Nanoscale Phase Separation in Bulk Heterojunction Organic Photovoltaic Device based in Si-Bridging Copolymer

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Introdução

Since the synthesis of the fullerene derivative [6,6]-phenyl C61 butyric acid methyl ester (PC61BM), bulk heterojunction (BHJ) devices have shown the most promising structure for organic photovoltaic. Combined with low band gap copolymer, the power conversion efficiency (PCE) exceeds 6%. In particular, copolymers using Si bridging atoms, like the poly[2,7-(9,9-bis(2-ethylhexyl)-dibenzosilole)-alt-4,7-bis(thiophen-2-yl)benzo-2,1,3-thiadiazole] (PSiF-DBT), are promising materials due to their broad absorption and their charge transport properties. BHJ devices using PSiF-DBT:PC61BM as active layer reached PCE of 5.4% for devices without thermal annealing [1]. The main reason for these improved optoelectronic properties is that large Si atom, and consequently large C-Si bonds, modify the entire geometry, leading to a more crystalline structure, allowing a better stacking between the chains. The efficiency of BHJ devices is strongly dependent on the blend morphology. A nanoscale phase separation is desired to ensure the best donor-acceptor contact leading to high exciton dissociation efficiency.

Resultados e Discussão

We present a study of BHJ device using PSiF-DBT:PC71BM as active layer. XPS (X-Ray Photoelectron Spectroscopy) and UPS (Ultraviolet photoelectron spectroscopy) techniques were used to probe both PSiF-DBT and PSiF:PC71BM films. XPS analysis of PSiF:PC71BM film shows that the chemical homogeneity of the film surface is improved with the temperature increase in thermal annealing. By analyzing the C-N and C-S contributions, which are representatives of the polymer, C-O and C=O representing the electron acceptor PC71BM in the blend, and the ratio of the areas between these atomic contributions ($A_{C\text{-}N\ +\ C\text{-}S}/A_{C\text{-}O\ +\ C=O}$), it is possible to indicate whether the film surface is rich in the polymer or PC71BM phases. The results of this analysis show that a more polymeric richer surface is achieved by thermal annealing. Photovoltaic characterization showed that as cast device has its PCE limited by its low value of short circuit density of current (J_{sc} = 4.06 mA/cm^2). Associated with a low value of open circuit voltage (V_{oc} = 0.48 V) and a fill factor (FF) of 42%, lead to a PCE of 0.82%. This occurs mainly because in the as cast film a desired morphology was not achieved. With a non favorable interface for exciton dissociation a limited value for both J_{sc} and V_{oc} is expected. As the annealing temperature increases a highly homogeneous film after 200^{o}C is observed, leading to a PCE of 2.5%. HOMO energy levels and respective work functions were obtained by UPS for the blends.

Conclusões

In agreement with XPS results, thermal annealing makes the film surface more chemically homogeneous impacting directly in devices performance. After the thermal treatment at 200°C a noticeable improvement is observed in J_{sc} and in V_{oc} (9.36 mA/cm^2 and 0.57 V, respectively) rising the PCE to 2.5%. Due to the more homogeneous surface a more suitable donor/acceptor surface was achieved making the exciton dissociation more efficient.

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[1] Wang, E.; Wang, L.; Lan, L.; Luo, C.; Zhuang, W.; Peng, J. and Cao, Y. *Applied Physics Letters* **2008**, *92*, 033307.