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Small Molecule Bulk Heterojuction: Impact of two thermodynamically stable morphologies on the efficiency of organic photovoltaics devices¹ NURADHIKA HERATH, VALERIA LAUTER, JIM BROWNING, ILIA IVANOV, JONG KEUM, KAI XIAO, JIAHUA ZHU, Oak Ridge National Laboratory, SANJIB DAS, GONG GU, University of Tennessee Knoxville — Structural characteristics of device active layers play a critical role in charge generation, separation and transport in organic photovoltaics (OPVs). Here we report on morphology and structure control of p-DTS(FBTTh₂)₂:PC₇₁BM films by means of thermal annealing and solvent additive processing. Depth-sensitive neutron reflectometry and X-ray diffraction are employed to characterize the thin film structures, and are correlated to the device performance. The neutron reflectometry results reveal that p-DTS(FBTTh₂)₂:PC₇₁BM films fabricated with 1,8-diiodooctane (DIO) reproducibly exhibit a 3-sublayer morphology similar to thermally annealed films without DIO. Moreover, DIO promotes the formation of a large population of p-DTS(FBTTh₂)₂ nanocrystals leading to a device efficiency (PCE) of 5.9 %. The thermally annealing generate p-DTS(FBTTh₂)₂ crystallites one order of magnitude larger than those formed with the DIO. Our results provide direct evidence that delicate size control of crystal domains closer to the optimum exciton diffusion length is as important as a high crystallinity of charge transport layers.

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