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X-ray Real-time Investigation of the Crystallization of Photovoltaic Polymer-fullerene films during Solvent Drying: the Effect of Processing Additives

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The fundamental concept of solution processed solar cells resides in the nanophase separation developing in the binary blend formed by a polymer (donor) and a fullerene derivative (acceptor) when the solvent evaporates, so-called bulk-heterojunction (BHJ). The performance of a BHJ solar cells arises from a complex interplay of the spatial organization of the segregated donor and acceptor phases and the local order/quality of the respective phases. A common practice to control the nanomorphology is the introduction of processing additives, such as octanedithiol (ODT).

We report real-time grazing incidence x-ray scattering (GIXS) study combined with optical interference that allows us to follow the evolution of the crystallinity.[1] We investigate in-situ the impact a ODT on the structure film formation of Poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3 - benzothiadiazole)] (PCPDTBT) as donor and [6,6]-Phenyl C71 butyric acid methyl ester (PC71BM) as acceptor. Such setup allows for a simultaneous determination of the crystallization dynamics and the solvent composition of the film. If processed from pure DCB solutions, PCPDTBT does not exhibit crystalline features due to fullerene clusters that impede dense chain packing. In the presence of 3wt% ODT we observe the microstructure of PCPDTBT emerges in several stages, which is interrelated with the aggregation behavior of the fullerene component.

References

- [1] B. Schmidt-Hansberg , M. Sanyal , M. F. G. Klein , M. Pfaff , N. Schnabel , S. Jaiser , A. Vorobiev , E. Müller , A. Colsmann , P. Scharfer , D. Gerthsen , U. Lemmer , E. Barrena , W. Schabel , *ACS Nano* **2011** , 5 , 8579 .

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