



Precisely control the morphology and crystallization of temperature-dependent aggregation bulk heterojunction by using co-solvent system for optimized light intensity distribution and its effect on thick active layer polymer solar cells



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ABSTRACT

The effects of co-solvent on the morphology, crystallization and light intensity distribution of thick bulk heterojunction (BHJ) polymer solar cells (PSCs) based on polymer of [(5,6-difluoro-2,1,3-benzothiadiazol-4,7-diyl)-alt-(3,3000-di(2-octyldodecyl)-2,20,50,200,500,2000-quaterthiophen-5,5000-diyl)](PffBT4T-2OD):[6,6]-phenyl-C71-butyric acid methyl ester (PC₇₁BM) are studied. By adjusting different co-solvent systems in thick BHJ layer, it is found that the polymer crystallization, fullerene absorption and PffBT4T-2OD:PC₇₁BM BHJ morphology are optimized by using a co-solvent of chlorobenzene (CB): dichlorobenzene (DCB):1,8-diiodooctane (DIO). The optimized BHJ thickness of 250 nm is analyzed by using transfer matrix theory, resulting in enhanced *FF* and *PCE* of 66.7% and 9.16%, respectively. This phenomenon is due to the active layer can absorb 90% of the incident light with a thickness of 250 nm, which contributes to the light intensity distribution and exciton generation rate.

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1. Introduction

Inexhaustible and environmentally friendly polymer solar cell (PSC) is a candidate for future clean-energy technologies due to the prominent advantages, such as lightweight, low cost-effect, flexible thin-film device, and large-scale manufacturing using solution process (Lu et al., 2015; An et al., 2016; Fan et al., 2017; Tumbleston et al., 2014; Huang et al., 2013). Over the past few decades, the progress of PSCs has made great achievements in materials (Scharber, 2016), morphological control (Li et al., 2005), interfacial engineering (H. Wang et al., 2016) and device construction (Yang et al., 2015) to realize high power conversion efficiency (*PCE*) beyond 12% (Ye et al., 2016; Nian et al., 2016; Zhang et al., 2016). However, the commercial products of PSCs are rare on the market yet, as to the difficulty of fabricating a homogeneous and pinhole-free bulk heterojunction (BHJ) layer.

Achieving high efficiency in low bandgap PSCs with a thick active layer is particularly important for commercial applications (Zheng et al., 2014). H. Yan et al. demonstrated a polymer of poly PffBT4T-2OD [(5,6-difluoro-2,1,3-benzothiadiazol-4,7-diyl)-alt-(3,

3000-di(2-octyldodecyl)-2,20,50,200,500,2000-quaterthiophen-5,5000-diyl)] with a temperature-dependent aggregation property, leading to a high *PCE* up to 10.8% with the thickness of 300 nm BHJ (Liu et al., 2014). Reynolds and So et al. investigated that the charge carrier combination losses and low charge carrier lifetime limit the performance of thick-film low-bandgap PSCs (Small et al., 2013). Cao et al. demonstrated a narrow bandgap pi-conjugated polymer with high mobility and promoted self-organization, exhibiting remarkable *PCE* over 10% with the BHJ thickness over 300 nm to 1 μm (Jin et al., 2016). Thus, the PSCs with a homogeneous and pinhole-free thick BHJ received widespread attention due to its compatibility with large-scale roll-to-roll processing.

It is reported that the PffBT4T-2OD based thick active layer PSCs are generally dissolved in chlorobenzene (CB), dichlorobenzene (DCB) (Liu et al., 2014; Ma et al., 2015) and *o*-xylene (Sprau et al., 2015). Although there are some works reported that the CB: DCB and *o*-xylene could adjust the morphology of PffBT4T-2OD: PC₇₁BM blends (Liu et al., 2014; Sprau et al., 2015), no systematical study and comparison with their effects on the crystallization, morphology, and light absorption of active layer. Also, to the best of our knowledge, the superiority of ternary mixed solvents treatment is the incorporation of two steps tuning of mor-

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phology, and the long-range ordered structure with favorable domain size and good domain purity could be obtained (Ye et al., 2012). This deposition protocol is very important for organic solar cells. However, the detailed protocol also needs to be controlled to different material systems (Earmme et al., 2014; Hong et al., 2014; Kim et al., 2016), and the procedure of this work can be used for temperature-dependent aggregation polymer. Furthermore, the concentration of solutions has a great impact on the network formation of the polymer and phase separation of PffBT4T-2OD:PC₇₁BM blends, due to their different contacts and entangles property of the solution (Liang et al., 2014). Therefore, the research work of PffBT4T-2OD:PC₇₁BM blends based on different co-solvents with different concentrations required carrying out urgently. In addition, the thickness optimization, the optical distribution, and the exciton generation rate of PffBT4T-2OD:PC₇₁BM PSCs by using the optical analysis are not mentioned up to present. Thus, the optimizing thickness of PSC based on PffBT4T-2OD:PC₇₁BM BHJ with transfer matrix method is far-reaching.

In this work, different co-solvent systems and optical simulation were adopted to PffBT4T-2OD:PC₇₁BM BHJ. By using different co-solvent systems in the thick BHJ layer, the highest crystallization of polymer and the smoothest morphology of PffBT4T-2OD:PC₇₁BM BHJ layer were optimized by using a co-solvent of CB:DCB:DIO. Furthermore, the light intensity distribution and exciton generation rate were analyzed by using transfer matrix theory, the PSC with a 250 nm BHJ layer showed a highest *FF* of 66.7% and *PCE* of 9.16%. The mechanism of co-solvent based PSCs was elucidated by characterizing both the blend morphology of BHJ active layers by atomic force microscopy (AFM), and the crystallization by X-ray powder diffraction (XRD) as well as Ultraviolet–visible (UV–Vis) absorption spectra. Changes in the photovoltaic property of the OPV device were evaluated. The optical distribution and exciton generation rate of PffBT4T-2OD:PC₇₁BM BHJ film were analyzed by transfer matrix method. More importantly, this procedure could pave a path to the optimization of other high performance temperature-dependent aggregation polymeric materials.

2. Experimental details

The architecture of the PSC and the chemical structures of materials used in the active layer are shown in Fig. 1. The device configuration is indium tin oxide (ITO)/zinc oxide (ZnO) (40 nm)/PffBT4T-2OD:PC₇₁BM (100–300 nm)/MoO₃ (15 nm)/Ag (100 nm). The ITO-coated glass substrates were cleaned according to a routine cleaning procedure (Lu & Yu, 2014). Prior to the deposition of organic layer, the substrates were treated with UV light for 10 min. The ZnO precursor was prepared by dissolving zinc acetate

dehydrate (Aldrich, 99.9%, 1 g) and ethanolamine (Aldrich, 99.5%, 0.28 g) in 2-methoxyethanol (Aldrich, 99.8%, 10 mL) under vigorous stirring for 12 h for the hydrolysis reaction in the air (M. Wang et al., 2016). A thin layer of sole-gel ZnO (30 nm) was spin-coated on the top of ITO-coated glass substrates and baked at 200 °C for 1 h in ambient. Then, the substrates were transferred to a high-purity N₂ filled glove box. The PffBT4T-2OD (99.9%, 1-Material Inc., Mw = 100 kg/mol) was blended with PC₇₁BM (99.9%, Solarmer) at a weight ratio of 1: 1.2 and dissolved in CB (anhydrous, 99.8%), DCB (anhydrous, 99.8%) and both of them with the addition of 3% DIO, with a total concentration of 9, 12, 15, 20, 26, 32 mg/ml, respectively. The blends were also dissolved in *o*-xylene with an addition of 1% AA, with a total concentration of 9 mg/ml. The PffBT4T-2OD:PC₇₁BM blends solutions were stirred at 110 °C at least 3 h (Liu et al., 2014; Sprau et al., 2015). Then, the solutions were spin-coated on ZnO thin layer. The polymer/fullerene films were then annealed at 80 °C for 5 min before being transferred to a vacuum chamber of a thermal evaporator inside the same glovebox. Finally, MoO₃ (99.98%, Aldrich) layers were deposited on the top of the active layer at a rate of 1 Å/s under a vacuum pressure of 3.0×10^{-3} Pa, followed by the deposition of Ag anode at a rate of 10 Å/s in the same vacuum chamber. The area of our device is determined (~ 0.02 cm²) by using a shadow mask during thermal deposition, and the size of each device was measured with a vernier caliper specifically (Zeman et al., 2013).

The current density–voltage (*J*–*V*) characteristics of PSCs were measured with a simulated light source (CHF-XM35, Beijing Trustech) with an AM 1.5G at a calibrated light intensity of 100 mW/cm² (Ye et al., 2015). The EQE spectra were measured under the lump light passing through a monochromator, which was calibrated by a standard Si solar cell. Electrical data were recorded with a Keithley 4200SCS Source Measure Unit (Tektronix, Shanghai, China) under ambient conditions. The UV–Vis absorption spectrum of the active layers were measured by using UV–Vis spectroscopy (Shimadzu UV1700). The film preparation condition for XRD (D1-HR XRD, Bede, Inc.) and AFM (MFP-3D-BIO, Asylum Research) measurements were kept the same as the device fabrication for comparison. The optical properties of each layers are represented by the index of refraction ($\tilde{n} = n + ik$) of each material, which were measured using a variable angle spectroscopic ellipsometer (VASE). All measurements were carried out under the ambient condition without encapsulation.

3. Results and discussion

As PffBT4T-2OD shows strong temperature-dependent aggregation property in solution, and the co-solvents have different boiling point, leading to the near-ideal polymer: fullerene morphology containing highly crystalline and pure yet reasonably small polymer domains (Liu et al., 2014). Also, when different co-solvents were utilized, the aggregation of polymer before liquid–liquid phase separation was different, and the domains were diverse (Franecker et al., 2015).

To verify the different aggregation and domain size of PffBT4T-2OD:PC₇₁BM blends based on different co-solvent systems, their microcosmic morphologies were characterized by AFM, as shown in Fig. 2. The BHJ film based on DCB:CB:DIO co-solvent system possesses medium domain size with a root mean square (RMS) of 1.31 nm, and the topography of BHJ film based on the co-solvents of DCB:DIO and CB:DIO present smaller domain size with similarly increased RMS of 1.59 nm and 1.51 nm, respectively. The increased surface roughness is attributed to the molecular aggregation in different co-solvents, and the co-solvent of DCB:CB:DIO resulting in a planar and intermixed polymer–fullerene (Zheng et al., 2016). However, the topographic feature of BHJ film

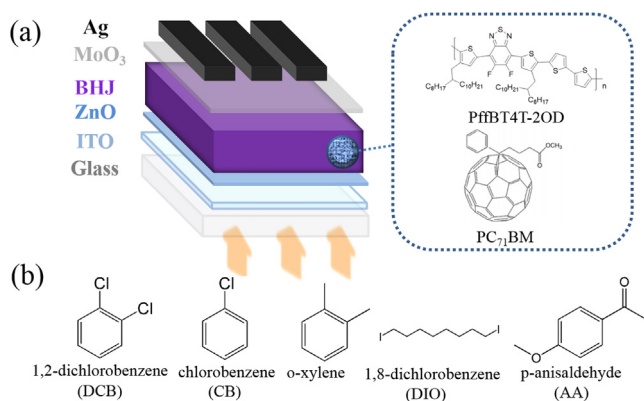


Fig. 1. (a) Device architecture and molecular structure of active layer materials. (b) Chemical structure of the solvents and additives investigated in this work.

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