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine] (PTAA) is used as an HTL, and its purpose is to collect holes from the active layer while N,N′-Bis(N,N-dimethylpropan-1-amine oxide)perylene-3,4,9,10-tetracarboxylic diimide (PDINO) is applied as an ETL with the function of collecting electrons from the active layer. ITO and Ag are used as the anode and cathode, respectively. The proposed OSC is shown in Figure 1. To calculate the output performance of an OSC, the following input parameters are required for simulation, which are shown in Table 1.

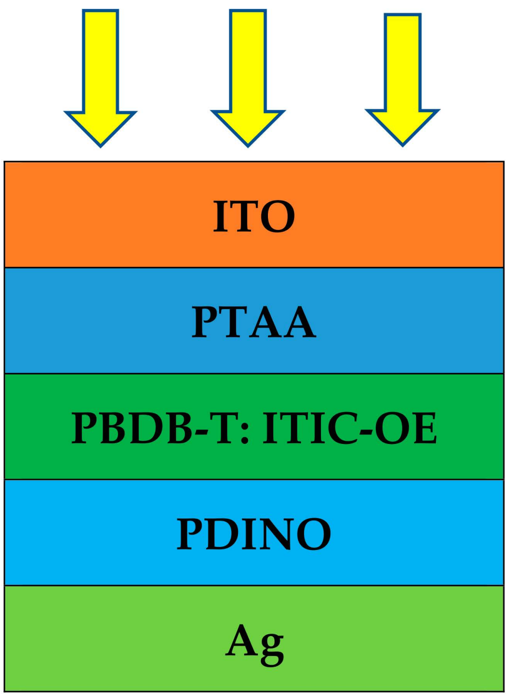


Figure 1. Structure of proposed OSC.

Table 1. Input parameters for simulation.

Parameters	HTL [18,19]	ETL [20]	Active Layer [16,21]
Thickness, d (nm)	40	50	70
Acceptor density, N_A (1/cm^3)	1×10^{17}	-	0
Donor density, N_D (1/cm^3)	-	2×10^{21}	0
Band gap, Eg (eV)	2.96	2.98	1.2
Electron mobility, μ_n (cm^2/Vs)	1×10^{-4}	2×10^{-6}	1.2×10^{-5}
Hole mobility, μ_p (cm^2/Vs)	4×10^{-3}	1×10^{-3}	3.5×10^{-4}
Dielectric permittivity, ε	9	5	6.1
Electron affinity, χ (eV)	2.3	4.11	4.030
Defect density, N_t (1/cm^3)	1×10^{14}	1×10^{14}	1×10^{13}

3. Results and Discussion

The active layer plays a vital role in determining the device's performance. Based on a previous research study, it was observed that the thickness of the active layer had an impact on photovoltaic characteristics such as Jsc, Voc, FF and PCE. In this study, the thickness of HTL varied up to 40 nm. However, HTL thickness has a minor impact on the performance of the proposed OSC. After HTL optimization, the thickness of the active layer is adjusted up to 70 nm to observe its effect on the OSC performance. From the simulation study, it is observed that by increasing the thickness of the active layer, the Voc and FF decrease while the Jsc and PCE increase, which is illustrated in Figures 2a,b and 2c,d, respectively. The decrease in Voc is due to defects and traps in the active layer or the fact that charge carriers have to cover a longer distance, which increases resistance. The reduction in FF is due to an increase in series resistance because it causes a voltage drop across the solar cell when a current flows through it. This voltage drop decreases the output voltage, which reduces the maximum power that the solar cell can generate. However, despite these reductions in FF and Voc, Jsc and PCE increase due to improved light absorption and the generation of photo-generated carriers.

In general, polymers often contain defects that can trap charge carriers and affect the quality of the active layer. Here in this investigated structure, the defect density (N_t) of the active layer is changed from 10^{10} (1/cm^3) to 10^{13} (1/cm^3) to observe the effect of defect density on the active layer. It is analyzed that as the defect density increases, the lifetime (τ_n) and diffusion length (L_n) of charge carriers decreases, as shown in Table 2. The defect density acts as a recombination site because it introduces energy levels within the band gap of the material. These energy levels can trap charge carriers (electrons and holes), which facilitate their recombination and can reduce the output performance of solar cells. When the defect density (N_t) increases, the Jsc and PCE decrease, as illustrated in Figure 3a,b.

Solar cells are exposed to higher temperatures when placed outside the door. So, it is essential to check the performance of the solar cells at high temperatures. In real weather conditions, the temperature may reach 400 K. So, in this simulation study, the temperature was varied from 300 to 400 K. From the simulation study, it is observed that variation in temperature affects the performance of OSCs, as illustrated in Figure 4a,b. The results of the simulation study indicate that as temperature increases, both the Voc and PCE decrease. The decline in Voc can be attributed to the increase in reverse saturation current density. At higher temperatures, electrons are excited due to the instability of the band gap, and the charge carrier recombination increases, which reduces the PCE.

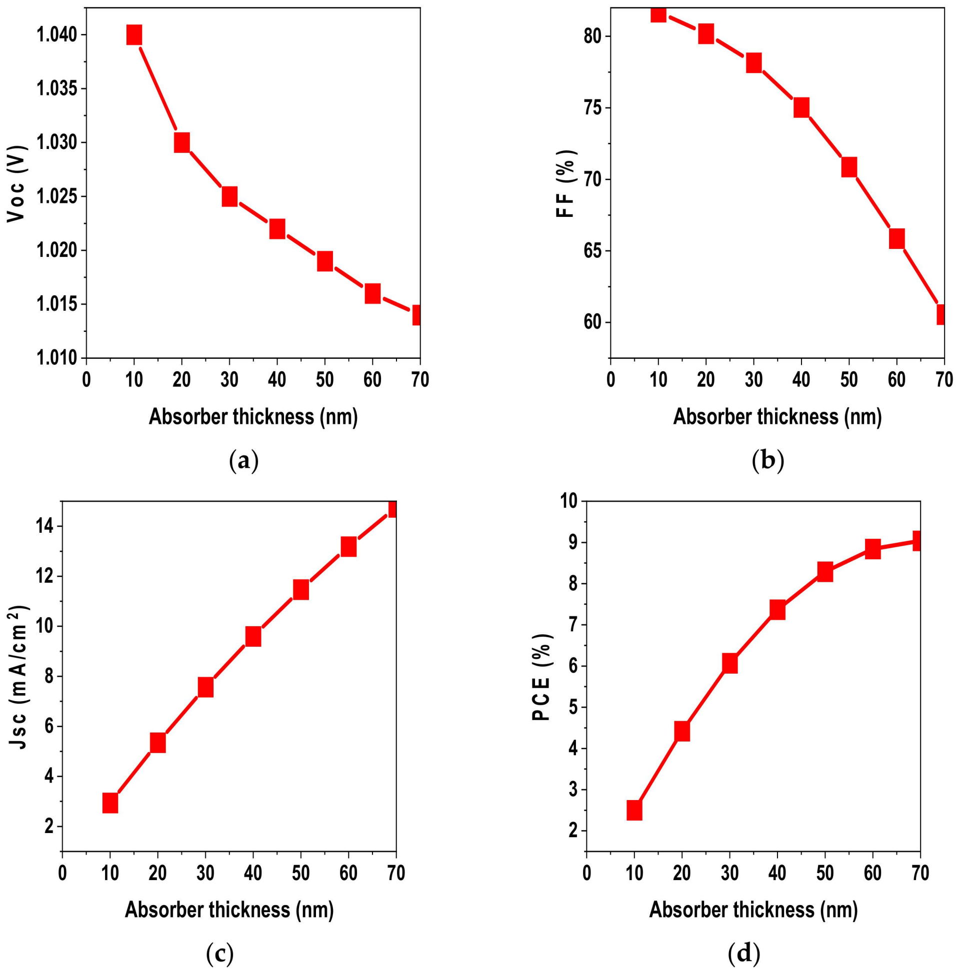


Figure 2. Active layer thickness as a function of (**a**) Voc; (**b**) FF; (**c**) Jsc and (**d**) PCE.

Table 2. Variation of defect density for charge carrier diffusion length and lifetime.

N_t (1/cm^3)	10^{10}	10^{11}	10^{12}	10^{13}
L_n (nm)	560	180	56	18
τ_n (µs)	10,000	1000	100	10

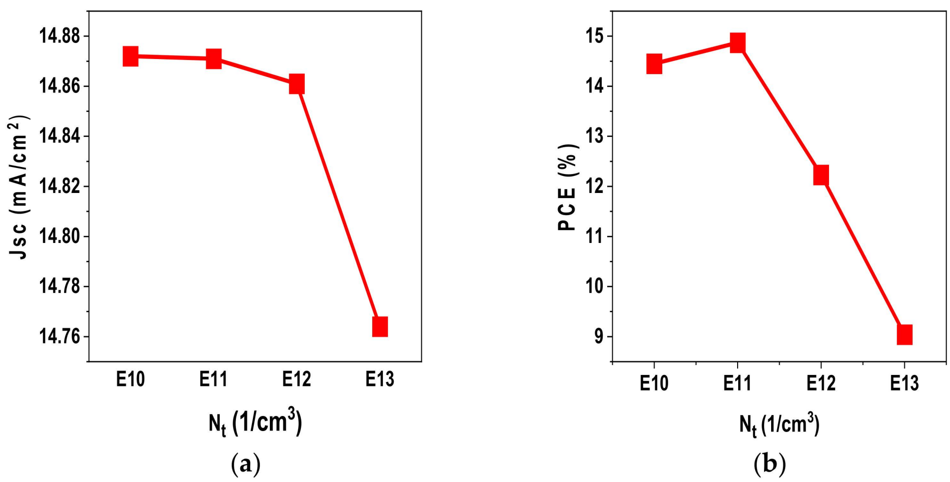
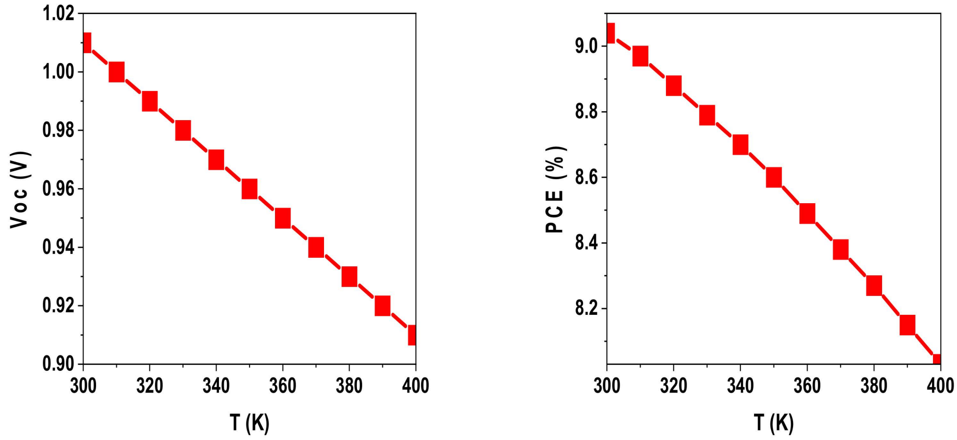


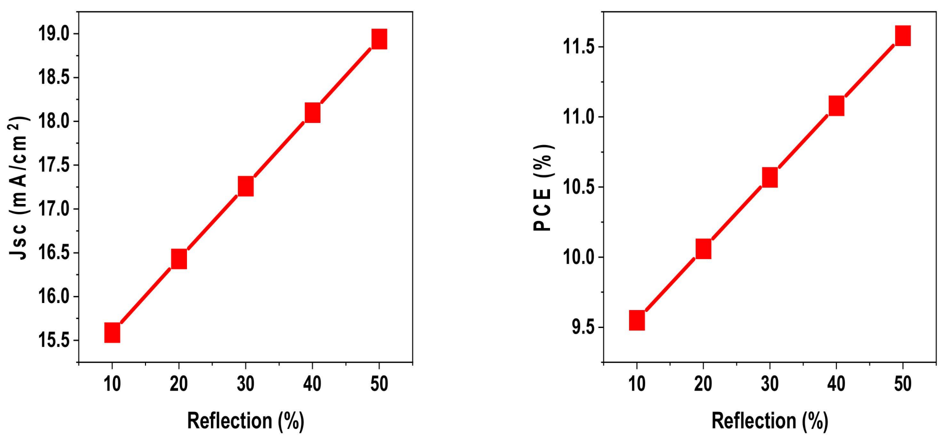
Figure 3. Effect of defect density on (**a**) Jsc and (**b**) PCE.



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

Figure 4. Effect of temperature on (**a**) Voc and (**b**) PCE.

Reflective coatings play a key role in enhancing the PCE of OSCs. Typically, these coatings are applied on the back side of the solar cell with the primary function being the redirection of unabsorbed light back through the solar cell [22]. This process significantly increases the light path within the cell. As a result of this extended light path, unabsorbed photons can interact with the active layer, thereby increasing the chances of the electron-hole generation process and enhancing the overall photocurrent. In this simulation study, the backside reflective coating is altered from 10% to 50% to study its effect on OSC parameters. Figure 5a,b demonstrates that through the addition of reflective coating, the Jsc and PCE improved.



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

Figure 5. Effect of reflection coating on (**a**) Jsc and (**b**) PCE.

4. Parametric Optimization and Comparative Analysis with Experimental Results

The optimized parameters for the proposed OSC are shown in Table 3. The simulated results are compared with the experimental results (ITO/PEDOT: PSS/PBDB-T: ITIC-OE/PFN-Br/Ag), which is performed for the same active layer [16]. From the simulation results, it is observed that simulation results are in close agreement with experimental results. The experimental and simulated results are shown in Table 4.

Table 3. Optimized parameters of proposed OSC structure.

Parameter	Value
Thickness of active layer, nm	70
Thickness of HTL, nm	40
Defect density, $1/cm^3$	1×10^{13}
Temperature, K	300
Reflective coating, %	50

Table 4. Comparative analysis of experimental and simulation results.

Parameters	Simulation without Reflective Coating	Simulation with Reflective Coating	Experimental [16]
Voc (V)	1.0140	1.0276	0.85
FF (%)	60.42	59.50	67
Jsc (mA/cm^2)	14.76	18.940	14.8
PCE (%)	9.04	11.58	8.5

5. Conclusions

In this simulation study, an OSC (ITO/PTAA/PBDB-T: ITIC-OE/PDINO/Ag) is simulated and its PCE is enhanced by optimizing the parameters such as the thickness of the active layer and HTL, the defect density of the active layer and temperature; PCE is also enhanced through backside reflective coating. From the simulation study, it is observed that HTL layer thickness has little impact on the photovoltaic parameters, so the HTL thickness is optimized up to 40 nm. Active layer thickness is changed up to 70 nm; it is observed that by increasing the thickness of the active layer, the output performance parameters such as Voc and FF decrease while Jsc and PCE increase. The decrease in Voc may be due to defects and traps in the active layer, while FF decreases due to an increase in series resistance. The increases in PCE and Jsc are observed due to the improved light absorption. The active layer defect density affects the performance of the OSC. It is observed that as the defect density increases, the performance parameters of solar cells decrease. The optimized value of the defect density is 1×10^{13}; below this value, the performance of an OSC is improved but it is difficult to design such a type of solar cell with low defects. Temperature has an impact on the performance of solar cells. The ideal temperature for solar cell operation is 300 K. So, a simulation study was performed for 300 to 400 K temperature. It was observed that by increasing the temperature, the performance parameters decreased. Backside reflective coating is a technique used to enhance the Jsc and PCE of OSCs. The reflective coating value was changed from 10% to 50%. Due to reflective coating, the absorption capacity and optical path length were enhanced, which improved the PCE. The simulated results are compared with the experimental results, which are available in the literature. These simulation results are in close agreement with practical results and this software can be used for the performance enhancement of OSCs.

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