ICAM2009
11th International Conference on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25

Substrate induced phase separation and crystals orientation in ultrathin polymeric films for photovoltaics

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Abstract – The effect of substrate nature on crystalline orientation and phase separation of P3HT and PCBM has been investigated. In particular a strongly hydrophilic substrate and a strongly hydrophobic one were employed. Hydrophobic substrate has been found to induce, at a given annealing temperature, a lower phase separation degree as well as a better packing of P3HT lamellae. We suggest these effects are caused from the different surface free energy between thin films and molecules which affect the ability of polymer to crystallize as well as migration of PCBM molecules away from the high surface free energy substrate (hydrophilic one).

Since the discovery of photoinduced charge transfer between conjugated polymers and fullerene molecules [1] the interest in development of plastic solar cells as low-cost, light and flexible alternative to conventional silicon ones has strongly increased. Actually the most investigated couple is given by poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) which respectively act as the electron donor and electron acceptor moieties. In order to reach high enough efficiency, which would allow the commercial distribution of such cells, two main structural parameters of P3HT-PCBM thin films must be optimized: phase separation and crystallinity which can indeed respectively affect photoinduced charge transfer yield [2] and conductivity.
Recently, while many studies have been focused on the effect of substrate on the vertical phase separation [3-5] of P3HT-PCBM thin films, no attention has been paid on the simple phase separation degree which can be affected by the substrate nature too.
In this paper, we report on investigation of the effect of strongly hydrophilic and strongly hydrophobic substrates on the structure of P3HT-PCBM ultrathin films. Combined AFM and GIXRD analysis have shown a marked effect on both phase separation and crystals orientation. In particular on hydrophobic substrate the phase separation, at a given temperature, is lower than on hydrophilic one and the in plane orientation of P3HT lamellae is higher. A possible explanation of this effect can be due to the different surface free energy between substrates and thin film. We already have showed that such difference in surface free energy can affect the P3HT mobility and, therefore, the packing of lamellae and their in plane orientation.
In P3HT-PCBM thin films, the obtained results suggest that PCBM spherical molecules may migrate away from the high surface free energy substrate, the hydrophilic one, and therefore increase their concentration at the film-air interface leading to such strong phase separation. This suggests that, in order to choose the optimal experimental parameters for developing high efficiency solar cells, the substrate nature must be considered not only because of the induced vertical phase separation but also because of the different degree of phase separation and crystals orientation. Hydrophobic substrate would in fact allow higher annealing temperature than hydrophilic one leading to high crystallinity (i.e. to high light absorption yield and conductivity) without any loss in charge transfer due to a too strong phase separation deriving from the PCBM diffusion which is well known to be the limiting process in high efficiency solar cells [6]

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