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Microstructure foundations of high carrier mobility in polymers. ERIC LIN, DEAN DELONGCHAMP, R. JOSEPH KLINE, DANIEL FISCHER, LEE RICHTER, ANDY MOAD, NIST, MARTIN HEENEY, IAIN MCCULLOCH, Merck Chemicals, JOHN NORTHRUP, PARC — The microstructure of organic semiconductor films can impact charge carrier mobility because it defines the persistence and quality of \pi bond overlap in the source-drain plane. Important aspects of microstructure include the intermolecular packing arrangement within crystals, the surface-relative crystal orientation, and the overall crystal size and connectivity. We combine complementary microstructure measurements including polarized absorption spectroscopies, scanning probe techniques, and X-ray diffraction to investigate the microstructure details of polymer semiconductors for organic thin film transistors (OTFTs). Here, we demonstrate this approach by solving the packing arrangement of a polymer semiconductor, poly(2,5-bis(3-alkylthiophen-2yl)thieno[3,2-b]thiophenes) (pBTTTs), with hole mobility of (0.2 to 0.6) cm 2/Vs. NEXAFS combined with FTIR spectroscopy reveals nearly all-trans side chains that strongly tilt. With the XRD lamellar spacing, we show that vertically adjacent layers interdigitate. A general consideration of side chain configuration reveals a striking signature packing motif that sets high performance polymers such as pBTTT apart from the lower performance poly(3-alkylthiophenes).

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