Layer by layer characterisation of the degradation process in PCDTBT:PC\textsubscript{71}BM based normal architecture polymer solar cells

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This work demonstrates the stability and degradation of OSCs based on poly(N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4,7-di-2-thienyl-2,1,3-benzothiadiazole)) (PCDTBT): (B6)-Phenyl C\textsubscript{6} butyric acid methyl ester (PC\textsubscript{71}BM) photoactive blend layers as a function of ageing time in air. Analysis of the stability and degradation process for the OSCs was conducted under ambient air by using current-voltage (I-V) measurements and x-ray photoelectron spectroscopy (XPS). The interface between photoactive layer and HTL (PEDOT:PSS) was also investigated. Device stability was investigated by calculating decay in power conversion efficiency (PCE) as a function of ageing time in the air. The PCE of devices decrease from 5.17 to 3.61\% in one week of fabrication, which is attributed to indium and oxygen migration into the PEDOT:PSS and PCDTBT:PC\textsubscript{71}BM layer. Further, after ageing for 1000 h, XPS spectra confirm the significant diffusion of oxygen into the HTL and photoactive layer which increased from 3.0 and 23.3\% to 20.4 and 35.7\% in photoactive layer and HTL, respectively. Similarly, the indium content reached to 7.9\% on PEDOT:PSS surface and 0.4\% on PCDTBT:PC\textsubscript{71}BM surface in 1000 h. Core-level spectra of active layer indicate the oxidation of carbon atoms in the fullerene cage, oxidation of nitrogen present in the polymer matrix and formation of I\textsubscript{2}O\textsubscript{5} due to indium diffusion. We also observed a steady fall in the optical absorption of the active layer during ageing in ambient air and it reduced to 76.5\% of initial value in 1000 h. On the basis of these experimental results, we discussed key parameters that account for the degradation process and stability of OSCs in order to improve the device performance.

1. Introduction

Solar energy harvesting has become one of the major areas of research for the current and upcoming technologies. In this context, polymer-based organic solar cells (OSCs) have drawn special interest due to their tunable properties, low manufacturing cost, roll to roll production compatibility, solution processed and lightweight [1–3]. To date, the progress in the OSCs development has been intensified and power conversion efficiencies (PCEs) of more than 10% have been successfully demonstrated [4,5]. In order to bring the OSCs into the market with full success, along with the high efficiencies and low manufacturing cost, longer devices lifetime is much needed [6].

Basically, the polymer solar cells employ bulk heterojunctions (BHJ) of blended donor (D) and acceptor (A) components as a photoactive layer which is sandwiched between two electrodes. In order to enhance the functionality of these devices often interfacial layers namely hole transport layer (HTL) and electron transport layer (ETL) are introduced at the interface between the photoactive layer and electrodes [7,8]. However, a short lifetime of the OSCs is observed to be one of the stability constraints since there is always a presence of degradation process throughout the device. The unique degradation mechanisms affecting the photoactive layer, interfacial layers and the electrodes is rather a complex phenomenon and are not yet fully understood. These multilayers and interfaces of metal/organic, organic/organic materials significantly influence the overall performance [9]. Recent reports on the lifetime stability of OSCs highlighted two major problems regarding the device stability. Firstly, the extrinsic stability which requires proper encapsulation of devices to prevent the environmentally