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ScienceDirect

Solar Energy 126 (2016) 64–72

SOLAR ENERGY

www.elsevier.com/locate/solener

Brief Note

An analytical model for bulk heterojunction organic solar cells using a new empirical expression of space dependent photocarrier generation

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Received 19 October 2015; received in revised form 15 December 2015; accepted 29 December 2015
Available online 13 January 2016

Communicated by: Associate Editor Frank A. Nüesch

Abstract

We present an analytical model for bulk heterojunction organic solar cells on the basis of an empirical expression of space dependent carrier generation rate. By developing the empirical formula of the carrier generation rate and successfully incorporating that in the transport equations, we bring in the spatial distribution effect of generation rate into the current–voltage (J–V) characteristic of this solar cell. The proposed empirical expression helps us to derive a J–V curve expression, especially for the cases where carrier generation rate cannot be described by any physics-based closed form analytical expression and/or where the spatial distribution of the generation rate profile is to be extracted and used directly from published/available data. We justify the model by comparing with numerical simulations and published data.

Keywords: Organic solar cell; Bulk heterojunction; Empirical carrier generation rate; Analytical model; Current–voltage characteristic

1. Introduction

Bulk heterojunction (BHJ) organic solar cells (OSC) based on polymer:fullerene (or fullerene derivatives) composites have been receiving extensive attention due to their promising advantages (e.g. thin, light weight, flexible and low cost fabrication in large areas) over conventional photovoltaic devices (Kippelen and Brédas, 2009; Krebs, 2009; Li et al., 2012; Park et al., 2009; Hausermann et al., 2009). Recently, above 10% efficiency has been achieved for tandem polymer BHJ solar cells (Li et al., 2012; You et al., 2013; Chen et al., 2014). In general, for a BHJ photoactive layer, an electron donating material (typically conjugated polymer) and an electron accepting material (such as fullerene or fullerene derivatives) are diluted in a same solvent and spin coated as one layer (Hausermann et al., 2009). The major advantage of this BHJ active layer is the increased donor–acceptor (D–A) interfaces. When photons are absorbed in this active layer, excitons (tightly bound electron–hole pair having short life, ~10 nm diffusion length) are generated. However, due to the presence of adequate D–A boundaries, the excitons easily approach to the interfaces (in spite of their short life) and subsequently convert into free electrons and holes (Li et al., 2012). This particular mechanism has given this configuration exceptional internal quantum efficiency (fraction of collected carriers per absorbed photon). Recently, almost 100% internal quantum efficiency has been reported by a research group for their BHJ structure (Park et al., 2009). It indicates the potentiality of this device to achieve high power conversion efficiency.

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http://dx.doi.org/10.1016/j.solener.2015.12.050
0038-092X/

Further optimization and engineering of this BHJ OSC are indispensable for the commercialization of organic photovoltaic cells. Apart from experimental studies, extensive theoretical modeling and simulation are also required to optimize this device for better performance (Li et al., 2012; Park et al., 2009). In literature, several numerical modeling and simulations have been done for this device (Hausermann et al., 2009; Koster et al., 2005; Monestier et al., 2007; Sievers et al., 2006). However, compared to the numerical models, very few works (Marsh et al., 2008; Kumar et al., 2009; Altazin et al., 2011; Arnab and Kabir, 2014; Chowdhury and Alam, 2015) have been done for analytical models of BHJ OSC devices. Kumar et al. (2009) developed their model on the basis of empirical arguments by using analogy with classical p–n junction models. More physically based models have been proposed by Marsh et al. (2008) and Altazin et al. (2011). However, none of these models (Marsh et al., 2008; Kumar et al., 2009; Altazin et al., 2011) have considered the spatial distribution of carrier generation rate (with respect to position) in the active layer. Arnab and Kabir, (2014) have considered exponential decay of light intensity (known as Beer–Lambert law) within the active layer similar to the traditional solar cells consist of bulk materials (generally in μm range). However, it has already been described in literature (Li et al., 2012; Chowdhury and Alam, 2015) that Beer–Lambert law cannot model the carrier generation rate profile within the OSC device, since the reflection and interference effects become important due to its thin film (generally in nm range) based multilayer structure. Because of the reflection and interference effects, carrier generation rate profile shows oscillating nature (instead of exponential decay) with respect to the position. Transfer matrix method (Li et al., 2012; Monestier et al., 2007; Sievers et al., 2006; Pettersson et al., 1999) is generally used to model these optical phenomena. Recently, we have reported more generalized analytical model of BHJ OSC incorporating optical transfer matrix formalism explicitly (Chowdhury and Alam, 2015). However, closed form expression obtained from transfer matrix method is not always suitable to calculate the optical electric field, since this approach is based on several assumptions (Li et al., 2012; Pettersson et al., 1999). Complex numerical simulations may be required to obtain accurate carrier generation rate profile (Li et al., 2012). Therefore, when carrier generation rate cannot be predicted by any physics-based closed form expression, it may turn out to be necessary to use generation rate profile obtained from available data or complicated numerical simulations. Moreover, for some particular cases it may become indispensable to use the published data of carrier generation rate profile into the transport equations to derive a model. All these carrier generation rate profiles are required to be represented by some sort of arithmetic expression to derive an analytical model of OSC. For these cases, a generalized empirical formula of carrier generation rate profile becomes a useful tool to derive the J–V characteristic expression of BHJ OSC. However, no such formula, which accounts for the above cases, has been proposed yet in literature. It is important to mention that Furlan and Amon (1985) proposed an empirical expression of generation rate for traditional solar cells (where generation rate experiences exponential decay with respect to position) to improve the computational efficiency. However, this expression cannot be applied to the thin film based structures (because of the oscillating nature of carrier generation profile (Li et al., 2012; Monestier et al., 2007; Pettersson et al., 1999). Therefore, in this work, we have developed a new empirical form of generation rate for BHJ OSC structure and incorporated it in the transport equations to derive the J–V characteristic expression. In addition, the empirical expression has been studied for different active layer thicknesses to justify its generous applicability and the obtained results have been compared with numerical studies and published data (Monestier et al., 2007).

2. Theory

In this section, we provide a detail derivation of our BHJ OSC model using the proposed empirical formula of carrier generation rate. We consider the BHJ OSC configuration shown in Fig. 1(a) (not in scale) for our study. The active layer used in this study is based on poly(3-hexyl thiophene):[6,6]-phenyl-C_{61}-butyric acid methyl ester (P3HT:PCBM) blend having a weight ratio of 1:1. Indium tin oxide (ITO) and aluminum (Al) layers are used as anode and cathode, respectively. Similar to the previous studies poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) is considered as the injecting layer (Hausermann et al., 2009; Kumar et al., 2009; Altazin et al., 2011). The complete cell structure is ITO (180 nm)/PEDOT:PSS (45 nm)/P3HT:PCBM (different thickness)/Al (100 nm) (Monestier et al., 2007). Corresponding energy levels of different layers (Fig. 1(b)) have been taken from literature (Li et al., 2012; Hausermann et al., 2009; Li and Liu, 2011; Brown et al., 1999). Excitons are generated when the device is exposed to photons with sufficient energy. These generated excitons are tightly bounded due to the low dielectric constant of organic materials (Liu and Li, 2011). Subsequently, the excitons diffuse to the donor–acceptor interface, then dissociate into bound electron–hole (e–h) pairs (also known as polaron pairs) (Li et al., 2012; Koster et al., 2005). At this stage, electron and hole of an e–h pair are situated in different molecules (electron in the acceptor material and hole in the donor material) (Li et al., 2012). However, they remain in the bounded condition. These e–h pairs are meta-stable – they can either decay to the ground state or can be dissociated into free charge carriers. This dissociation process is considered as an electric field and temperature dependent phenomena (Koster et al., 2005). Afterward, the free charge carriers (electrons and holes) are diffused and drifted to their respective electrodes (Li et al., 2012; Koster et al., 2005; Altazin et al., 2011). The P3HT:PCBM blend has