Phase separation during the drying process of the photoactive layer in polymer solar cells

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Introduction

Organic polymer solar cells (PSCs) offer a promising alternative to their inorganic counterparts due to their potential for low cost and light weight photovoltaic devices. Efficiencies above 5% have been reported [1, 2] as well as successful realized tandem concepts for a wider light absorption range and energy conversion efficiency [3, 4]. But still there are big challenges in optimizing and fabricating these devices.

We report the determination of the drying kinetics (evaporation time) for several solvents and blending ratios of P3HT:PCBM (poly(3-hexylthiophene-2,5-diyl) and [6,6]-phenyl-C61-butyric-acid-methyl-ester). As well the solubility of both components in several solvents is investigated as a precondition for describing the solid-liquid phase equilibrium. This is of importance for the drying process (solidification) where the solubility limit is crossed.

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Experimental

Commonly used application techniques for organic layers of PSCs are spin coating, knife coating (doctor blade) and ink-jet printing. In this work the active layer was deposited via knife coating or inkjet printing. For spin coating and knife coating one solvent, e.g. dichlorobenzene, chlorobenzene or chloroform, already leads to high performance of the photoactive layer. Ink-jet printing requires solvent mixtures, e.g. dichlorobenzene-mesitylene, chlorobenzene-tetrahydronaphthalene, providing the droplet formation and spreading on the substrate in addition to a high solubility and slow solvent evaporation [5, 6]. We investigate relevant polymer-fullerene-solvent systems regarding the drying kinetics and phase separation which occurs during the solvent evaporation and the resulting morphology of the photoactive layer.
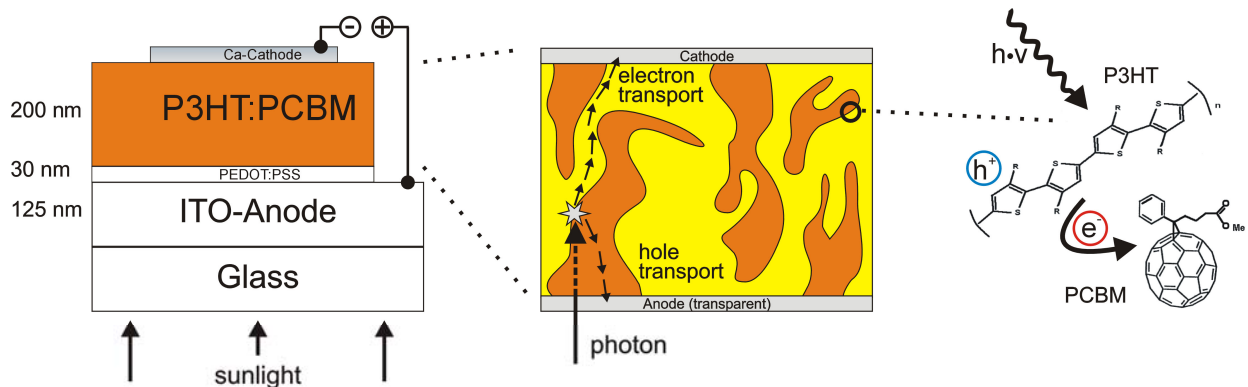

Figure 1: Structure of a polymer solar cell with approximate film thicknesses. Electron donor (P3HT) and acceptor (PCBM) are blended together to maximize the interface where exciton dissociation into electrons and holes takes place. For an efficient photocurrent, each material must provide a continuous path for electron and hole transport to the respective contact. Isolated domains can collect charges and cause recombination.

The nanomorphology of the photoactive layer is a key parameter for solar cell efficiency (s. Fig. 1). Morphology changes with the blending ratio, the chosen solvents and the solvent evaporation time [7]. We demonstrated the influence of drying kinetics on solar cell

characteristics qualitatively with different drying processes of the photoactive layer of P3HT:PCBM solved in dichlorobenzene. In this work vapor-liquid-phase equilibria and diffusion coefficients of solvents in the polymer-fullerene matrix are determined by means of a magnetic suspension sorption balance. Based on this data the solvent concentration during drying can be calculated in time and space for defined drying conditions.

To control the bulk structure of the polymer-fullerene-blend during the drying process our investigations also focus on the characterization of solid-liquid-phase-equilibria of P3HT and PCBM with suitable solvents to determine phase diagrams of these polymer-fullerene-solvent-systems. Screening experiments (s. Fig. 2) of binary mixtures regarding solubility of P3HT and PCBM in different solvents also showed a gelification of P3HT solutions at low temperatures. We now determine the temperature dependency of solubility whereas samples of saturated solution are retained at each temperature. The concentration analysis is accomplished via size exclusion chromatography which is sensitive for very low amounts.
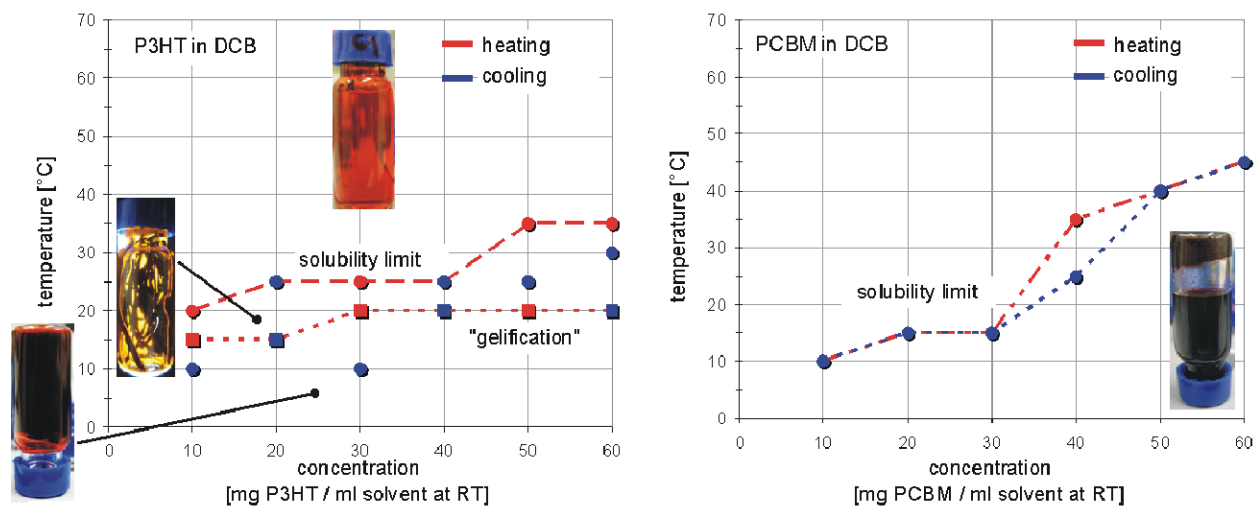

Figure 2: Screening the phase behaviour of P3HT and PCBM in binary solutions. Exemplarily plotted for dichlorobenzene (DCB).

Conclusion

The determination of polymer-fullerene-solvent phase equilibria and solvent diffusion coefficients enables the calculation of solvent concentrations in time and space during drying of the organic film. This is relevant for investigating the development of phase separation caused by crossing the solubility limit. In addition the drying and rewetting process of a continuous Roll-to-Roll process can be described with the same data.

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