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Bulk-heterojunction solar cells with different active layer blends: Comparison of experimental and theoretical results

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ABSTRACT

Bulk-heterojunction (BHJ) organic solar cells (OSCs) were fabricated with various active layer materials. Solar cells of configuration ITO/PEDOT:PSS/P3HT:PC$_{61}$BM/Al, ITO/PEDOT:PSS/P3HT:PC$_{71}$BM/Al and ITO/PEDOT:PSS/PCDTBT:PC$_{71}$BM/Al were fabricated. Current density-voltage (*J-V*) characteristics were measured in the dark and under illumination in ambient conditions. A single theoretical model was able to explain the *J-V* characteristics of all freshly prepared cells using realistic parameters. Copyright © 2015 VBRI Press.

Keywords: Organic solar cells; theoretical analysis; P3HT; PCDTBT; PCBM; drift-diffusion model; freshly prepared.

Introduction

Photovoltaic devices based on composites of conjugated polymer/fullerene have emerged as promising candidates for solar cell applications [**1**]. The theoretical analysis of *J-V* characteristics is an important practice for understanding the charge conduction mechanisms and thus facilitating better device design for enhanced efficiency and stability. Various theoretical models have been suggested to explain the behavior of OSCs [**2-6**]. In the present work we have attempted to explain the conduction phenomenon of P3HT:PC$_{61}$BM, P3HT:PC$_{71}$BM and PCDTBT:PC$_{71}$BM based solar cells with a single theoretical model [**6**].

Experimental

The solar cells were fabricated with vertical layer configuration as ITO/PEDOT:PSS/Active Layer/Aluminum. Indium tin oxide (ITO) (10 Ω/sq) coated glass substrates were cleaned with soap solution in ultrasonic bath and then rinsed in deionized (DI) water for 15 minutes each. The substrates were then boiled in acetone (10 minutes), isopropanol (10 minutes) and trichloroethylene (10 minutes), followed by an oxygen plasma treatment (5 minutes) prior to film deposition. A ~50 nm thick film of poly(3,4-ethylenedioxythiophene)-poly(styrene sulfonate) (PEDOT:PSS) was spin coated at 2000 rpm for one minute and then annealed in vacuum at a temperature of 120 °C for 20 minutes. For all the active materials, o-dichlorobenzene was used as solvent. The active layer blend ratios and concentrations have been chosen from previously optimized conditions [**7, 8**]. The active layer of P3HT:PC$_{61}$BM (20 mg/ml and 1:1 ratio) and P3HT:PC$_{71}$BM (20 mg/ml and 1:1 ratio) were spin coated at 600 rpm for one minute to get a film thickness of ~150 nm (dried in vacuum oven at 100 °C for 30 min), while the active layer of PCDTBT:PC$_{71}$BM (12 mg/ml and 1:4 ratio) was spin coated at 1000 rpm for one minute to maintain a film thickness of ~100 nm (dried in vacuum for 24 hours). The aluminum electrodes (~100 nm) were finally thermally evaporated in a vacuum of 10^{-6} torr. Solar simulator, SS50AAA, with 100 mWcm^{-2} intensity and Keithley-2400 source meter were used for taking *J-V* measurements. The measurements were taken immediately after aluminum contact deposition (referred as freshly prepared samples) at room temperature. All the chemicals are procured from Sigma Aldrich chemicals.

Theoretical Model

The continuity equation for electron current in dark is given by,

$$J_D = q\mu n(x)F + qD_n\frac{\partial n(x)}{\partial x}$$

where, μ is the charge carrier mobility, *n(x)* is electron density, *F* is the electric field and D_n is the diffusion coefficient. This equation has been further solved by assuming a constant electric field both in the dark and under illumination, and following equation has been obtained for OSC in the dark [**6**],

$$J_D = \frac{q^2 D_n N_C (V_{bi} - V) \exp\left(\frac{-\varphi}{kT}\right)\left(\exp\left(\frac{qV}{nkT}\right) - 1\right)}{dnkT\left(1 - \exp\left(\frac{-q(V_{bi} - V)}{nkT}\right)\right)} \quad (1)$$

where, J_D is the dark current density, k is Boltzmann constant, T is temperature in Kelvin, n is the diode ideality factor, V_{bi} is the built-in voltage, V is the applied voltage, d is sample thickness, N_C is the effective density of states, φ are the electron injection barriers at the electrodes and D_n is the diffusion coefficient. Also $Dn = \mu \frac{KT}{q}$ where, μ is the charge carrier mobility.

Under illumination the J-V characteristics for OSCs is given by [**6**],

$$J_L = \frac{q^2 D_n N_C (V_{bi} - V) \exp\left(\frac{-\varphi}{kT}\right)\left(\exp\left(\frac{qV}{nkT}\right) - 1\right)}{dnkT\left(1 - \exp\left(\frac{-q(V_{bi} - V)}{nkT}\right)\right)} - J_L(V) \quad (2)$$

where, JL(V) is the photo-generated current density and has been calculated under ideal conditions by,

$$J_L(V) = |J_{SC}|\mu\tau \frac{(V_{bi} - V)}{d^2}$$

τ is the lifetime of the charge carrier, JSC is the short circuit current density.

Results and discussion

Fig. 1 shows the experimental current density-voltage (*J-V*) characteristics of P3HT:PC$_{61}$BM OSC in the dark and under illumination.

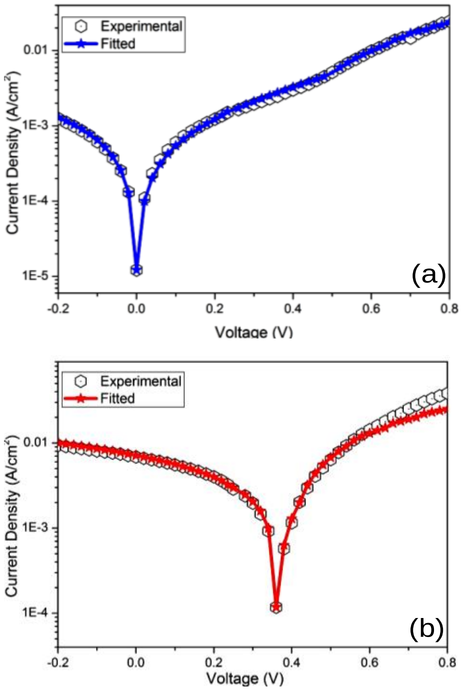

Fig. 1. Experimental and fitted *J-V* characteristics of freshly prepared P3HT:PC*61*BM OSC (a) dark characteristics (b) illuminated characteristics.

The open circuit voltage values (V_{oc}) and short circuit current density (J_{sc}) was found to be 0.38 V and 5.03 mA/cm^2 respectively. It was observed from the figure that theoretical curves agree well with the experimental data. The realistic parameters used for the theoretical calculations using equation 1 and equation 2 were [**6, 9**] T=295K, $N_c = 10^{19}$cm^{-3}, n=1.8, V_{bi}= 0.47V, d= 150 nm, $\tau = 2.5\times10^{-5}$ s, $\mu = 9.9\times10^{-5}$ cm^{2}v^{-1}s^{-1}.

The *J-V* characteristics of freshly prepared P3HT:PC$_{71}$BM OSC was shown in **Fig. 2**. The values of V_{oc} and J_{sc} for P3HT:PC$_{71}$BM OSCs were found to be 0.44 V and 3.25 mA/cm^2 respectively. It was observed that the experimental data is well explained by drift-diffusion model. The realistic parameters used for the fitting of P3HT:PC$_{71}$BM OSC were [**6, 9**] T=295K, N_c= 10^{19}cm^{-3}, n=1.7, V_{bi}= 0.45V, d= 100 nm, τ= 2.0×10^{-5}s, μ= 1.0×10^{-4} cm^{2}v^{-1}s^{-1}.

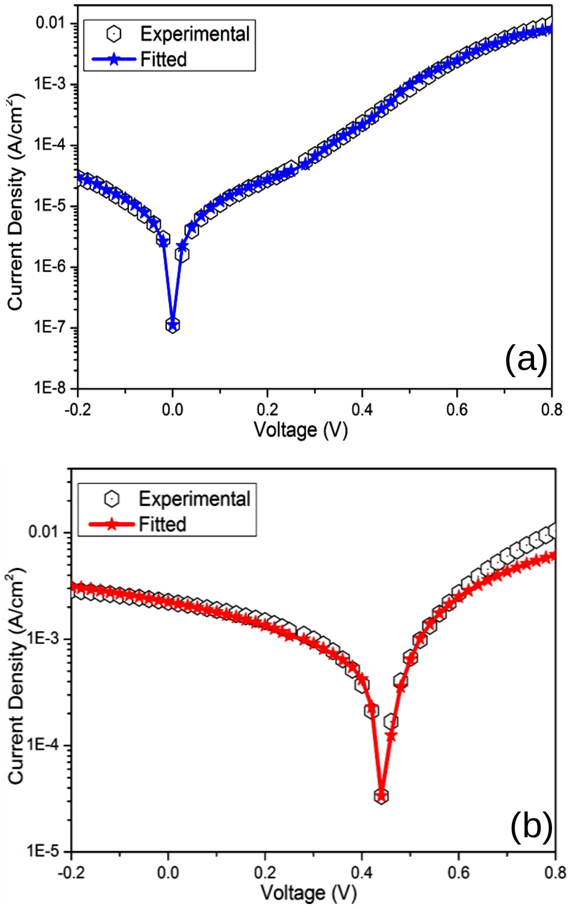

Fig. 2. Experimental and fitted *J-V* characteristics of freshly prepared P3HT:PC$_{71}$BM OSC (a) dark characteristics (b) illuminated characteristics.

Fig. 3 shows the dark and illuminated *J-V* characteristics of PCDTBT:PC$_{71}$BM OSC. It was observed that V_{oc} has improved to 0.67 V and J_{sc} to 9.21 mA/cm^2. Experimental *J-V* characteristics were shown to be in good agreement with the theoretical curves. The realistic parameters taken for theoretical calculation were [**10-11**] T=295 K, N_c = 10^{20} cm^{-3}, n=1.8, V_{bi}= 0.66V, d= 100 nm, τ = 9.0×10^{-5} s, μ = 1.0×10^{-4} cm^{2}v^{-1}s^{-1}. Higher value of V_{oc} and J_{sc} of PCDTBT:PC$_{71}$BM OSC can be attributed to the larger difference between HOMO of acceptor and LUMO of donor in these solar cells as compared to previous solar cells, which further influences charge dissociation and charge transport [**12**].

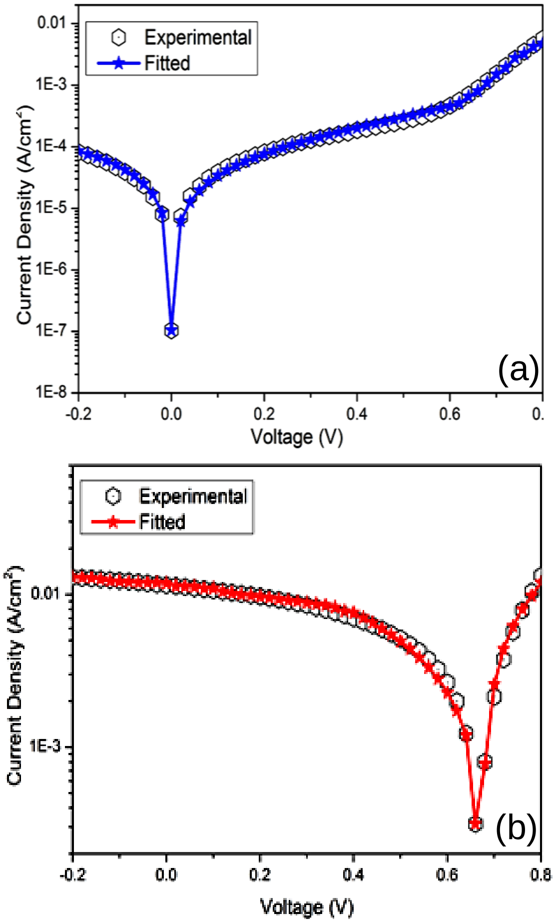

Fig. 3. Experimental and fitted J-V characteristics of freshly prepared PCDTBT:PC71BM OSC (a) dark characteristics (b) illuminated characteristics.

Fig. 4 shows the energy band diagram of the three donor acceptor combinations used for the active layer of the devices. The theoretical value of V_{oc} in conjugated polymer-fullerene solar cell is given by the following empirical formula [**13**],

$$eV_{oc} = \left[\left|E_{HOMO}^{Donor}\right| - \left|E_{LUMO}^{Acceptor}\right|\right] - 0.3eV \tag{3}$$

where, E is the energy level, e is the elementary charge, and 0.3 eV is an empirical value for efficient charge separation.

Equation 3 implies that greater the difference between HOMO of the donor and LUMO of the acceptor, higher will be the value of V_{oc}. It can be observed from **Fig. 4** that the PCDTBT:PC_{71}BM combination has highest energy difference which can be correlated with the highest V_{oc} obtained experimentally for this system. Further, the short circuit current (I_{sc}) in OSC depends upon the dissociation efficiency of exciton, which in turn is determined by the offset between the LUMO of the donor and the LUMO of the acceptor [**14**]. Generally, the minimum difference required between LUMO of donor and acceptor is 0.3 eV, and any energy difference greater than this will simply result in wasted energy [**15**]. Therefore, it can be observed from **Fig. 4** that PCDTBT:PC_{71}BM has the optimum energy offset values, thereby giving highest values of V_{oc} and J_{sc} as compared to the other two combinations. In conclusion, it is very interesting to observe that *J-V* characteristics of all freshly prepared solar cells can be exclusively explained by a single drift-diffusion theory.

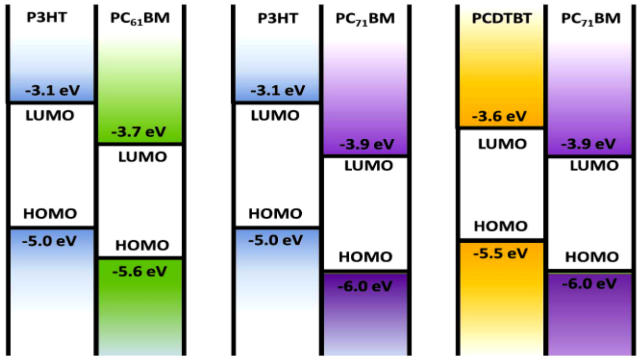

Fig. 4. Energy band diagram of P3HT:PC_{61}BM, P3HT:PC_{71}BM and PCDTBT:PC_{71}BM active layers.

Conclusion

Organic solar cells with different active layer materials were fabricated in the ambient conditions. Single theoretical model has been used to explain the *J-V* characteristics of various OSC. It was observed that the experimental curves were in good agreement with the theoretical generated curves using realistic parameters. Higher V_{oc} and J_{sc} in PCDTBT:PC_{71}BM OSC was due to the optimum difference between HOMO and LUMO of donor and acceptor material in these solar cells.

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