Evolving Trends in Engineering and Technology *Online: 2014-12-01*
ISSN: 2349-915X, Vol. 3, pp 30-36
doi:10.18052/www.scipress.com/ETET.3.30
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Recent Modeling of MDMO-PPV: PCBM Solar Cells Versus Mixture Ratio, Electric Field and Incidence Angle with Hopping Model

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Keyword: Hopping model, organic polymer solar cells, electric field, mixture ratio

ABSTRACT. It is a matter of controversy why excitons can efficiently dissociate into free carriers at an intrinsic polymer/fullerene interface. While extensive characterization is performed in the course of many reported experimental studies, correlation of performance and physical parameters among studies done in different laboratories is low, pointing out the need to address some aspects of BHJSC active materials that have received relatively some attention.
In this paper, we discuss the modeling of MDMO-PPV/PCBM(Poly(2-methoxy-5-(3,7-dimethyloctyloxy)-1,4-phenylenevinylene)/ soluble C60 derivative, methanofullerene, [6,6]-phenyl C61-butyric acid methyl ester organic devices. In our approach, we apply two recent methods so called transfer matrix method and hopping model to calculate the exciton dissociation probability, and photocurrent density versus mixture ratio, electric field and angle of incidence. The results show that EDP (exciton dissociation probability) in solar cells without PEDOT-PSS (Poly (ethylendioxythiophene)-Poly(styrene sulfonic acid)) HTL hole transporting layer is better than the cells with additional layer in enhancing the performance of MDMO-PPV/PCBM solar cells. When the weight ratio of MDMO-PPV is less than 3:5 and 2 :5 respectively, the best exciton dissociation probability, and photocurrent density of solar cell is obtained

1. INTRODUCTION

Polymer solar cells (PSCs), considered as a promising source of renewable energy, have attracted much attention because of their low-cost, compatibility with flexible substrates and large-area applications[1,4]. Recently, the power conversion efficiency of the bulk heterojunction (BHJ) PSCs around 7.4% has been realized [5,6].
The photovoltaic effect involves the generation of electron and hole pairs and their subsequent collection at the opposite electrodes. In inorganic materials, the photon absorption produces free charge directly. The conjugated semiconducting polymers used in photovoltaic typically have low dielectric constants, which causes Frenkelexcitons to be created upon light absorption [7]. These Coulombically bound electron–hole pairs have a binding energy of approximately 0.5 eV [8]. Higher efficiency devices were prepared from MDMO-PPV/[6]PCBM blends reaching 3.1% in the so-called bulk heterojunction geometry, PEDOT: PSS (Figure.1) is solution processible and possesses a suitable work function to act as an effective hole transporting layer in the word of organic solar cells[9].

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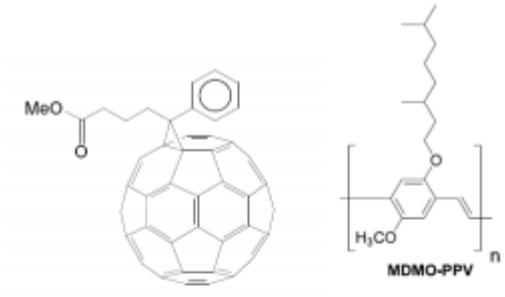

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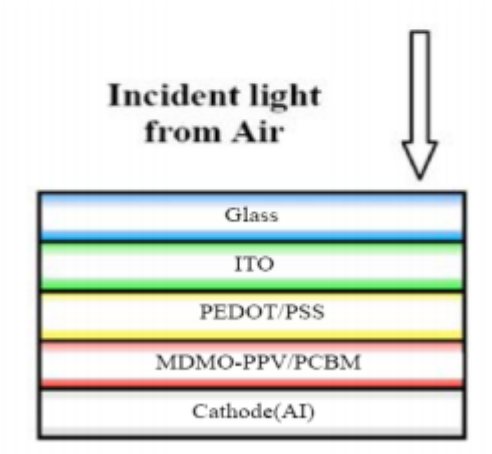

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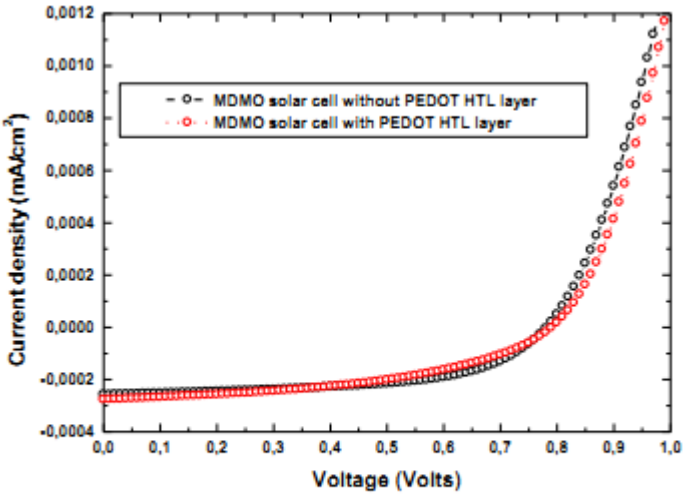

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Figure 1 Chemical structures of the used conjugated organic polymers, namely, PCBM(C60) and MDMO-PPV (a) Schematical diagram of an organic solar cell (b) Current density versus bias of the studied solar cells (c) [9]

In this paper we present an overview of recent achievements in experimental and theoretical studies of a hopping transport mechanism and there relaxation parameters by an analytical model, which is done in the next section introducing mixture ratio and incidence angle in addition to electric field contributed by S.D Baranovskii et al [13]. Finally, outlooks for the development of organic electronic devices based on the studied materials are given.

2. Model and calculation method

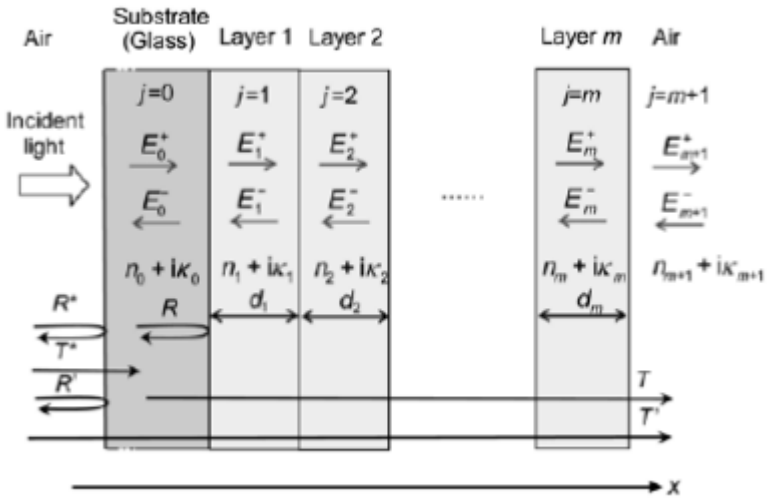

Figure 2 Geometry of a general multilayer structure [12]

To investigate the effect of applying an HTL layer to a cell as described above, a method of determining the optical transmission and reflection properties of a multilayer system is required that also includes the interference effects. The approach used here is the multiplication of the matrixes [9] that describe how the wave propagates by the whole device. Figure.2 shows the arrangement of propagation of the forwards and towards fields in the back of the device under AM 1.5 solar spectrum.

We start by decomposing the optic electrical field into an upstream and a downstream component [10]. The equation (1) gives the sum of the electric field in the positive and the negative directions respectively as

$$E_j(x) = E_j^+(x) + E_j^-(x) \tag{1}$$

The total system transfer matrix Swich relates the electric field between the substrate (j=o) and ambient side (j=m+1) by

$$\begin{bmatrix} E_0^+ \\ E_0^- \end{bmatrix} = S \begin{bmatrix} E_{m+1}^+ \\ E_{m+1}^- \end{bmatrix} \tag{2}$$

where S is the product of all interface and layer matrices that light propagates through orderly.

$$\begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} = S \begin{bmatrix} E_{m+1}^+ \\ E_{m+1}^- \end{bmatrix} \tag{3}$$

$$T' = \frac{T^* T}{1 + R^* R} \tag{4}$$

$$R' = \frac{R^* + R}{1 + R^* R} \tag{5}$$

with

$$T^* = [2/(1+n_0)]^2$$

and

$$R^* = [(1-n_0)/(1+n_0)]^2$$

According to Fresnel relation for transmission and reflection and n0 is the real index of reflection of the substrate.
For other details, the readers can overview references [10-11].
The calculation of the exciton dissociation probability is according to the following equation [13]

$$\eta(E) \approx \left[1 + (\nu_0 \tau_0)^{-1} \exp\left(\frac{-E_b - \beta\sqrt{E}}{k_B T}\right)\right]^{-1} \tag{6}$$

$$C = \frac{e^2}{4\pi\varepsilon\varepsilon_0 k_B T r_0},$$

$$B = \frac{eEr_0}{k_B T},$$

and $$\beta = \left(\frac{e^3}{\pi\varepsilon\varepsilon_0}\right)^{1/2}$$

where
υ_0 is the attempt-to-escape frequency, E_b is the exciton binding energy,
k_B is the Boltzmann constant,
T is the temperature,
e is the elementary charge,
ε is the dielectric constant,
ε_0 is the permittivity of vacuum,
r_0= 1 nm.
The mixture molar ratio of the donor to the totals implemented in the hopping model for the first time is defined as [14]

$$\zeta = \frac{\varepsilon - \varepsilon_{HOS}}{\varepsilon_{DOP} - \varepsilon_{HOS}} \tag{7}$$

where ε_{DOP} and ε_{HOS} are the dopant and host dielectric constant, respectively.

The photogenerated current is equal as given in [17]

$$J_{ph} = eGL\left[\frac{\exp(eV/k_B T)+1}{\exp(eV/k_B T)-1} - \frac{2k_B T}{eV}\right] \tag{8}$$

where
V is the effctivepotensial,
k_B the Boltzman constant,
T the temperature
eGL represents the saturated photocurrent.

3. Results and discussion

MDMO-PPV composite materials were evaluated as electron donor/acceptor materials in ITO-free organic bulk heterojunction solar cells by using glass as substrates. We are interested in this work to the mixture ratio in order to optimize exciton dissociation probability (EDP) and photocurrent of MDMO-PPV based solar cells using analytical hopping model, where physical constants are taken from [13,14,15] and wavelenght was fixed at 600nm[16].

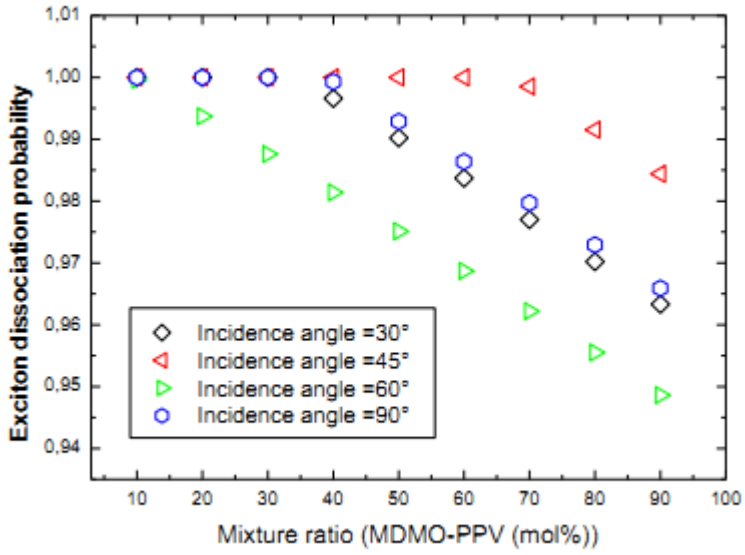

Figure 3 Exciton dissociation probabilty versus mixture ratio at different angles of incidence with PEDOT/PSS additional layer

Figure 3 show that the best values of the EDP are reported for less than 40% of mixture rato at angle of incidence 45°, 90° and 30° respectively. Figure 4 shows that the best values of the EDP are reported for less than 60% of mixture ratio at angle of incidence 60° and 90° respectively when EDP is acceptable for 30° and 45°. The clear difference is the effect of the PEDOT: PSS layer when it affect the dissociation probability earlier (decreasing rapidly at mixture ratio more than 45%). Several electrical properties are reducing at this range in the work presented by[14].

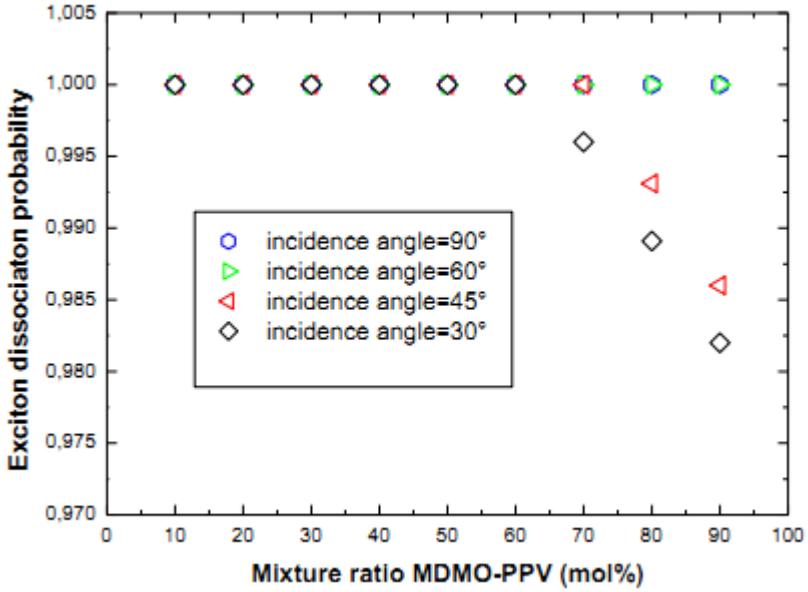

Figure 4 Exciton dissociation probability versus mixture ratio at different angles of incidence without PEDOT/PSS additional layer

From the results reported here and by ploting the photocurrent density versus electric field in a log-log diagram, we show that a good linear correlation between the last parameters was governed, and a general equation modeling the phenomena for all incidence angles is written as

$$\frac{J_{ph1}}{J_{ph2}} = 0.87 \tag{9}$$

J_{ph1} and J_{ph2} are the calculated photocurrent for solar cells with and whithout additional layer in PEDOT: PSS respectively.
The same result(~0.89) is giving by dividing experimental values of the two cells fabricated by [9] which the thickness of the HTL layer is 140nm at V=1 volt. The majority of the photocurrent optimizations results (Figure.5) are given by 0.9 of the mixture ratio and r_0=1.1 nm for any incidence angle.

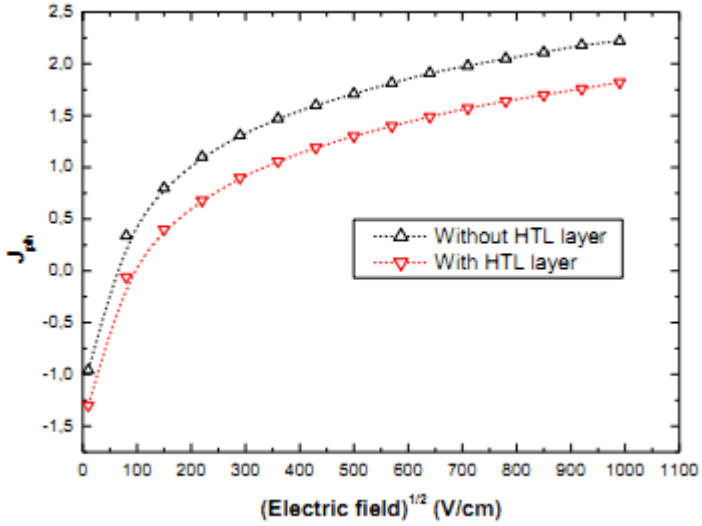

Figure 5 Normalized photocurrent versus electric field with the following parameters: Incidence angle is 30° λ =600 nm and V=1volt with/without HTL layer.

Conclusion

In conclusion, we have shown that the electric field dependence of MDMO-PPV/PCBM based solar cells, in the range from 0 to 1000 V/cm, can be used in terms of a model coupling mixture ratio of donor materials and incidence angle by hopping transport to enhance exciton dissociation probability and photogenerated current density in disordered materials. We show that the best exciton dissociation probability is performed at less than 40% of mixture ratio for solar cells with and without HTL layer. The same analytical model that covers all relevant processes among photons, excitons and charges provides a powerful framework for extracting material and device parameters by a combined experimental and simulation approach.

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