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Interdiffusion in bilayers of PCBM fullerene and poly(3-hexyl thiophene) P3HT EDWARD J. KRAMER, NEAL D. TREAT, MICHAEL A. BRADY, UCSB, MICHAEL F. TONEY, SSRL, MICHAEL L. CHABINYC, CRAIG J. HAWKER, UCSB — Bulk heterojunction (BHJ) photovoltaic materials, typified by blends of PCBM and P3HT, are often regarded as immiscible in the absence of casting solvent. We use dynamic secondary ion mass spectrometry and grazing incidence wide angle X-ray scattering to probe the interdiffusion of bilayers of P3HT and deuterated dPCBM. We find that the as cast P3HT film is semicrystalline, while the dPCBM film is amorphous, and that there is complete interdiffusion between dPCBM and P3HT after annealing for 300 s at $T = 150^\circ\text{C}$, a typical treatment to improve device efficiency. This interdiffusion occurs without disrupting the ordered lamellar stacking in the P3HT crystallites, showing that PCBM is miscible with amorphous P3HT at this temperature (the size and/or perfection of the P3HT crystallites actually increases during the annealing). At $T < 150^\circ\text{C}$ rapid diffusion of dPCBM into P3HT still occurs but the dPCBM concentration reaches an apparent solubility limit after long anneals, a limit that decreases with decreasing temperature. This result suggests that dPCBM will phase separate from amorphous P3HT in the BHJ on cooling from 150°C to room temperature.

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