



Poster abstract

P.22 Mixing at polymer-fullerene interfaces: The impact of molecular weight

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Polymer-fullerene organic photovoltaics (OPVs) are potential candidates for the development of low-cost and flexible solar cells. Much research is being performed on devices where the active layer consists of a blend of conjugated polymer and fullerene (acting as electron-donor and electron-acceptor respectively). Ideally, a bicontinuous nanoscale morphology is desired, in order to optimise charge separation and charge transport. However in real devices, such as those containing poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61 butyric acid methyl ester (PCBM), there is the potential for considerable complexity in the film morphology, due to the miscibility of species, surface segregation, and aggregation/crystallisation of both components. In our studies we are seeking to take a step back from this complexity by probing the model system of polystyrene (PS) and PCBM. Here, only the fullerene can crystallise, and our work focusses on determining the interfacial mixing of the PS and PCBM on silicon substrates by annealing and performing neutron reflectivity measurements. We have discovered that a consistent composition profile is established rapidly (on a much faster timescale than that on which the PCBM crystallises) on annealing. This profile (parameterised by the width of the interface between two layers of uniform composition) is independent of the annealing temperatures used to-date (140 °C and 170 °C), is independent of the initial PS film thickness, and does not alter significantly, even as the PCBM crystallises [1]. This behaviour suggests that the observed interfacial width and layer compositions are governed by the equilibrium thermodynamics between the PS and (the amorphous part of) the PCBM (i.e. our hypothesis is that the bilayer structure is that of a liquid-liquid equilibrium between two co-existing phases). To test this hypothesis further, we have recently performed a series of neutron reflectivity measurements as a function of the molecular weight of the PS. We will present the results of these measurements and initial data analysis, as a function of PS molecular weights in the range 2000 to 300,000.

- [1] Mön, D., Higgins, A. M., James, D., Hampton, M., Macdonald et al . Bimodal crystallization at polymer-fullerene interfaces. *Phys. Chem. Chem. Phys.*, 17, 2216–2227 (2015)