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Self-healing polymer sealant for encapsulating flexible solar cells

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ABSTRACT

Herein we demonstrate the utility of polyisobutylene (PIB) as a fully printable self-healing sealant for protecting organic photovoltaic devices from degradation under ambient conditions. These sealants can be applied on flexible substrates using drop casting, spin coating or blade coating. PIB-based crosslinked sealants show excellent device stability, especially the low molecular weight PIB.

1. Introduction

The power conversion efficiencies of organic photovoltaic (OPV) devices continue to increase for single junction [1] and tandem cells [2]. Low cost large area fabrication process on flexible substrates [3] makes this technology more exciting and attractive to the solar cell community. There are three major areas of research in OPVs; (1) improving device efficiency by tuning absorption spectra [4,5], (2) device architecture and processing [6,7] and (3) encapsulation for long-term stability [8,9]. Although in last two decades, tremendous efforts have been made to increase the efficiency by synthesizing low band-gap polymers [10,11] and engineering various processing conditions [12,13] for large area roll-to-roll (R2R) printing, there are only very few reports (less than 5% of the total published work on OPVs) on the device stability [9]. The stability of OPVs can be broadly classified into two categories; chemical stability [14] and mechanical stability [15]. Active layers of OPVs such as polymers and small molecular semiconductors and electrode materials such as calcium and aluminum are susceptible to oxidation due to presence of oxygen and moisture in air. Reducing the oxygen and moisture penetration into the active layer can improve the chemical stability of these OPVs. It has previously been shown that oxygen and moisture can diffuse through the electrodes into the polymer active layers [16]. There have been some reports on device architecture where inverted type geometry containing oxide from both sides of the active layers show higher chemical stability over conventional architecture due to less diffusion of oxygen [17]. But the most common practice to prevent oxygen and moisture diffusion into the active layer is by encapsulating the device active area with gas impermeable materials [18]. Though transparent glass is almost impermeable and can be used as encapsulating materials [19], it is incompatible with large-scale R2R printing. There are polymers such as polyvinyl alcohol (PVA) [20], polyurethane [21], poly(methyl methacrylate) PMMA or PMMA-polyolefin which have been used as a coating materials to protect organic active layers from degradation. However these polymers are also susceptible to degradation and crack formation upon prolonged exposure to unfavorable weather condition [22]. Therefore there is a need for new encapsulating materials, with high flexibility and excellent barrier properties to oxygen and moisture to realize stable and flexible OPVs for commercial applications. Polyisobutylene (PIB) based networks have good flexibility and strong adherence to the substrates, excellent damping and barrier properties, thermal stability and also high chemical and solvent resistance [23]. Kim et al. recently reported desiccant-filled linear PIB edge sealant for organic electronics. But the sealant has to be dissolved in a solvent before applying on organic electronics. Furthermore, the sealant is susceptible to damage caused by the harsh environment, as it is not self-healing [24]. Recently, Banerjee et al. has reported a PIB-based self-healing polymer based on reversible [2+2] cycloaddition of coumarin [25] demonstrating light-induced self-healing properties, but the device stability is not studied.

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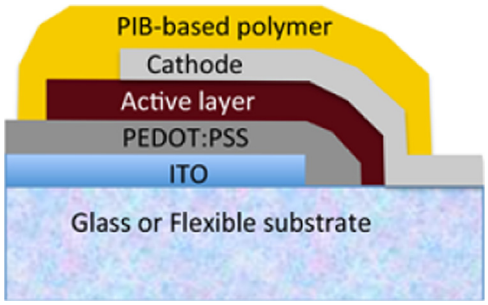

Fig. 1. Schematic diagram of an encapsulated polymer solar cell.

Herein, we demonstrate the use of a new class of UV curable "solventless" PIB-based self-healing sealant from coumarin functionalized tri-arm star PIB to improve the stability of OPVs under environmental conditions. These sealants are compatible to R2R printing [26,27] for fabrication of stable and flexible OPVs for commercial applications. We also studied the impact of the molecular weight of PIB on the gas permeability and hence device stability.

2. Experimental detail

2.1. Synthesis of UV curable tri-arm star PIBs

Coumarin functionalized tri-arm star PIBs $(PIB\text{-}MUMB)_3$ with number average molecular weight (M_n)=2000 g mol^{-1} [$(PIB\text{-}MUMB)_3$-2k], 5000 g mol^{-1} [$(PIB\text{-}MUMB)_3$-5k] and 10,000 g mol^{-1} [$(PIB\text{-}MUMB)_3$-10k] were synthesized (Scheme S1 in the Supporting Information) following a procedure reported earlier [25]. Table S1 and Fig. S1 depict the molecular characterization data and SEC chromatograms of the $(PIB\text{-}MUMB)_3$ samples, respectively. ^{1}H NMR spectrum of a representative $(PIB\text{-}MUMB)_3$-2k sample (see Fig. S2) revealed the characteristic peaks of coumarin moiety at 2.39 and at 6.82 and 7.48 ppm (for –OCOCH– and for aromatic signals) suggesting efficient functionalization of PIB.

2.2. Device fabrication

Poly[3-hexylthiophene-2,5-diyl] (P3HT) (M_w=36 kDa, rr=96%, $Đ$=2.7) from Rieke Metals, Inc. and [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) from Nano-C Inc. were used as received for the fabrication of bulk hetero-junction (BHJ) polymer solar cell for this stability study. Devices were fabricated following a standard protocol reported in the literature [28]. A hole-transporting buffer layer, poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) was spin coated at 3000 rpm for 35 s on pre-cleaned indium tin oxide (ITO) substrates. A P3HT/PCBM blend (1:1 by weight) from chlorobenzene (20 mg mL^{-1} concentration) was spin coated on a PEDOT:PSS coated ITO substrates at 1000 rpm for 60 s. As cast samples were then annealed under chlorobenzene solvent vapor (solvent assisted annealing) for 5 min in air. Polymer film was removed from the edges of the substrate to prevent oxygen and moisture penetration through the active layer after encapsulation as shown in Fig. 1. A thin layer of Ca (5 nm) at 0.5 Å s^{-1} followed by a thick layer of Al (100 nm) at 3 Å s^{-1} was deposited thermally in a physical vapor deposition chamber attached to a N_2 filled glove box at a chamber pressure of 1×10^{-6} mbar. Devices were then encapsulated with the polymers by drop coating onto the substrates inside a glove box and kept in vacuum for 10 min for degassing (Fig. 1). Encapsulated devices were then exposed to 365 nm UV light (~3 mW cm^{-2}) for 20 h for photo-crosslinking in air. Device efficiency was studied

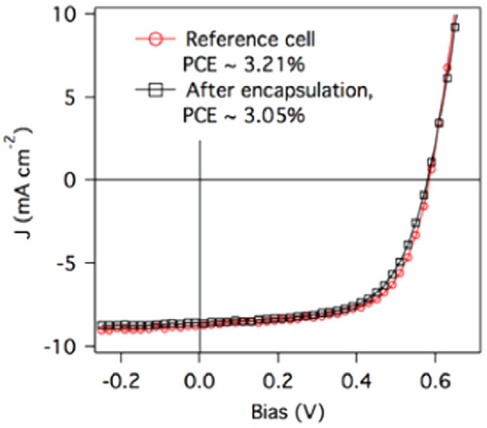

Fig. 2. P3HT/PCBM BHJ solar cell light *J–V* characteristics before and after encapsulation with PIB-based polymer sealant and photo-crosslinking under 365 nm UV lamp inside a glove box. Measurements were carried out under AM1.5G solar simulator at 100 mW cm^{-2} light intensity.

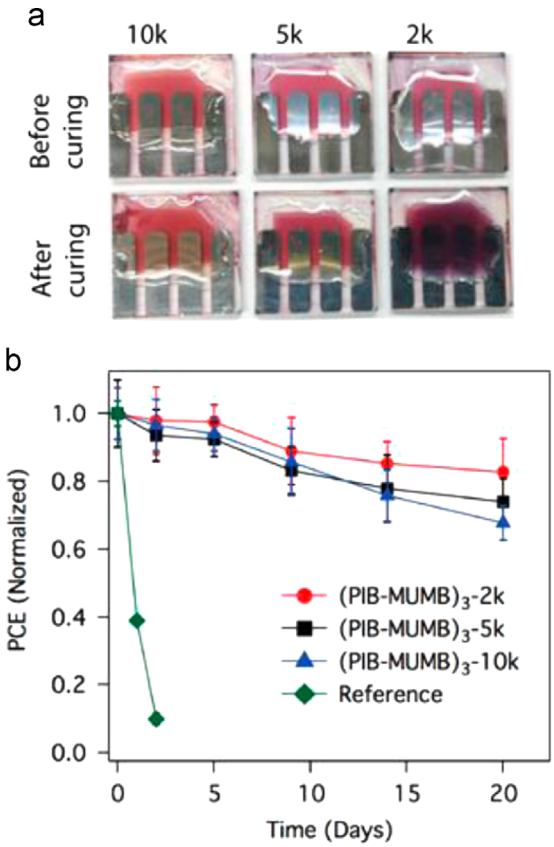

Fig. 3. (a) Encapsulated device before and after photo-crosslinking. (b) Device stability in air. Error was calculated based on 4 devices data from the same substrate.

periodically under AM1.5G solar simulator at 100 mW cm^{-2} light intensity and stored in ambient conditions over 20 days.

3. Results and discussion

3.1. Photo-crosslinking of tri-arm star PIBs

Coumarin functionalized tri-arm star PIB was used as the base material to develop the sealant. Photoreversible dimerization of