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GPVDM Simulation of Thickness Effect on Power Conversion Efficiency of PEDOT:PSS/P3HT:PCBM Solar Cell Performance

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Abstract. In this research, polymer solar cells (PSC) by configuring ITO/PEDOT:PSS/P3HT:PCBM/Al changed to optimize their performance. Modifications are made by varying the thickness of each layer so as to increase the ideal thickness with optimal power conversion efficiency (PCE) value. The researchers used GPVDM software to study several power conversion efficiency (PCE) parameters of ITO/PEDOT:PSS/P3HT:PCBM/Al solar cells. The results of this research show that the power conversion efficiency (PCE) can be increased by adjusting the thickness of the coating, this research showed the power conversion efficiency (PCE) was increased from 4.16% to 4.81%.

Keywords: PSC, PCE, GPVDM software, layer thickness modification

INTRODUCTION

Solar energy is a reliable alternative energy source because it is abundant and environmentally friendly. In this perspective, developing solar cells is one of the best approaches to convert solar energy into electrical energy based on the photovoltaic effect. Until now, the advancement of solar cell technology is growing so rapidly. Solar cell technology is becoming very important in industry, society, and the environment [1]. Efforts have been made to substantially increase the efficiency of solar cells. To explore the potential of solar cells we do not only work experimentally but also in simulation. In this study, researchers worked in a simulation. This is because the solar cell is a device that can only work according to its function in the right environment. Thus, we must consider the interconnection and packaging technology with due regard to the material properties.

The focus of this research is the simulation of polymer-based solar cells with the configuration ITO/PEDOT:PSS/P3HT:PCBM/Al which refers to the research conducted by [2], have investigated J-V characteristics of P3HT:PCBM been modeled by solving the drift and diffusion equation for a constant electric field in the active layer. And the other research of polymer-based solar cells has been done by [3] by experiment, polymer solar cells (PSCs) with the configuration of ITO/PEDOT:PSS/P3HT:PCBM/back electrode with different back electrodes of silver (Ag), aluminum (Al), and Ag/Al alloy with various weight percentages were investigated. And [4], were analyzed and the simulation system of current-voltage (I-V) characteristics of organic photovoltaic cell was established by GPVDM software. Result of this research showed that the increase in efficiency is caused by optical absorption in the pure polymer layer and hence efficient charge separation at the polymer bulk-heterojunction interface between the poly(3,4 ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) and poly(3hexylthiophene):phenyl-C61-butyric acid methyl ester (P3HT:PCBM) layer.

P3HT:PCBM, these two materials are often used by researchers because they have a high absorption rate in the visible light region and have a tendency to be stable. These advantages of polymer material properties provide benefits for the advancement of modern solar cells, in addition to being cheaper and more environmentally friendly

[5]. In this research, GPVDM simulator is used to simulate solar cells based on ITO/PEDOT:PSS/P3HT:PCBM/Al, such as the last research has been done but on perovskite solar cells [6]. Modifications to the thickness of each layer are carried out to achieve performance optimization in terms of the value of its power conversion efficiency and obtained the ideal thickness.

MATERIALS AND METHOD

In this research, researchers use one of the organic solar cells, namely polymer-based solar cells. Polymer solar cells are solar cells that use two polymer materials as an active layer where the polymer functions to absorb sunlight and generate electrons when sunlight hits the surface of the solar cell [7]. The electrons will then flow through a pair of electrodes, namely aluminum (Al) as the cathode below, and go to the transparent anode above it to produce an electric current. The active layer is formed by two polymeric materials into a bulk heterojunction structure by being mixed to form a composite film [8]. The polymer materials used in this research, P3HT or poly(3-hexylthiophene) which is a derivative of polythiophene as an electron donor and mixed with PCBM or [6,6]-phenyl-C61-butyric acid methyl ester which is a derivative of poly (p-phenylene vinylene) [9]. The structure of ITO/PEDOT:PSS/P3HT:PCBM/Al solar cells can be seen in Figure 1.

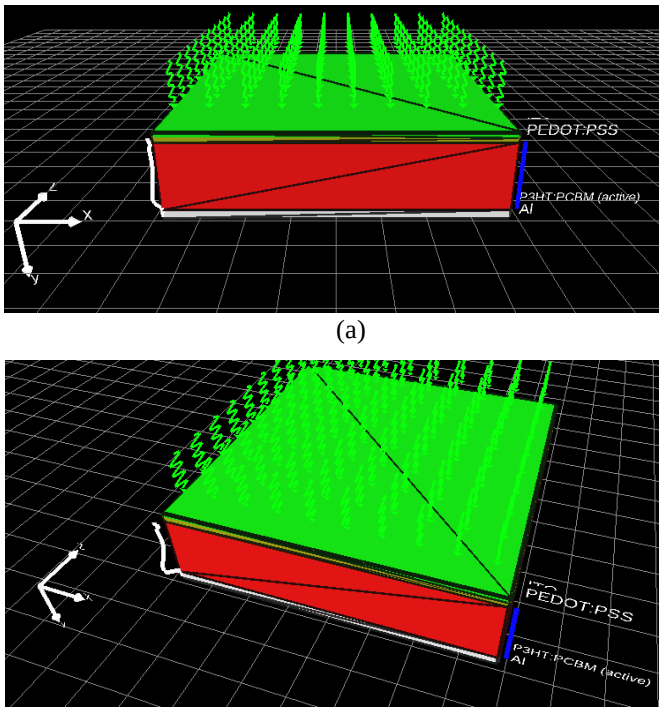

FIGURE 1. ITO/PEDOT:PSS/P3HT:PCBM/Al solar cell structure (a) frontside (b) upside

Simulations were carried out using the General Purpose Photovoltaic Device Model (GPVDM). GPVDM simulator is a 1D/2D optoelectronic device model, which can be used to simulate solar cells, LEDs, diodes, FETs, etc. This simulator is based on solving Poisson equation (1) to obtain voltage $\emptyset$,

$$\frac{d}{dx}(\epsilon_0\epsilon_r).\frac{d\emptyset}{dx} = q(n-p) \quad (1)$$

where front anode $(x = 0)$ dan back cathode $(x = d)$, ϵ_0 is the permittivity of free space, ϵ_r is relative permittivity, q is the elementary charge, n and p is free electron and hole population [10].

Something not less important in solar cells is the offset of band edges of the HOMO and LUMO levels will prove responsible for the improvement of all photovoltaic properties of the organic solar cells. Since a deep HOMO level is desirable for obtaining high open-circuit voltage (V_{OC}) since the maximum value of the V_{OC} is

determined by the energy difference between the HOMO (Highest Occupied Molecular Orbital) level of the donor and LUMO (Lowest Unoccupied Molecular Orbital) level of the acceptor. Drift diffusion equation (momentum conservation equation) for electron

$$J_n = q\mu_e n\frac{\partial E_c}{\partial x} + qD_n\frac{\partial n}{\partial x} \quad (2)$$

for hole

$$J_p = q\mu_h n\frac{\partial E_v}{\partial x} + qD_p\frac{\partial p}{\partial x} \quad (3)$$

E_c dan E_v define the carrier mobility and define $E_c = -\chi - \emptyset$ and $E_v = \chi - E_g$, where χ is a difference of LUMO mobility and vacuum level and E_g is the difference of HOMO and LUMO mobility.

To describe carrier trapping, d-trapping recombination used SRH recombination model for electron and hole, which assume a steady-state distribution of trapped charge carries in the trap states.

$$R_T = \frac{np - n_i^2}{\tau_{P0}\left[n + n_i \exp\left(\frac{E_t - E_i}{kT}\right)\right] + \tau_{n0}[p + n_i \exp\left(\frac{E_i - E_t}{kT}\right)]} \quad (4)$$

This form of the SRH equation is therefore not suitable for time-domain simulations, where trapping or recombination via trap states dominate charge dynamics. As the charge carriers can not go out of equilibrium [11].

So, to describe carrier trapping, d-trapping recombination we use SRH recombination model for electron and hole. But, SRH equation is not suitable for time-domain simulation. So, to solved this problem the charge density of each trap state needed to split space up into energy slices and solved the SRH equation explicitly in the time domain. Each trap state gets its rate equation

$$\frac{\partial n_t}{\partial t} = r_{ec} - r_{ee} - r_{hc} + r_{he} \quad (5)$$

r_{ec} is the rate at which free electrons get trapped, r_{ee} is the rate at which electrons can escape from the trap back to the free electron population, r_{hc} is the rate at which free holes get trapped and r_{he} is the rate at which holes escape back to the free hole population. Electron recombination rate (R_e) in equation 2 can be calculated by subtracting the total number of electrons that escape all traps into the carrier free electron population from the total number of electrons captured from the free carrier population into all traps [12]. An analogous procedure is carried out to calculate R_h for free holes. For more detail equation resolving and device modeling can be found more detail in [13-16].

TABLE 1. Parameters simulation [13]

Parameters	P3HT:PCBM
Layer thickness (m)	$1x10^{-7}$
Relative permittivity ε_r	3,8
Bandgap energy (eV)	1,1
Electron affinity (eV)	3,8
Electron mobility (m^2/V.s)	$2,48x10^{-7}$
Hole mobility (m^2/V.s)	$2,48x10^{-7}$
Donor concentration (m^{-3})	$4,86x10^{26}$
Acceptor concentration (m^{-3})	$4,86x10^{26}$

RESULT AND DISCUSS

The Optimation method used in our simulation is to fix all parameters and modify one by one until we have the parameters that give maximal PCE and from this result can be determined the ideal layer thickness design of ITO/PEDOT:PSS/P3HT:PCBM/Al. Figure 2 presented the curve of effect PEDOT:PSS layer thickness on PCE.

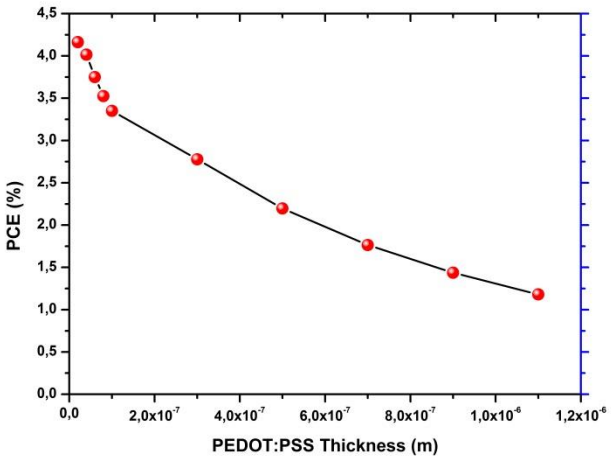

FIGURE 2. Effect PEDOT:PSS layer thickness on PCE

From Figure 2 we can note that a PEDOT:PSS layer thickness of $2x10^{-8}$ m gives the maximal value of PCE 4,16% with a fill factor of 75,78%, an open circuit voltage of 0,617 V, and a short circuit of -88,99 V. So, PEDOT:PSS layer with a thickness $2x10^{-8}$ m was set and further modified the P3HT layer thickness to obtain curve in Figure 3.

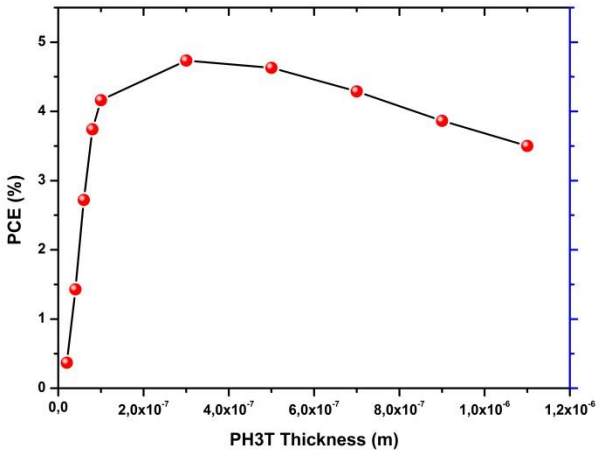

FIGURE 3. Effect P3HT layer thickness on PCE

From Figure 3 we obtained a maximal value of PCE which is 4,73% corresponding to P3HT layer thickness of $3x10^{-7}$ m, with fill factor 60,84%, an open circuit voltage of 0,6 V, and a short circuit of -129,3 V. Then, PEDOT:PSS layer thickness was set at $3x10^{-7}$ m, and changing the ITO layer thickness we obtained curve in Figure 4.

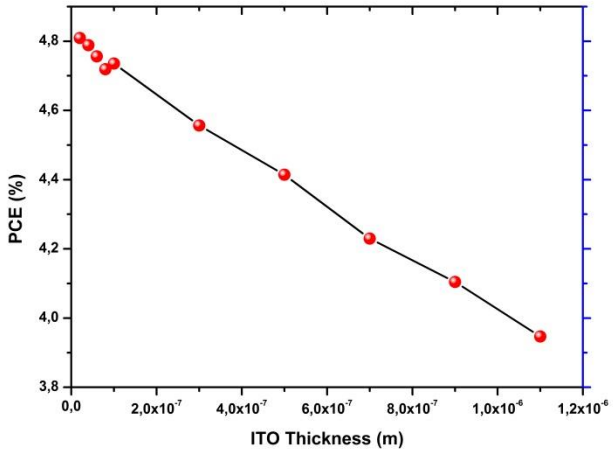

FIGURE 4. Effect ITO layer thickness on PCE

In Figure 4 the maximal PCE is 4,8% in the ITO layer thickness of $2x10^{-8}$ m, with fill factor 60,77%, an open circuit voltage of 0,6 V, and a short circuit voltage of -171,7 V.

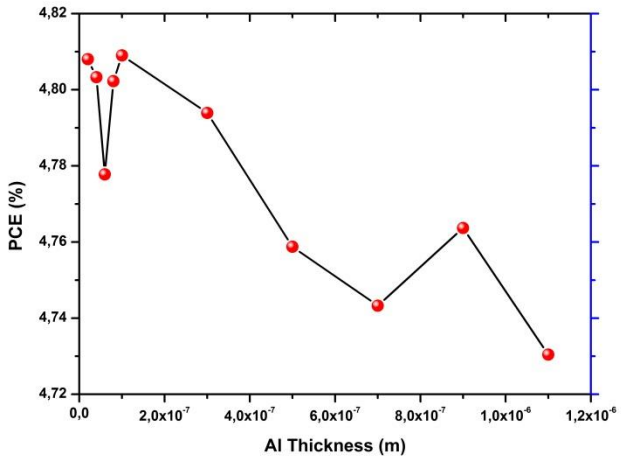

FIGURE 5. Effect Al layer thickness on PCE

In the last setting, ITO layer thickness was set to $2x10^{-8}$ m and Al layer thickness was modified. Figure 5 shows the maximum PCE of 4,81%, with a fill factor is 60,8%, an open circuit is 0,6 V and a short circuit is -131,7 V at $1x10^{-7}$ m of Al thickness.

Figures 2 to 5 is presented different layer thickness effects on PCE PEDOT:PSS/P3HT:PCBM/Al solar cell where we saw that efficiency increased from 4,16% to 4,81% optimized parameters. Ideal layer thickness design of PEDOT:PSS/P3HT:PCBM/Al solar cell is: PEDOT:PSS layer thickness of $2x10^{-8}$ m, P3HT layer thickness of $3x10^{-7}$ m, ITO layer thickness of $2x10^{-8}$ m, and Al layer thickness set to $1x10^{-7}$ m.

SUMMARY

In this paper, the capabilities of GPVDM for analyzing PCE of PEDOT:PSS/P3HT:PCBM/Al solar cells have been presented. The coding used in GPVDM can simulate the relevant physics phenomena in submicron and nanoscale device scales. Intuitive scripts in this application provide users to define their devices. The simulation result from GPVDM shows that the power conversion efficiency (PCE) can be increased by adjusting the thickness of the coating, this research showed the power conversion efficiency (PCE) was increased from 4.16% to 4.81%. From the simulation result, PCE PEDOT:PSS/P3HT:PCBM/Al solar cell ideal thickness design at PEDOT:PSS layer thickness of $2x10^{-8}$ m, P3HT layer thickness of $3x10^{-7}$ m, ITO layer thickness of $2x10^{-8}$ m, and Al layer thickness set to $1x10^{-7}$ m.

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