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Simulation and optimization of the performance of organic photovoltaic cells based on capped copolymers for bulk heterojunctions

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ABSTRACT

Recently many investigations have been done to improve the performance of solar cells photovoltaic. One of this devices developed is the Bulk Heterojunction (BHJ) solar cells based on poly (3-hexylthiophene) (P3HT)/[6, 6]-phenyl C_{61}-butyric acid methyl ester (PCBM) blend which have been fabricated by spin-coating. It is known that the nanostructure of the active layer of this device has an important impact on the photovoltaic performances. In this work, we analyze the results obtained on solar cells using a copolymer P3HT-*b*-PS based on poly (3-hexylthiophene) (P3HT) as a donor block and polystyrene (PS) as a soft block, their compatibility with the blend of P3HT/PCBM at various weight percentages (0%–5%). The addition of this weight percentage is in order to improve the performance of polymer solar cells. It has been demonstrated that the addition of a small amount of P3HT-b-PS (from 0.5%–1.5%) led to an increase in photovoltaic efficiency compared to devices made from P3HT/PCBM only. To study the impact of the added amount of the P3HT-b-PS on the performances of the fabricated organic cells, we used an equivalent circuit model based on single diode model with five photovoltaic parameters. Then, we extracted these physical parameters of the organic photovoltaic cells such as the saturation current density, the series and shunt resistances, the ideality factor and the photogenerated current density from the experimental characteristics (J–V) in the dark and under illumination. We proposed and developed the used procedure based on this model and we resolved the analytic equations of the density-current using the Lambert W-function. A good agreement between the theoretical model and the experimental data of electrical characteristics is obtained illustrating the enhancement of the addition of a small amount of P3HT-b-PS ($\leq$1.5%) in the P3HT/PCBM blend on the characteristics of BHJ organic photovoltaic cells.

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1. Introduction

In the course of these recent years, polymer solar cells because of their advantages of low-cost manufacturing, lightweight, near-transparent, colorful and good flexibility [1–4] have attracted a comprehensive interest of scientific communities. Bulk heterojunctions (BHJs) consisting of a mixing of poly (3-hexylthiophene) (P3HT) as electron donor (D) and 6, 6-phenyl C_{61}-butyric acid methyl ester (PCBM) as electron acceptor (A) [5] constituted the most investigated structures in the field of organic photovoltaics. The reached power conversion efficiencies (PCE) with this kind of solar cells is up to 5% [6]. Indicating that in these devices, the nanostructure of the active layer plays an important role on several physical parameters of the photovoltaic process [7–11]. A good organization of the donor and acceptor materials allows limiting the electron-hole recombination by generating a phase separation whose characteristic size is equivalent to the diffusion length of the exciton. The control of the morphology of the P3HT/PCBM blend is therefore particularly important.

Recently the use of D/A block-copolymers as compatibilizer in the P3HT/PCBM blends offers a particularly attractive strategy to control the morphology and increase stability of devices [12–18]. The efficiency of polymer solar cells have improved by synthesizing rod-coil block copolymers and adding them to the P3HT/PCBM blends as a surfactant [12]. Furthermore, it has been shown that with adding of donor-acceptor block copolymer P3HT-b -poly (acrylate perylene bisimide) as a compatibilizer leads to an improvement in phase separation in the active layer [13].

An enhancement of phase separation and thermal stability have been realized as well as increased internal quantum efficiencies by using the P3HT-b-P4VP as nanostructuring agent in the active layer P3HT/PCBM [14]. It has been shown that adding 5 wt% polystyrene-*block*-poly (3-hexylthiophene) (PS-*b*-P3HT) to P3HT: PCBM blends increases the PCEs from 3.3% to 4.1% [15]. These results have been attributed to the increase in miscibility of P3HT and PCBM driven by the copolymer compatibilizer. Other works have developed a P3HT-b-C_{60} diblock copolymer based on regioregular poly (3-hexylthiophene) (P3HT) and [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) and have used as a compatibilizer for the P3HT/PCBM blend [16]. It has been shown that the additions of P3HT-b-C_{60} significantly reduce the decrease of PCE for long-time thermal annealing and were able to suppress phase segregation after prolonged annealing.

The rod–coil block copolymer has been used as compatibilizer. It is based on a regio-regular poly (3-hexylthiophene) electron-donor rod block and a C_{60}-grafted coil block. The effect of the compatibility agent on performance of organic photovoltaic cells and the control the morphology of the polymer/fullerene have been studied [17]. More recently, a study of the effect of P3HT-b-PS-b-C_{60} and P3HT-b-PS diblock copolymers as additives on classical P3HT: PCBM bulk heterojunction solar cell has been reported [18]. It has been shown that the addition of small amounts of the P3HT-b-PS and P3HT-b-PS-b-C_{60} increases the crystallinity of P3HT and homogenized the vertical distribution of P3HT and PCBM in the active layer. Moreover, it has been demonstrated that the C_{60} functionalization P3HT-b-PS-b-C_{60} is the most effective way to control the phase separation, the crystallinity and to enhance the donor–acceptor interfacial area within the P3HT: PCBM blends.

To investigate and describe the nonlinear behavior of the organic photovoltaic cells based on polymer bulk heterojunctions, several mathematical models have been proposed in the literature. These models differ in the calculation procedure and the number of parameters involved in the calculation of the current–voltage characteristic [19–21]. These parameters are usually the series and shunt resistances, the ideality factor, the density of the saturation current of the diode and the photocurrent density. The extraction of these parameters from the illuminated and dark current-voltage characteristics is a crucial to improve the performance and optimize the photovoltaic parameters of the device.

A method based on the Lambert W-function has been proposed to calculate the different parameters of an organic solar cell [22]. Later, a mathematical technique that introduces new formulations to extracting the intrinsic and extrinsic parameters of the plastic solar cells has been developed [23]. In this method, the Co-content (CC) function has first been calculated from the exact explicit analytical expressions and then extracted the parameters by curve fitting. Recently, a new method has been used to extract all the parameters of a solar cell under one constant illumination level [24]. This method relies on calculating the differential value dV/dI from the experimental data. Furthermore, other method for extract the solar cell parameters under dark conditions based on the simulation of current-voltage curve using the single diode model, considering the series resistance [25]. Other works presented three methods to determine the four parameters of a solar cell (the saturation current I_0, the series resistance R_s, the ideality factor n, and resistance shunt R_{sh}) from dark experimental data [26]. These methods include analyzes and tests that give a good agreement with the experimental results, with various levels of success of the calculation.

The main aim of this work is to describe the usefulness of P3HT-b-PS copolymer as a compatibilizer in the P3HT/PCBM blend with an analysis of the observed effect on the organic cell parameter in the dark and under illumination. These parameters will be used to calculate the current–voltage in the dark and under illumination and will be simulated using the Lambert W -function to obtain the theoretical curves.

2. Theory and calculation

The J–V characteristic of solar cells measured in dark and under illumination can be presented by a two diode model or by a single diode model [27], the single diode model (known also as the five parameters model) is, however, the most widely used model for solar cells [28,29].