Solid-State Electronics 104 (2015) 53–60

Contents lists available at ScienceDirect

Solid-State Electronics

journal homepage: www.elsevier.com/locate/sse

Effect of chiral photosensitive liquid crystalline dopants on the performance of organic solar cells

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ARTICLE INFO

Article history:
Received 17 June 2014
Received in revised form 10 November 2014
Accepted 14 November 2014
Available online 4 December 2014

The review of this paper was arranged by Dr. Y. Kuk

Keywords:
Liquid crystals
Organic solar cells
Azo compounds
Photosensitive composite
Bulk heterojunction solar cells

ABSTRACT

In order to design a new type of an organic solar cell device and to contribute for its performance optimization, i.e. transport and optical properties, a composite organic solar cell have been designed. It has been fabricated in two modifications from poly(3-hexylthiophene) and [6,6]-phenyl C_{61}-butyric acid methyl ester mixtures (P3HT:PCBM) and two chiral photosensitive liquid crystalline (PCLC) materials used as additives. Doping of the P3HT:PCBM solar cell by a specific PCLCs led to a distinct adjustment (increase or decrease) of power conversion efficiency in comparison to that of an undoped cell and it is also strongly depends on the viscosity of the PEDOT:PSS used. In order to control the properties of the resulting composite P3HT:PCBM solar cells doped by PCLCs, the photovoltaic and impedance spectroscopy studies have been done for active layers annealed at different temperatures. Differential scanning calorimetry (DSC) in combination with polarized optical microscopy (POM) has been used to examine the morphology of an active layer. Thermal annealing of the sample within a mesophase temperature range can remove defects, optimize the morphology of the active layer, and hence might be responsible for the increase of photocurrent and cell efficiency.

1. Introduction

At present the design of new types of organic solar devices and optimization of their performance, i.e. transport and optical properties, by various functional additives is currently belongs to a highlighted field of research [1–3]. During last years a lot of attempts have been done to improve the efficiency of the photovoltaic devices keeping their price at reasonably low level.

From all the types of polymeric solar cells being under active consideration, mainly the bulk heterojunction (BHJ) devices are actively investigated as the most favourable ones for practical purposes [4–8]. The most common way to design BHJ polymeric solar cell is to blend two materials, namely a poly(3-hexylthiophene) denoted as P3HT (working as a donor) and [6,6]-phenyl C_{61}-butyric acid methyl ester denoted as PCBM (acting as an acceptor). Using donor and acceptor allows to increase an interfacial area between two compounds which potentially can result in an improvement of power conversion efficiency (PCE) of the resulting device. The flexibility and low cost fabrication of organic PVs (OPVs) have attracted enormous attention from both academy and industry as alternatives for conventional inorganic solar cells [9]. Also, there are several attempts to design a flexible and stretchable organic solar cells, namely OPVs with a specific stretchable electrodes which demonstrated quite robust mechanical properties, while maintaining excellent OPV performance [10].

Liquid crystalline (LC) materials of different molecular shape (rod-like, disk-shaped or sanidic type) have been already used as smart dopants for an improvement of organic photovoltaics (PV) [9,11–27]. Both low molar mass compounds and macromolecular ones like LC polymers have been used as donor or as acceptor dopants in organic solar cells. The value of PCE for the organic PV based on LCs has been found within 0.03–3.97%. However, there is a relatively small number works until now dedicated to an effect of LC compounds on organic photovoltaics behaviour. In particular a rod-like (or so called calamitic) LC compounds are not extensively investigated as additives due to their specific molecular shape [23–25]. There are just a few examples of a calamitic LC compounds used as additives in solar cells with P3HT:PCBM active layer, namely (i) 4-cyano-4′pentylbiphenyl (5CB), 4-cyano-4′-octylbiphenyl (8CB) exhibited nematic or SmA and N mesophases, respectively (PCE = 3.2–3.7%) [23], (ii) chiral (S)-5-octyloxy-2-[{4-(2-methylbuthoxy)-phenylimino}-methyl]-phenol exhibited the ferroelectric tilted SmC* phase (PCE = 2.9%) [24], and azomethines with benzothiazole ring possessing the paraelectric orthogonal SmA phase (PCE = 0.1%) [25].

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http://dx.doi.org/10.1016/j.sse.2014.11.010
0038-1101/

On the other hand, an effect of azobenzene group in dye compounds on the performances of PV, where the dye was applied as a donor [2,28,29] have not been extensively investigated so far. The obtained values of PCE were lower than the value obtained for the device based on P3HT:PCBM. It is quite exciting that a few materials with the N=N group have been also applied in PCBM [30] as smart dopants. However, the value of PCE was lower than in the case of application as an acceptor PCBM in active layer based on P3HT.

Taking into consideration actual trends in design of organic solar cells, it is very important and promising to apply new low molar mass organic compounds in photovoltaics. This can be reached by morphology control of active layers, investigation of the intermolecular interactions and material's miscibility with the aim to increase the OPV performance [31–33].

The subject of LC materials [34–36] and their applications in flat-panel displays and non-linear optical systems has become of huge importance during the last two decades. In our days, LC materials are widely applied for devices such as PC displays and flat high-resolution TV sets [37–40]. Numerous low molar mass compounds [41–47], polymeric compounds [48–54] and even dendrimers with different shape [3], symmetry and consequently with different mesomorphic behaviour have been designed and investigated as self-assembling materials possessing extraordinary mesomorphic, optic and structural properties. Compounds of different molecular shape and structure can exhibit one or a sequence of mesophases such as nematic (N), smectic (Sm), and columnar. Chiral liquid crystalline materials derived from the lactic acid can form a broad variety of mesophases such as chiral nematic but also various smectics (i.e. nano-layered phases). Due to their smart properties and advantages with respect to other conventional chiral LC materials [40,42,43,46,63] such materials can be evidently utilized as a smart dopants. Obviously, an introduction of double bond or —OH polymerizable groups on one of the alkyl chain [43,48–51,62] or incorporation of a photosensitive azo group in the molecular core [50,51,55–57,64] can strongly increase the potential functionality of this class of chiral LC materials and make them useful for photonics, telecommunications and non-linear optics [39]. Due to their properties complying with specific demands, lactic acid derivatives are actively used as strongly effective dopants for tuning properties of the resulting mixture [43–45,58] or nanocomposites [59,60].

The main objective is thus proposing a synergy between chiral liquid crystalline photochromic compounds with azobenzene group derived from the lactic acid and organic solar cells in order to produce smart BHJ devices and to study an effect of PCLC type on the photovoltaic parameters such as the open circuit voltage (V_{oc}), the short circuit current (J_{sc}), a fill factor (FF) and the power conversion efficiency (PCE). Herein, two photosensitive chiral liquid crystal compounds with azo bond (denoted as AZO1 and AZO2 – see subsection 2.1) [55], have been used as acceptor additives in active layer P3HT:PCBM organic solar cells.

Photoisomerization of an azo group from E to Z states drastically changes the shape of molecules from rod-like to bent-shape and thus toughly affects the mesomorphic and structural properties of the resulted composite materials. Thus, new polymer solar cell devices containing photosensitive chiral liquid crystalline (PCLC) additives were fabricated and their properties were established and discussed.

In this study, we tried to improve the PV performance of BHJ solar cells based on P3HT:PCBM by adding specific PCLC as an additive to the active layer of device. To summarize, we constructed 25 organic PV devices and investigated them in four main aspects, namely (i) amount of PCLC in active layer, (ii) viscosity of applied PEDOT:PSS, (iii) role of PCLC in active layer and (iv) annealing of an active layer at various temperatures. To our best knowledge, there have been no detailed studies on properties of the solar cell designed with such a smart additive as a photosensitive LC material.

2. Experimental

2.1. Materials and characterization methods

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS, viscosity 100 cP), poly(3-hexylthiophene-2,5-diyl) (P3HT, regioregular) and [6,6]-phenyl C_{61} butyric acid methyl ester (PCBM) were purchased from Sigma–Aldrich and used as received. PEDOT:PSS was purchased additionally from Ossila company (viscosity 5–12 cP). Methanol, acetone, and chloroform were purchased from POCH Company and used as received. Special ITO glass substrates were purchased from Ossila Company. Surface resistance of ITO was about 20 Ohm/square. Details on the synthetic route and basic mesomorphic properties of 4-((4-(octyloxy)phenyl)diazenyl)phenyl 4-(2-(dodecyloxy)propanoyloxy)benzoate compound (denoted here as **AZO1**) and 4-((4-(decyloxy)phenyl)diazenyl)-2-methylphenyl 4-(2-(dodecyloxy)propanoyloxy)

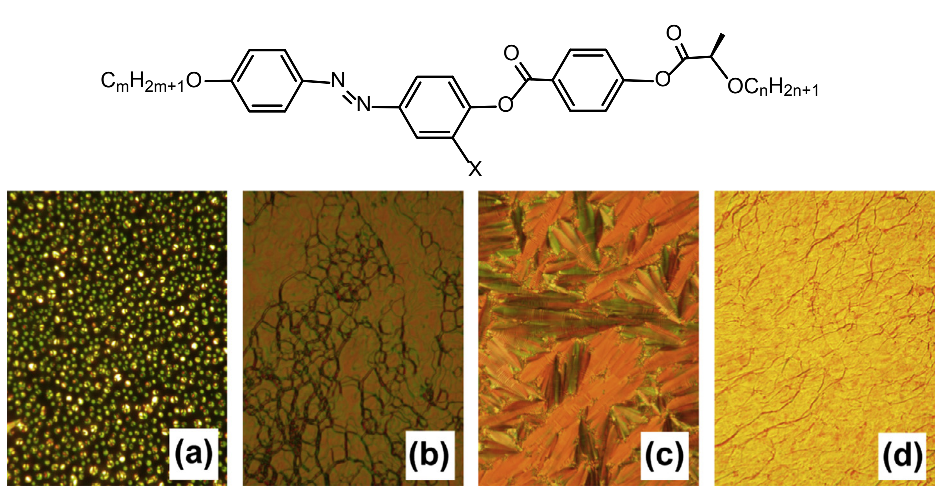

Fig. 1. Chemical formula of chiral LC photosensitive compounds **AZO1** (m = 8, n = 12, X=H) and **AZO2** (m = 10, n = 12, X=CH_3) and microphotographs of the characteristic textures obtained at POM on cells with planar alignment: (a) droplet texture of the isotropic-N* phase transition for **AZO1**; (b) oily streaks texture of the N* phase for **AZO1**; (c) broken fan texture with dechiralization lines of the ferroelectric SmC* phase for **AZO1**; (d) oily streaks texture of the N* phase for **AZO2**.