Investigation of the effects of charge carrier mobility on the performance of P3HT: PCBM based organic solar cell

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Abstract

Effect of charge carrier mobility on P3HT: PCBM based organic solar cell has been investigated in this study. Numerical simulation for the structure ITO/PEDOT: PSS/P3HT: PCBM/Al has been done using simulating software GPVDM (General Purpose Photovoltaic Device Model). Hole mobility has been varied from $5x10^{-8}$ $m^2V^{-1}S^{-1}$ to $100x10^{-8}$ $m^2V^{-1}S^{-1}$at fixed electron mobility $2x10^{-8}$ $m^2V^{-1}S^{-1}$ and vice-versa. Short circuit current density, open circuit voltage, fill factor, efficiency have been studied to understand the dependency of carrier mobility on device performance. Result shows that efficiency is greatly influenced by charge carrier mobility.

***Keywords*:** Mobility, GPVDM software, Organic solar cell

1. Introduction

In recent years Organic based solar cell technologies have been a very attractive area of research. Bulk hetero-junction (BHJ) OSC is being widely investigated in recent days [1]. In BHJ light absorption and generation of excitons occurs at the donor-acceptor blend. Excitons are splitted at donor-acceptor interface and separated charges are transported to opposite electrodes though active material. Among various acceptor-donor (A/D) combinations, P3HT(Poly(3-hexylthiophene-2,5-diyl)) as acceptor and PCBM(Phenyl-C61-butyric acid methyl ester) as donor have been seen to be quite efficient due to its high hole mobility, large absorption in red region, high crystalline degree etc [2]. Between the electrodes and active layer, PEDOT: PSS (poly (3, 4-ethylenedioxythiophene) polystyrene sulfonate) is used as buffer layers to block the electron and hole transfer in wrong direction.

It is necessary to collect maximum no of generated charge carrier in order to have higher power conversion efficiency and thus mobility is considered as one of the ways to increase the charge carrier collection. To improve the device performance, one of the key parameter is charge carrier mobility and it should be optimized. This article investigates how the device performance is affected by charge carrier mobility.

To understand the device performance, numerical simulation has been done using GPVDM (General purpose photovoltaic device model) software which is constructed for the simulation of donor-acceptor materials based BHJ solar cells and is capable of simulating various electrical and optical characteristics. Effect of variation of different parameters on electrical and optical properties are being studied using GPVDM software recently [3,4]. It is designed to simulate bulk heterojunction organic solar cell such as those based on P3HT: PCBM material.

GPVDM is based on electrical model which is governed by Poisson's equation (equation 1) [5]

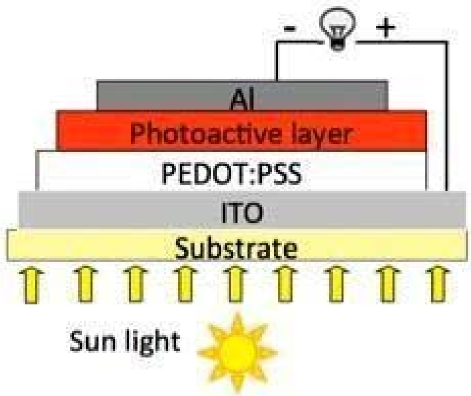

Figure 1: Bulk Heterojunction solar cell

and continuity equation for holes and electrons (equation 2 and 3) [5] and drift-diffusion phenomenon (equation 4 and 5) [6] which is as follows.

$$\frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \frac{q(N_A^- - N_D^+ + n - p + n_t - p_t)}{\epsilon} \quad (1)$$

$$\frac{dJ_p}{dx} = -q[R(x) - G(x)] \quad (2)$$

$$\frac{dJ_n}{dx} = q[R(x) - G(x)] \quad (3)$$

$$J_p(x) = -KT\mu_p \frac{dP}{dx} + q\mu_p pE(x) \quad (4)$$

$$J_n(x) = KT\mu_n \frac{dn}{dx} + q\mu_n nE(x) \quad (5)$$

Where, ψ is the electrostatic potential, ε is the permittivity and q is the charge of electron. n, p, n_t, p_t, N_D^+ and N_A^- are the free electrons, free holes, trapped electron, trapped holes, ionized donor like doping concentration and acceptor like doping concentration respectively.

2. Material used:

For electrical simulation P3HT: PCBM has been used as active layer, PEDOT: PSS acts as buffer layer and Al are used as counter electrode for easy collection of electron. The cell structure (Figure 1) consists of P3HT as the donor and PCBM as the acceptor material. The energy diagram is shown in Figure 2.

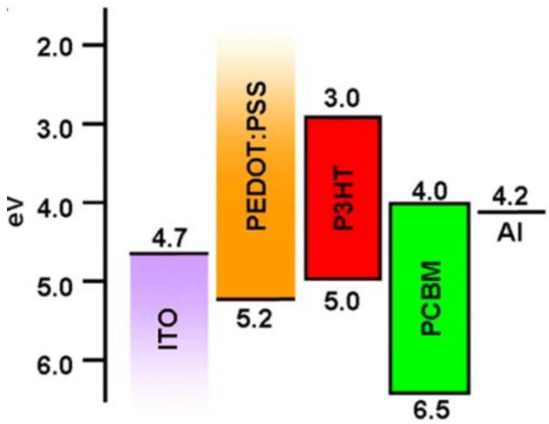

Figure 2: Energy level diagram of typical P3HT: PCBM Bulk Heterojunction OPV

As a transparent front electrode, Indium Tin Oxide (ITO) coated glass plate has been used due to its high transmittance in visible region and ability of conduction.

3. Electrical simulation

Layer thickness of ITO, PEDOT: PSS, P3HT: PCBM and Al have been used as 100 nm, 100nm, 220 nm and 100 nm respectively. At first we run the software for hole mobility from $5x10^{-8}$ $m^2V^{-1}S^{-1}$ to $100x10^{-8}$ $m^2V^{-1}S^{-1}$at fixed electron mobility $2x10^{-8}$ $m^2V^{-1}S^{-1}$. And then we vary the electron mobility from $5x10^{-8}$ $m^2V^{-1}S^{-1}$ to $100x10^{-8}$ $m^2V^{-1}S^{-1}$at fixed hole mobility $2x10^{-8}$ $m^2V^{-1}S^{-1}$. Using this numerical simulation different parameter such as short circuit current density, open circuit voltage, fill factor, efficiency has been studied to understand the dependency of carrier mobility on device performance.

4. Result and Discussion

As stated earlier, at first electrical simulation for P3HT: PCBM based organic solar cell with the variation of hole mobility has been done at constant electron mobility $2x10^{-8}$ $m^2V^{-1}S^{-1}$. As noticed from fig 3, short circuit current density is found to decrease with hole mobility which is due to the loss in free charges n and p due to the Langevin recombination which increases with charge mobility as shown in equation 6 [7,8]

$$R_D = \frac{e(\mu_n + \mu_p)}{\epsilon_0 \epsilon_r}(np - n_0 p_0) \tag{6}$$

Fig 4 shows the variation of open circuit voltage with hole mobility and it is found to decrease with hole mobility. This is in good agreement with equation 7 [9].

$$qV_{OC} = E_g - 2\left(E_{F,H} - E^D_{HOMO}\right) + K_B T \ln\left(\frac{\mu_n}{\mu_p}\right) \quad (7)$$

Fill factor is found to increase with the hole mobility due to the decrease in short circuit current density and open circuit voltage and has the tendency to become constant at higher hole mobility. The efficiency vs. hole mobility for P3HT: PCBM based solar cell has been shown in fig 6. A peak has been noticed at hole mobility $2\text{x}10^{-7}$ $m^2V^{-1}S^{-1}$ which corresponds to the 4.43% efficiency.

Next electrical simulation for study the P3HT: PCBM based solar cell performance with the variation of electron mobility has been investigated for constant hole mobility $2\text{x}10^{-8}$ $m^2V^{-1}S^{-1}$. For short circuit current density a similar behavior has been noticed which is also in good agreement with equation [6].

V_{OC} is found to increase with electron mobility up to $4\text{x}10^{-7}$ $m^2V^{-1}S^{-1}$after that it decreases very slowly. Fill factor vs. electron mobility has been found to vary in similar manner as shown in following fig 9. Though V_{OC} increases at first, but rapid decrease in J_{SC} results in increase in FF with electron mobility. Efficiency is found to increase with electron mobility up to $7\text{x}10^{-7}$ $m^2V^{-1}S^{-1}$ and then it becomes constant at nearly 4.95%.

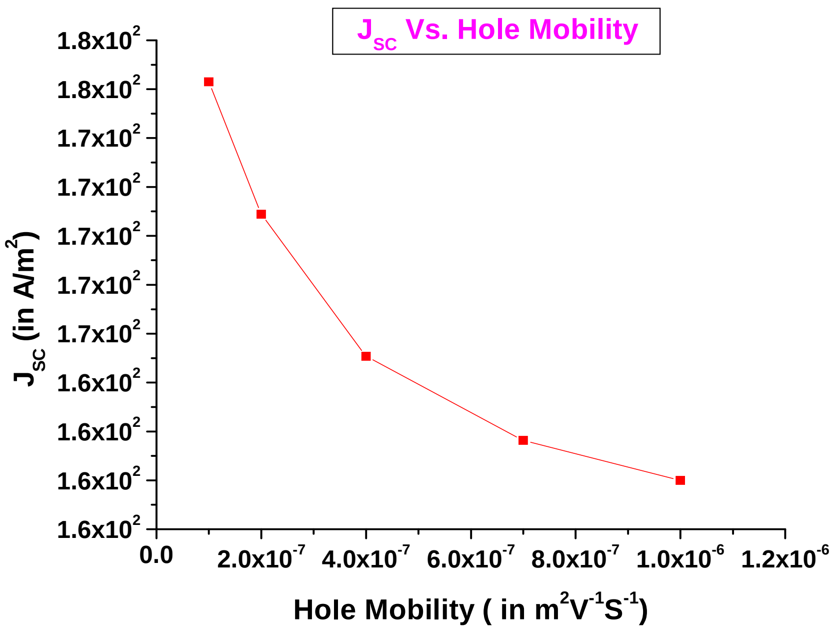

Figure 3: Short circuit current density vs. hole mobility

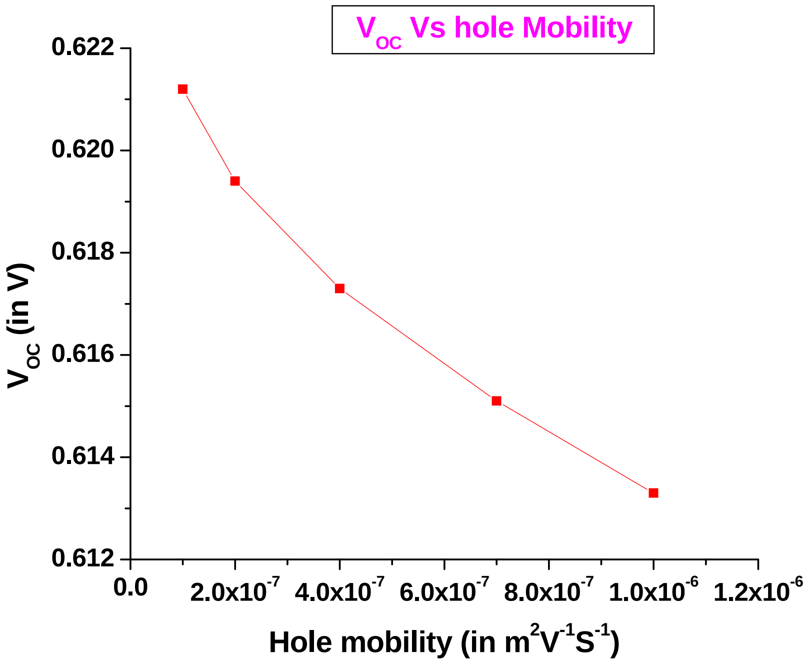

Figure 4: Open circuit voltage vs. hole mobility

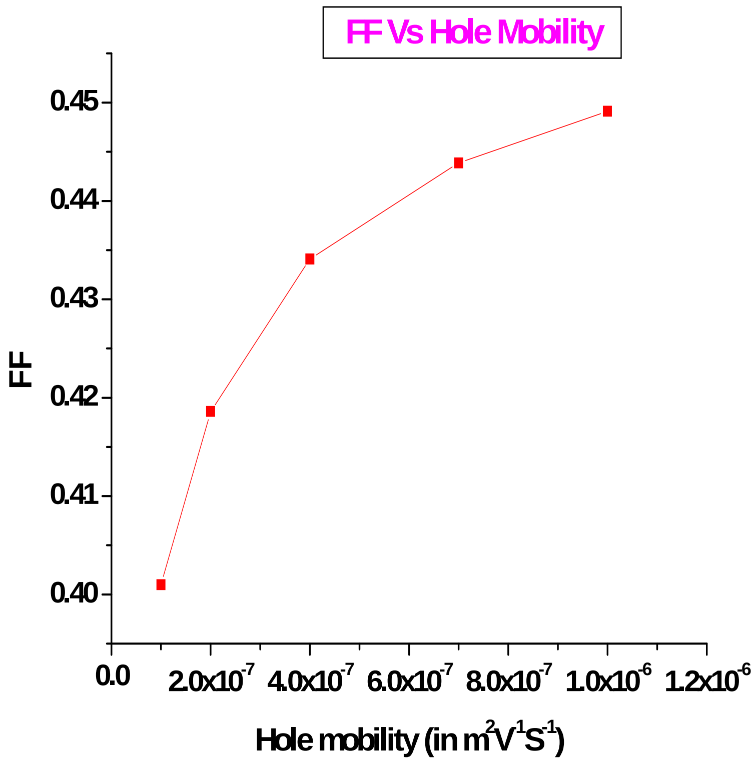

Figure 5: Fill Factor vs. hole mobility

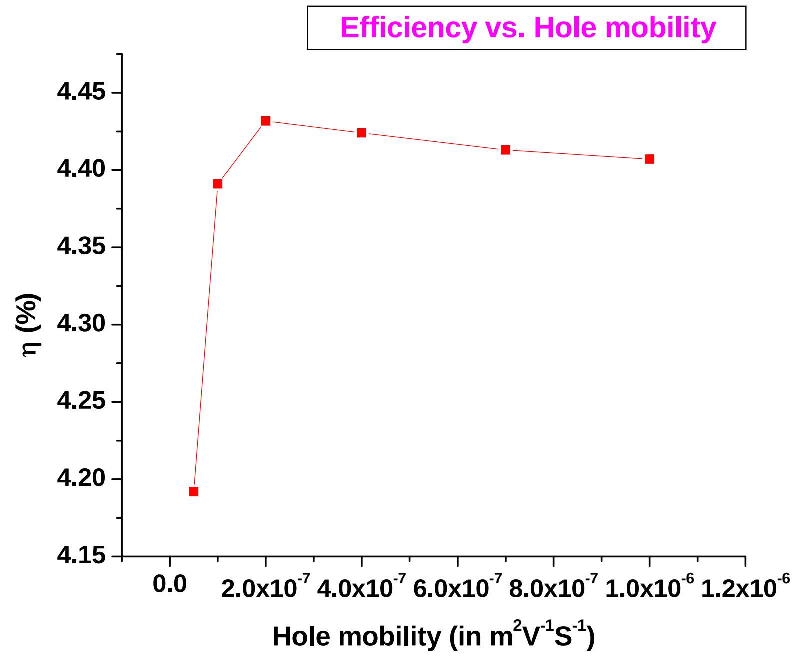

Figure 6: Efficiency vs. hole mobility

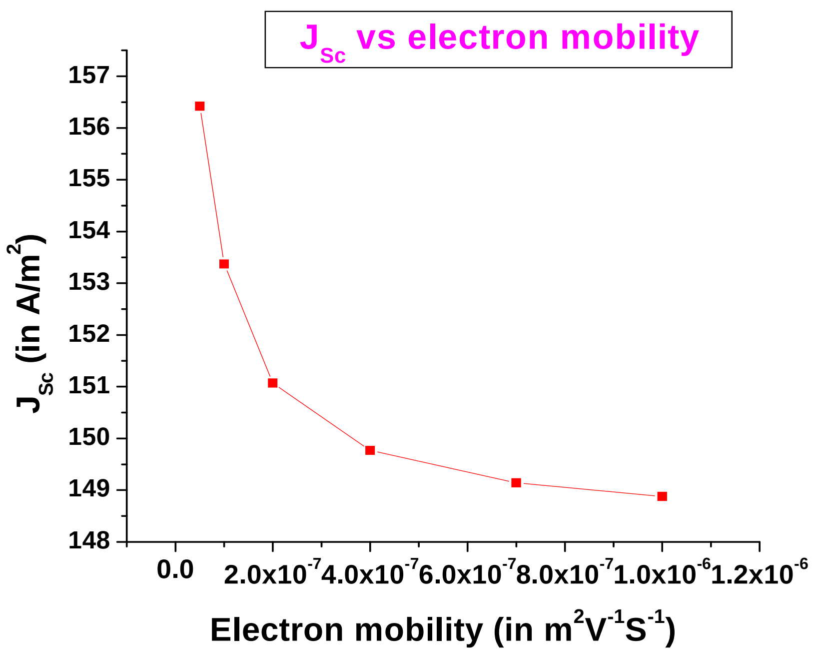

Figure 7: Short circuit current density vs. electron mobility

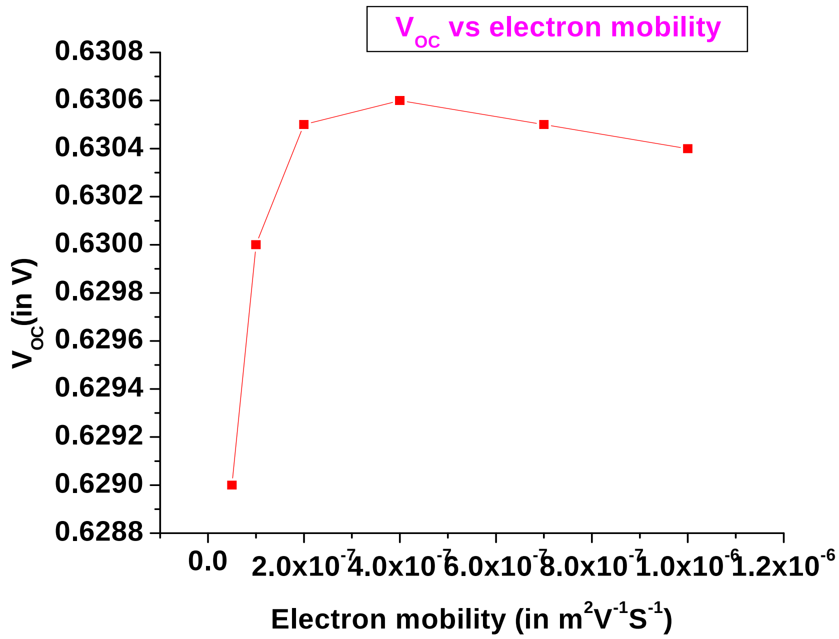

Figure 8: Open circuit voltage vs. electron mobility

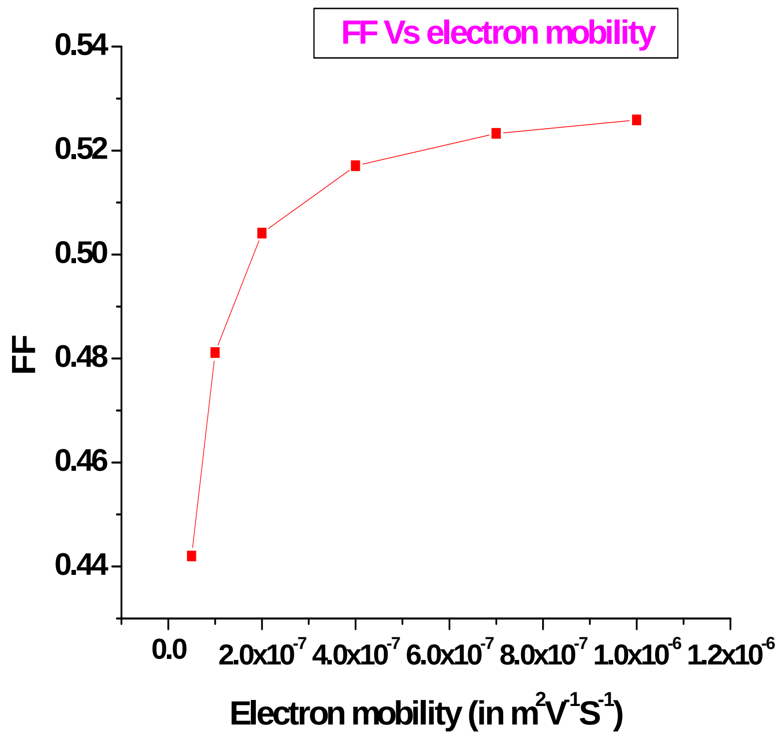

Figure 9: FF vs. electron mobility

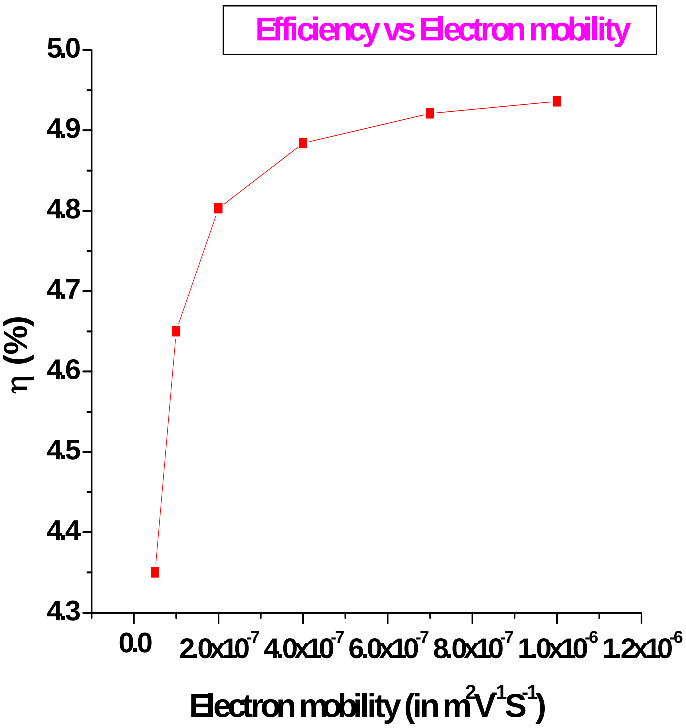

Figure 10: Efficiency vs. electron mobility

5. Conclusion

Investigation on the performance of P3HT: PCBM based organic solar cell ITO/PEDOT: PSS/P3HT: PCBM/Al structure has been done in this article. Both the effect of hole and electron mobility has been studied separately using simulating software GPVDM. Maximum 4.43% efficiency has been found for hole mobility $2x10^{-7}$ $m^2V^{-1}S^{-1}$ with fixed electron mobility $2x10^{-8}$ $m^2V^{-1}S^{-1}$. From electron mobility variation, 4.95% efficiency can be achieved with minimum electron mobility $7x10^{-7}$ $m^2V^{-1}S^{-1}$ for fixed hole mobility $2x10^{-8}$ $m^2V^{-1}S^{-1}$. Results suggest that both hole mobility and electron mobility strongly affects the P3HT: PCBM based organic solar cell. Thus to enhance the OSCs performance, charge carrier mobility has to be optimized.

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