Fullerene Crystallinity dictates Device Efficiency in Small Molecule OPV: the Decisive Role of Device Architecture

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Vacuum-deposited small molecule organic solar cells are a highly active field of research. The development of the photo conversion efficiencies (PCE) up to 8.3%[1] for single junctions and certified 12%[2] for a multi bulk-heterojunctions (BHJ) stack is impressive. The role of substrate heating during or after BHJ deposition for the active layer morphology and its impact on PCE has been a matter of discussion. The crucial influence of C_{60} crytsallinity on the charge separation has been recognized only very recently[3,4,5]. A possible influence of device architecture (e.g. the underlying layer) on BHJ morphology and crystallization has so far not been considered in the literature.

In this work, we show that the effect of substrate heating on PCE in small molecule organic solar cells ($F_4ZnPc:C_{60}$) is closely related to the improved free charge generation in ordered C_{60} regions. It strongly depends on device architecture, namely if the cell is built in inverted or non-inverted architecture. Based on our findings from analytical transmission electron microscopy and device characterization we demonstrate that (i) for non-inverted solar cells heating during deposition has a strong effect on phase separation in the BHJ but not on PCE, whereas (ii) in inverted cells heating has a strong effect on phase separation and induces local fullerene ordering, which improves the free charge generation and the PCE. Our findings elucidate why record efficiencies for vacuum deposited cells are typically achieved in inverted architecture, and have important implications for future development of organic solar cells.

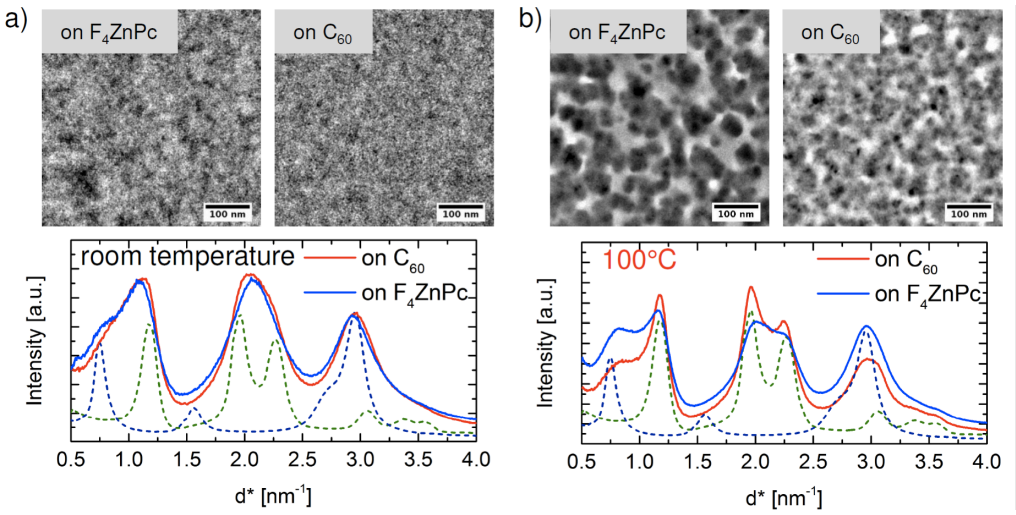

Fig. 1. TEM images and diffraction profiles of BHJs deposited on varying substrates at a) room temperature and b) at 100°C.

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