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A physics-based analytical model for bulk heterojunction organic solar cells incorporating monomolecular recombination mechanism

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ABSTRACT

We present an analytical model for bulk heterojunction organic solar cells incorporating the physics of recombination in the transport equations. Monomolecular recombination process is considered to be the dominant mechanism and treated explicitly. The proposed analytical model shows good agreement with the experimental data as well as with the numerical simulations. The improvements over the previous models are also presented to show the importance of considering the recombination process. The model can be used to find device characteristics such as current–voltage characteristic, efficiency etc. of bulk heterojunction organic solar cells avoiding the mathematical complexities of numerical models.

1. Introduction

In recent years, organic solar cells (OSCs) have got extensive attention due to their thin, light weight, flexible and low cost features which conventional silicon solar cells cannot provide [1–7]. The field of OSC can be divided into two major segments – bilayer heterojunction and bulk heterojunction (BHJ) solar cells [4]. The OSC based on bilayer configuration usually cannot provide high efficiency because the diffusion length of excitons (bound electron–hole pair) is very small (about 10 nm) and thus most of the excitons decay to the ground states before reaching to the donor–acceptor (D–A) interfaces of bilayer configuration. Conversely, excitons can easily reach to D–A interfaces in a BHJ configuration due to the presence of sufficient interfaces near to them [3]. Therefore, high efficiency is achieved in this configuration. The performance of BHJ OSCs have been improved significantly in the last few years [8–10] and the power conversion efficiency of up to 10.6% has been achieved recently for a tandem BHJ solar cell [3]. However, there are still many questions left unanswered regarding charge generation, recombination and transport mechanisms for these cells [11]. To understand these phenomena and optimize their performance accurate and efficient device models are required. The modeling of organic BHJ solar cells has been mainly limited to numerical studies and has been extensively investigated [4–7]. Few research groups [12–14] have also performed analytical and/or physically-based modeling of the current–voltage (J–V) characteristic of BHJ OSCs. Drift and diffusion charge transport has been ignored in the model given by Marsh et al. [12] which limits its capability. Kumar et al. [13] derived their model without accounting the carrier generation and recombination processes physically. Later, Altazin et al. [14] proposed a physically-based analytical model for BHJ OSCs assuming recombination rate is much smaller than the generation rate. However, no analytical model has been proposed yet for BHJ solar cells incorporating the recombination mechanism explicitly. In this work, we present an analytical model for BHJ OSCs incorporating the physics of monomolecular recombination in the transport equations. We follow the numerical model proposed by Liu and Li [15] to incorporate the recombination process and derive an analytical model from it. The poly(3-hexylthiophene):[6,6]-phenyl-C_{61}-butyric acid methyl ester (P3HT:PCBM) based solar cells have been used for this work. The model has been compared with established numerical model [5] and experimental data [15] to justify its validity.

2. Theory

In this section, we describe the development of our analytical model along with the OSC configuration. The BHJ OSC configuration shown in Fig. 1(a) (not in scale) has been considered for this study. The active layer is considered as a 1:1 weight ratio of 100 nm thick

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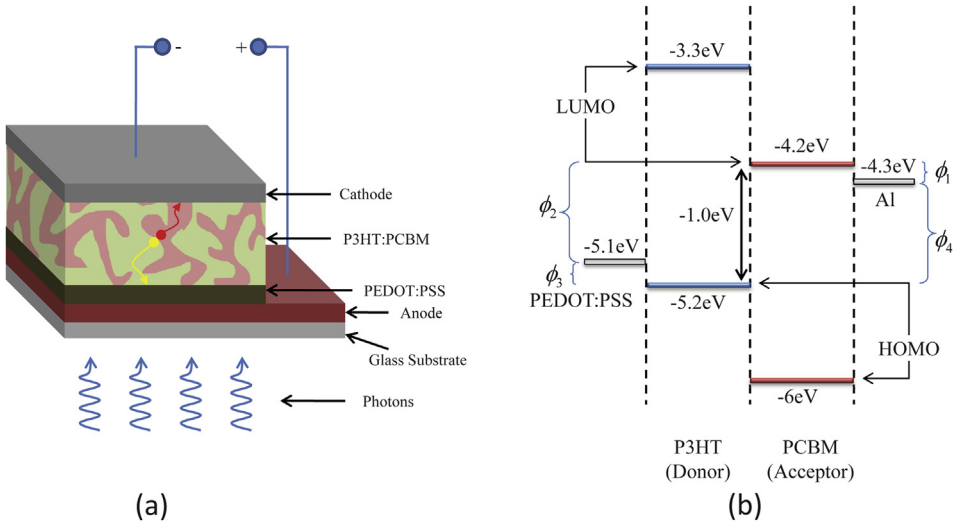

Fig. 1. (a) Configuration of P3HT:PCBM based BHJ OSC and (b) Schematic energy potential diagram of the considered cell (before the materials are brought into contact).

P3HT:PCBM blend sandwiched between aluminum layer (cathode) and poly(3,4–ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) layer. The PEDOT:PSS layer is covered by indium tin oxide (ITO). A schematic energy potential diagram of this structure (before the materials are brought into contact) is shown in Fig. 1(b). The energy potential values are taken from literature [4,15–17]. In this study, we have considered PEDOT:PSS as the injecting layer similar to the previous models [4,13,14]. When photons are absorbed by the active layer, tightly bounded electron–hole (e–h) pairs are generated. Afterward, these e–h pairs are separated in the form of free electrons and holes by the built-in potential at the interfaces between the donor and acceptor materials. Both charge carriers then travel to their respective electrodes as shown in Fig. 1(a).

To calculate the J–V characteristics of the device, one needs to find the charge density as a function of device parameters (such as electron and hole concentration (n and p, respectively) as function of position). The charge density can be calculated from the continuity equations [Eqs. (1) and (2)]:

$$-\frac{1}{q}\frac{\mathrm{d}J_n}{\mathrm{d}x} = G - R_n, \tag{1}$$

$$\frac{1}{q}\frac{\mathrm{d}J_p}{\mathrm{d}x} = G - R_p, \tag{2}$$

where G is the carrier generation rate, $R_{n(p)}$ is the recombination rate of electron (hole) and q is the unit charge. $J_{n(p)}$ is the electron (hole) current density which can be expressed as:

$$J_n = q\mu_n nE + qD_n\frac{\mathrm{d}n}{\mathrm{d}x}, \tag{3}$$

$$J_p = q\mu_p pE - qD_p\frac{\mathrm{d}p}{\mathrm{d}x}, \tag{4}$$

where $\mu_{n(p)}$, $D_{n(p)}$ and E are the electron (hole) mobility, electron (hole) diffusion coefficient and electric field within the active layer of device structure, respectively. We use the classical Einstein relation ($D_{n(p)}/\mu_{n(p)} = kT/q = V_T$) for the diffusion coefficients similar to previous authors [5,14,15], where k is the Boltzmann's constant, T is the absolute temperature and V_T is the thermal voltage.

It can be seen that Eqs. (1) and (2) cannot be solved analytically for bimolecular recombination mechanism (i.e., $R_n = R_p = r_b np$ in which r_b is the bimolecular recombination coefficient) even if we use uniform electric field approximation (E = constant). Therefore, the recombination terms were not explicitly considered in the previous works [13,14]. This approximation [14] seems to have done a quite fair job for matching the experimental J–V curve of Koster et al. [5]. However, it may not be valid for all cases; especially where monomolecular recombination mechanism is dominant and/or the recombination rate is comparable to the generation rate [15] which will be discussed more elaborately in the next section. Interestingly, we note that, for the case where monomolecular recombination mechanism is dominant and recombination rate is comparable to the generation rate, an analytical solution can be obtained.

To obtain a complete analytical model for J–V characteristic of BHJ cell, we have used constant generation rate and uniform electric field approximations which are generally the cases in thin active layers (up to ~200 nm). Since our active layer thickness is 100 nm (as described earlier), these approximations are also valid for this study. Similar assumptions have also been used by other authors for such devices [6,12–14]. Using uniform electric field approximation, the electrostatic field can be written as [13]:

$$E = \frac{V_a - V_{bi}}{L}, \tag{5}$$

where E is the electric field through the whole active layer, L is the active layer thickness, V_a is the terminal voltage (note that, conventionally V_a is termed as applied bias in literature), and V_{bi} is the built-in potential of the device. V_{bi} can be calculated from the difference of the electrodes work-functions [13,14,18].

Under the above realistic assumptions, the continuity equations can be written in the following form:

$$-V_T\mu_p\frac{\mathrm{d}^2p}{\mathrm{d}x^2} + E\mu_p\frac{\mathrm{d}p}{\mathrm{d}x} = G - r_m p, \tag{6}$$