Polyethylene induced structural modification of ternary polymer blends used in photovoltaic cells

A. Akhtar, E.M. Herzig, J. Zhang, D. Posselt[1], C.M. Papadakis, S.V. Roth[2] and P. Müller-Buschbaum

Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

[1]IMFUFA, Department of Science, Systems and Models, Roskilde University, PO Box 260,4000 Roskilde, Denmark

[2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Photovoltaic devices based on polymers provide a potential towards novel types of renewable, delocalized and competitive energy sources. The devices based on organic semiconductor systems such as poly(3-hexylthiophene) (P3HT):fullerene blends have been investigated by different research groups, because of their potential towards low cost and abundant possibilities for application [1]. Recently, it has been observed that by adding a third component to the binary photovoltaic system the mechanical properties can be altered without loosing the performance of the system [2]. Various investigations have shown that the morphology of the active layer is very important for device performance [1] therefore the morphology of such systems is examined to understand and further exploit the connection between morphology and performance. The addition of a third component can also improve the morphology of organic materials in solar cells, for large scale production cheap commodity polymers are of interest. It is reported that among different commodity polymers, high density polyethylene (HDPE) is a promising material for organic solar cells, because of the improvement in the photocurrent generation efficiency of such a system [2]. Furthermore, it is also expected that the use of HDPE instead of low density polyethylene (LDPE) provides a better control to the microstructure in the final photovoltaic cell, because of its highly crystalline nature [2].

In this work we investigate a ternary heterojunction system containing the conjugated polymer P3HT, the electron conductor PCBM and the commodity polymer HDPE. The system P3HT and PCBM was chosen because it is probably the best investigated polymer based system for photovoltaic applications.

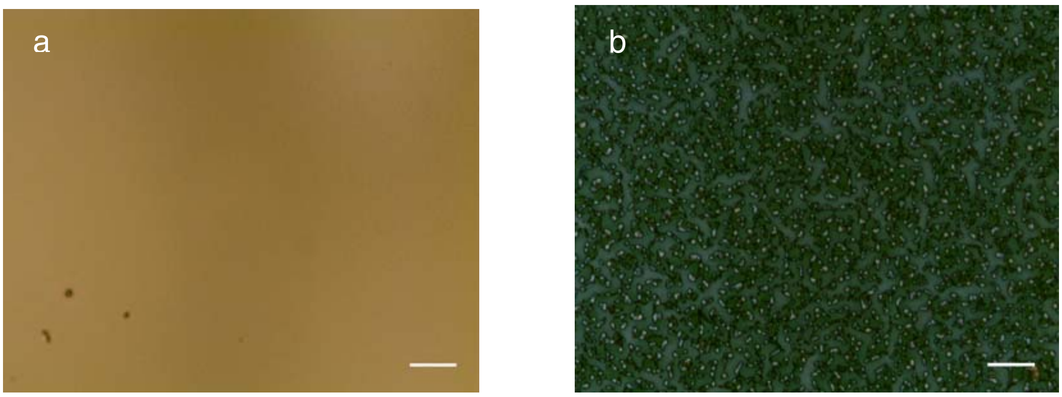

Figure 1: *Optical microscopy (scale bar 10 µm) of a) P3HT:PCBM (50:50) blend and b) P3HT:HDPE:PCBM (25:25:50) blend thin films on silicon.*

The choice of a common solvent for the ternary system is an important step to produce homogenous thin films. Because of the high crystallinity of HDPE high temperatures are needed to dissolve the polymer. This leads to the selection of a solvent with a high boiling point. In this investigation trichlorobenzene is used which has a boiling point around 180°C. Furthermore, the spin coating at normal temperature leads to an uncontrolled crystallization process which in turn leads to an inhomogeneous film. Therefore all necessary equipment and substrates (silicon and glass) are preheated to 120°C and spin coating is also carried out at the elevated temperature (120°C). To allow a reproducible, quantitative comparison between samples it is important to have films of equal thickness to rule out film thickness effects. The film thickness depends on several parameters, such as concentration and spin coater speed [3]. A process was established to produce films with equal thickness although the HDPE content is varied. To confirm this, the film thickness has been measured with ellipsometry. To establish the connection between performance and morphology two sample series are thoroughly investigated. In a first sample series the weight percentage of P3HT and HDPE (keeping HDPE concentration constant) is varied keeping PCBM constant at 50%. In a second sample series the HDPE content is varied, keeping P3HT and PCBM weight percentage constant.

The optical microscopy images show a clear structural change with and without HDPE (see figure1). Furthermore, the optical absorption spectra of both sample series show a clear change. While the overall absporption decreases with the decreasing amount of P3HT, the normalized plot shows an increase of order within the samples containing more HDPE. To gain more structural insights, both sample series are further examined with grazing incidence small angle X-ray scattering (GISAXS) at the P03 beamline. Lateral structural correlations and the vertical structure such as domain geometry, size distributions and spatial correlations are probed with GISAXS. The 2D GISAXS data (see figure 2) indicate that the structure changes with the addition of HDPE. The detailed analysis of the GISAXS data is in progress.

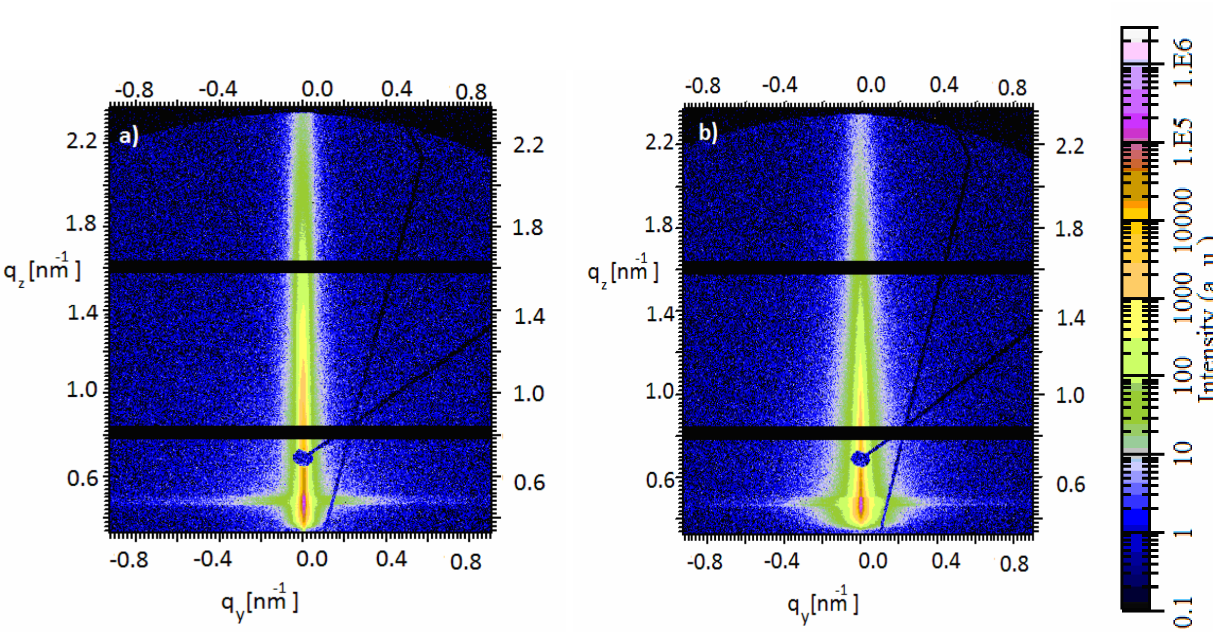

Figure 2: *2D GISAXS patterns of a) reference P3HT:PCBM (50:50) and b) maximum HDPE weight percentage P3HT:HDPE:PCBM (25:25:50).*

[1] M. A. Ruderer and P. Müller-Buschbaum, Soft Matter **7**, 5482-5493 (2011)

[2] S. Goffri, C. Müller, N. Stingelin-Stutzmann, D. W. Beriby, C. P. Radano, J. W. Andreasen, R. Thompson, R. A. J. Janssen, M. M. Nielsen, P. Smith, H. Sirringhaus, Nat. Mater **5**, 950-956 (2006)

[3] M. A. Ruderer, E. Metwalli, W. Wang, G.Kaune, S.V. Roth and P. Müller-Buschbaum, ChemPhysChem **10**, 664-671 (2009)