Structural development in molecular semiconductors for thin-film electronics

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Abstract:

Though both the molecular orientation and crystal structure of molecular semiconductors are known to impact charge transport in thin-film devices, controllably accessing different polymorphs and tuning both the in-plane and out-of-plane molecular orientations remain challenging, requiring careful selection of film deposition conditions, film thickness, and substrate chemistry. Without necessitating any specification of these parameters, we have been able to impose specific polymorphs and/or preferential molecular orientation by decoupling film formation from structural development and controlling the latter through post-deposition processing.

In the case of contorted hexabenzocoronene (HBC), we can access two distinct polymorphs and independently vary the distributions of its out-of plane molecular orientation. Starting with a thermally evaporated amorphous HBC film, thermal and solvent-vapor annealing induces the thin film to crystallize into distinct polymorphs; we can further transform between the polymorphs with subsequent rounds of processing. Because the molecular orientation distribution is primarily determined during the first processing step, subjecting already crystalline thin films to different post-deposition processing conditions allows us to access different polymorphs without altering the molecular orientation distribution, thus enabling us to decouple the influence of each on charge transport.

In the case of solution-processable triethylsilylethnyl anthradithiophene (TES ADT), we have been able to exploit its differential crystallization rates on substrates having different surface energies to guide the in-plane growth direction of neighboring crystals. The systematic engineering of solely low- and high-angle grain boundaries between neighboring crystals have allowed us to elucidate their relative contribution to charge transport.