SCAPS Simulation of P3HT:Graphene Nanocomposites-Based Bulk-Heterojunction Organic Solar Cells

Nur Shakina Mohd Shariff, Puteri Sarah Mohamad Saad, Mohamad Rusop Mahmood

***Abstract*— The discovery of bulk-heterojunction concept and conjugated polymer led to an increasing interest towards organic solar cells. Eventhough organic solar cells are less expensive than inorganic solar cells, the power conversion energy is still considered low. This research's main objective is to study the thickness and concentration effect of P3HT's layer towards the efficiency of the P3HT:Graphene solar cells. SCAPS is a simulation software that is used in this research to simulate the effect on the solar cells. The solar cell's structure is drawn in the simulation software and the parameters for each layers is inserted. From the overall results, the thickness of 100nm and the concentration of 1.0 x 10^{16} cm^{-3} yeild the optimum efficiency.**

***Index Terms*— Organic Solar Cells, P3HT, Graphene, SCAPS.**

I. Introduction

Since the discovery of conjugated polymers [1]-[2] and bulk-heterojunction [3], organic solar cells has become a major field of studies in photovoltaic. Organic solar cells is well known nowadays due to its favorable properties such as easy fabrication, less expensive and also lighter than inorganic based solar cells [4].

Most studied polymer till today is Poly(3-hexylthiophene) (P3HT), which in the last decade has been widely used in organic electronics and photonics. Its use in organic photovoltaic has most contribute to its popularity. P3HT is known to posses properties such as high electrical conductivity and high solubility in different solvent [4]. It also can be deposited under low deposition temperature by using cheap deposition technique [4]-[5].

This paper is about simulation of P3HT:Graphene thin film for photovoltaic usage submitted on 22nd August 2016. Accepted on 17th November 2016.

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P3HT possesses a high electrical mobility (μ_{hole} = 0.2 cm^2/Vs) but it is low compared to the electrical mobility of inorganic solar cells [4],[6]. Since P3HT is a donor material and a p-type semiconductor, it posses higher hole mobility than electron mobility. P3HT has a melting temperature of 240°C and is a semi-crystalline polymer [7].

Recent photovoltaic studies shows new materials that have organic-inorganic combination such as P3HT with carbon polymorph composites is developed in order to produce a higher efficiency [4]. Carbon polymorph composites such as Carbon nanotubes (CNTs) and Graphene is being widely researched. The discovery of Graphene in 2004 has led to many research on Graphene's properties. Graphene has an excellent electrical characteristic such as high conductivity and mobility than CNTs [4],[8]. It is also reported that Graphene is a superb electron acceptor [4]. In this research, P3HT is mixed with Graphene and is use as an active layer inside the solar cell.

The existence of Graphene in P3HT effects the capacitance of the thin film. Capacitance (*C*) is used to analyze the charge transport in organic photovoltaic devices. The capacitance-voltage characteristics gives a deep understanding into these devices when combined with current density-voltage (*J-V*) data [9] and also provide info of the device characteristic. Recent research has showed that at the peak in the *C-V* characteristic, the built- in voltage (V_{bi}) can be obtained [10]. As polarity changed, only one peak is visible when the bias is applied through the organic semiconductor [11][12][11][11][13].

Low power conversion efficiency is the main problem for organic solar cells. This is because of low photocurrent. Low photocurrent in P3HT is due to low electron mobility ($\mu_{electron}$ = $10^{-14} – 10^{-14}$ cm^2/Vs) [4],[6]. In order to increase the electron mobility, P3HT will be mixed with a high electron mobility material such as Graphene. It also has been stated that low photocurrent is due to low absorption of incident light power [6],[14]. These two problems is mainly affected by the thickness of the active layer in the solar cell. This research is to study the effect of P3HT:Graphene concentration and thickness towards the solar cell's characteristic.

II. METHODOLOGY

The simulation software that is used in this research is SCAPS. The structure of the solar cell is drawn in the software as shown in Figure 1. The parameters such as the bandgap, electron affinity and the electron concentration is fixed for each layer of the solar cell. The P3HT's thickness is measured from 60 nm to 100 nm and for each thickness of P3HT, the hole concentration is measured from $1x10^{13}$ till $1x10^{16}$ cm^{-3}. Effect of the concentration will also be measured since carrier concentration is linked with electrical mobility. The open circuit voltage (V_{oc}), short circuit current density (J_{sc}), fill factor (FF), efficiency (η), quantum efficiency (QE), the capacitance-voltage (C-V) and the capacitance-frequency (C-f) is calculated by the software. Equation (1) shows the efficiency (η) equation where P_{IN} is the input power. Equation (2) shows the quantum efficiency (QE) equation. P_o is the incident optical power and I_{ph} is the photocurrent.

$$\eta \equiv \frac{V_{oc} J_{sc} FF}{P_{IN}} \qquad (1)$$

$$QE \equiv \frac{h\upsilon I_{ph}}{eP_o} \qquad (2)$$

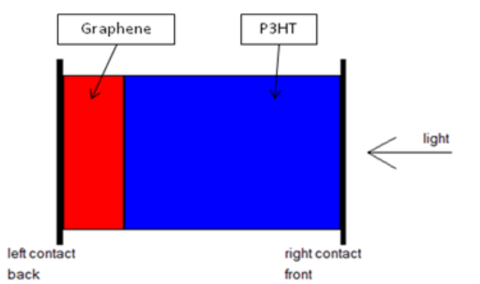

Fig. 1. Solar cell structure of P3HT/Graphene layer

III. RESULT AND DISCUSSION

According to the simulation result shown in Figure 2, the current density shows the gap between the dark current and under illumination increases when the thickness of the active layer increases. In order to generate more power, the gap between the dark current and under illumination should be bigger. Due to a bigger charge generation, the photocurrent will increase as the thickness of the P3HT:Graphene increases [6].

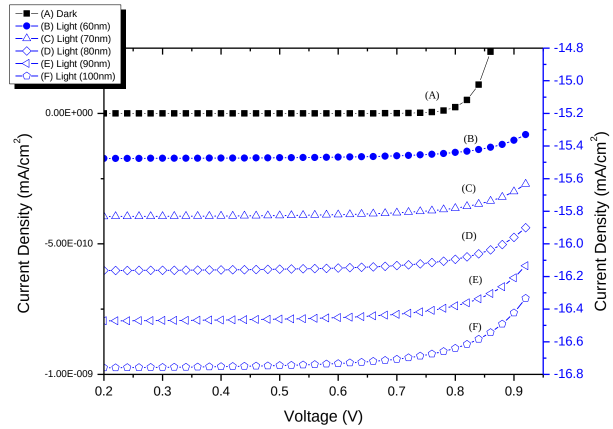

Fig 2 Current density (J_{sc}) for every thickness at dark current and under illumination at a hole concentration of 1.0 x 10^{16} cm^{-3}.

From Figure 3, the quantum efficiency shows that the more thicker the P3HT:Graphene layer, the higher the quantum efficiency. Quantum efficiency (QE) is only affected by the amount of the absorption light. Therefore more light will be absorbed to generate more photocurrent when the active layer is thicker. The QE drop till 0 at around wavelength of 580nm because there are no more light absorbed at higher wavelength. P3HT absorption is has also been proved to be at 300nm till 600nm [4].

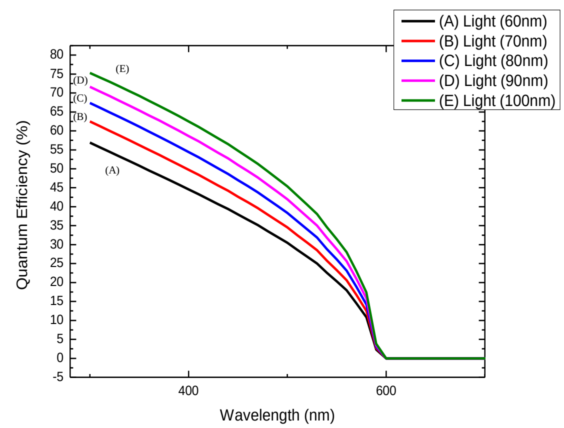

Fig. 3. The quantum efficiency (QE) at different thickness of the active layer.

The effect of the layer's concentration towards the open circuit voltage (V_{oc}) is shown in Figure 4. V_{oc} increases as the concentration of the active layer increases. From the graph in Figure 4, the thickness of 60 nm has the highest V_{oc} value at a concentration of $1x10^{16}$ cm^{-3} while the thickness of 100nm has the lowest V_{oc} value. The results shows that the thicker the active layer, the lower the voltage. Voltage usually is affected by the resistance. A thicker active layer has a lower voltage due to a higher series resistance [6].

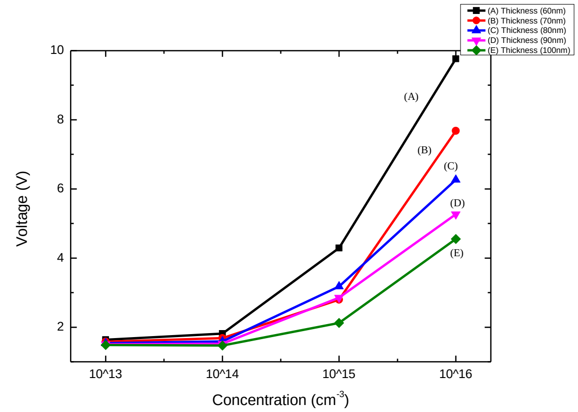

Fig. 4. The open circuit voltage (V_{oc}) for every thickness and concentration

Figure 5 shows the effect of the thickness towards the short circuit current density (J_{sc}). From the results, the highest current density value is the layer with a thickness of 100 nm while 60 nm has the lowest value. At 100 nm, the active layer has more area to generate current than the active layer that is only 60 nm thick. It also have more carrier concentration when the active layer is thicker. Therefore the current is higher. As stated from previous studies, when the thickness increased, the number of charges also increase due to more absorption [6].

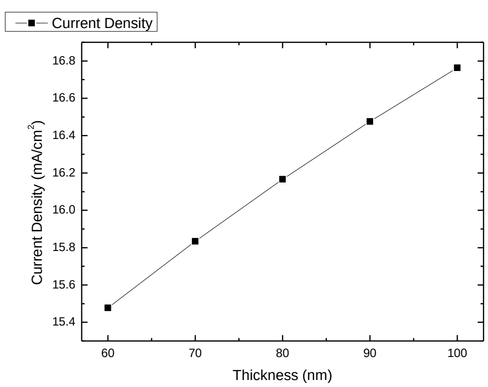

Fig. 5. The short circuit current density (J_{sc}) for every thickness

The fill factor results for every concentration is shown in Figure 6. As shown, the fill factor decrease rapidly as the concentration rises. The fill factor then decrease as the thickness and concentration of the active layer increase from $1x10^{14}$ cm^{-3} to $1x10^{16}$ cm^{-3}. Fill factor is the ratio of the maximum power from the solar cell to the product of V_{oc} and J_{sc}. The *FF* decrease when the charge mobility is raised in polymer solar cells [6]. When the charge mobility increases, more charges can move through faster and will result in a higher photocurrent.

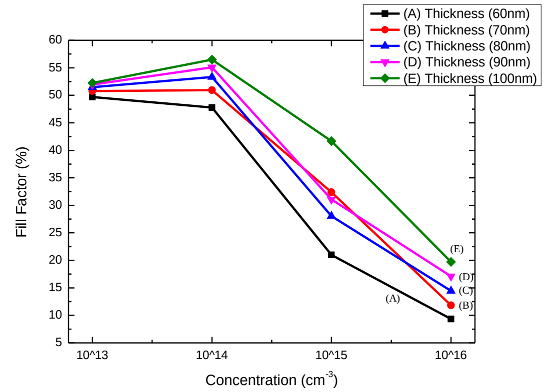

Fig. 6. Fill Factor (*FF*) for every thickness and concentration of P3HT

In Figure 7, the efficiency rises when the concentration increases. Highest efficiency achieved is 15% at a thickness of 100 nm. A higher efficiency lead to a better device performance because more sunlight can be converted into electricity. Figure 7 shows a higher power conversion efficiency is achieved when the active layer is thicker. The efficiency is the most important results because it shows the performance of a solar cell. A higher efficiency leads to a higher performance solar cell. Efficiency is mainly affected by J_{sc} and from Figure 5, the J_{sc} increase when the active layer gets thicker, due to that the efficiency also increased [6].

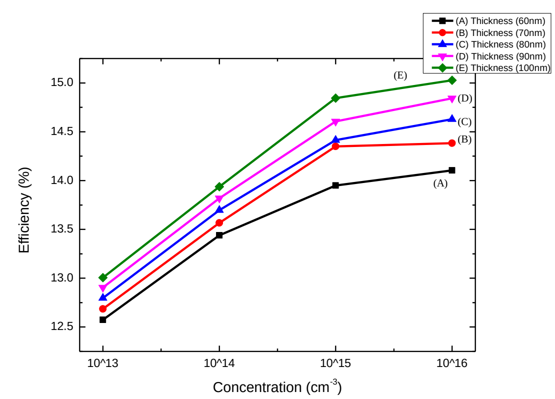

Fig. 7. The efficiency (η) for every thickness and concentration.

The effect of the P3HT's concentration towards the device's capacitance is shown in Figure 8. The thickness of the active layer is fixed at 100nm while the hole concentration is evaluated from 1.0 x 10^{13} cm^{-3} to 1.0 x 10^{16} cm^{-3}. From Figure 8, only (D) shows a drastic increase at 0.7 V while (A),(B) and (C) slowly decrease as the voltage increase. (D) also shows there is a built-in voltage inside solar cells. The capacitance increases in the forward direction and reach a peak at 0.86V. It has been reported that the peak came from mobile holes in donor materials [11].This occur due to the concentration of P3HT which increase from 1.0 x 10^{13} cm^{-3} to 1.0 x 10^{16} cm^{-3}. P3HT is p-type semiconductor and rich in hole concentration. The capacitance value also increase when the hole concentration increases. It seems that the capacitance decrease until it reach a voltage of 0.58V. At 0.58V, the capacitance increase rapidly at a concentration of 1.0 x 10^{16} cm^{-3} until it reach its peak at around 0.86V. The capacitance then decrease till 0.94V due to the limitation of the minority carriers concentration [10].

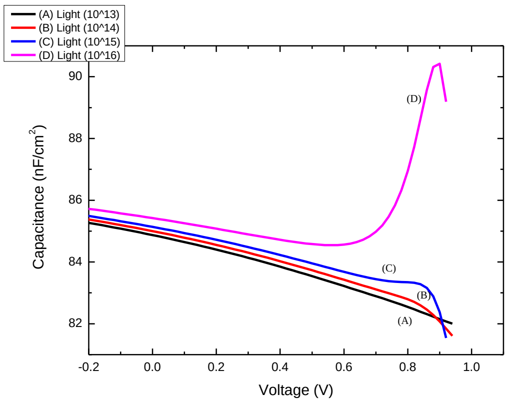

Fig. 8. C-V characteristic for every concentration

The effect of thickness towards the device's capacitance voltage is shown in Figure 9. Here, the voltage and concentration is fixed from -0.8V to 1.0V and 1.0 x 10^{16} cm^{-3} respectively. The thickness of P3HT is measured from 60 nm till 100 nm. As seen from Figure 9, 60nm has the highest capacitance while the lowest capacitance is at 100 nm. It can be concluded that as the thickness decreases, the capacitance increases. For very thickness, there is a slight rise at 0.84V but as the thickness decrease, the peak also decreases. As explained above the peak decrease because of the limitation of minority carriers concentration [10]. The hole concentration decreases as the thickness of the P3HT decreases. This will cause the peak to decrease. The peak voltage is related to the bias voltage V_{bi} therefore the peak for all thickness is the same [9]. The thickness of the active layer is inversely proportional to the capacitance. Therefore as the active layers gets thicker, the capacitance decerase.

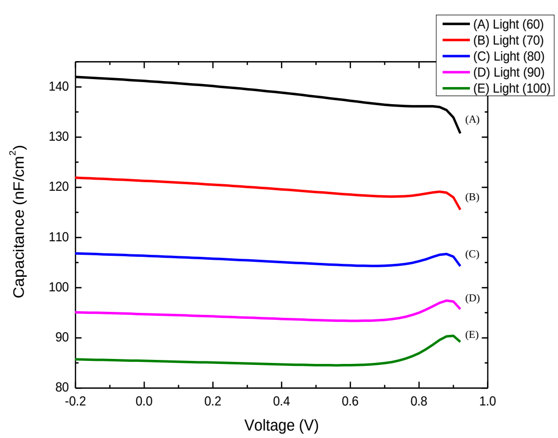

Fig. 9. C-V characteristic for different layer's thickness

The capacitance – frequency (C-f) result is shown in Figure 10. The highest capacitance value is at a concentration of 1.0 x 10^{16} cm^{-3} when under illumination. As the frecuancy increase, the capacitance does not show a major change. It can be seen in Figure 10 that even the concentration increases from 1.0 x 10^{13} cm^{-3} to 1.0 x 10^{16} cm^{-3}, the capacitance is static. The highest capacitance value is shown at (B) which is around 85.4125 nF/cm^2 while (E) shows the lowest capacitance value at 84.832 nF/cm^2. When the active layer is under illumination, the capacitance value remains constant due to fixed temperature in the simulation program.

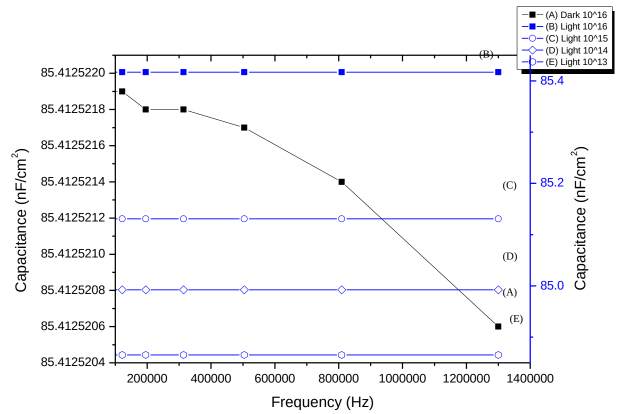

Fig. 10. C-f characteristic for every concentration.

Figure 11 shows the effect of P3HT:Graphene thickness towards the capacitance. The capacitance increase as the active layer's thickness increases. The thickness of 60nm has the highest capacitance while 100nm has the lowest. The capacitance of P3HT:Graphene remain the same in Figure 11 as the frequency increases. The capacitance value between (B) and (F) has a larger gap compared to the one in Figure 10. This shows the thickness has a higher effect than the carrier's concentration towards the solar cell's capacitance. As shown in Figure 11, (A) shows as frequency increases, the capacitance decrease. The graph is actually quite the same as (A) for all thickness under illiminaton. Its is seen as a straight line due to the decrease of capacitance is too small. It can be concluded from the graph that the thickness of the thin film has a small effect on the capacitance because it is mainly affected by the temperature [15]. As the active layer is thicken, the capacitance decrease because the distance between two electrodes of the solar cells increase. Due to that the capacitance to slowly decrease.

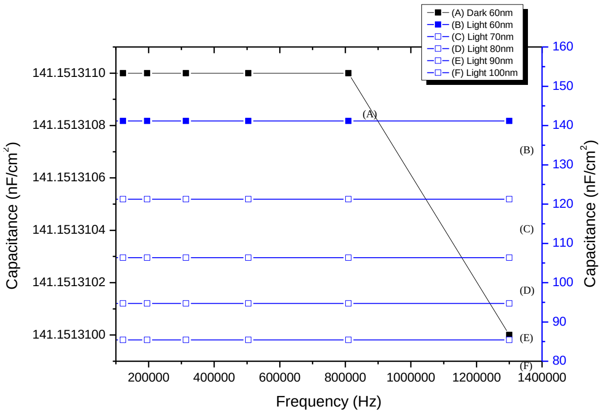

Fig. 11. C-f characteristic at every thickness.

IV. Conclusion

A simulation on the effect of the thickness and concentration towards the solar cell's characterization has successfully been done. It can be concluded that the thicker and the more higher the concentration, the higher the power conversion efficiency. When the thickness and the concentration of P3HT is increased, the total of carrier concentration increases. It will lead to a higher photocurrent. Therefore, the optimum thickness and concentration of P3HT layer that yield the optimum efficiency is at a thickness of 100 nm and concentration of 1.0 x 10^{16} cm^{-3}. For C-V measurements, the peak appears at both results. The capacitance value at forward bias shows a strong sign that the minority charge carriers plays an important role. For C-f measurements, the thin film's thickness & concentration have a little effect. The capacitance decrease as the thickness of the active layer increase. This is due to the increase distance from the two electrodes.

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