Phase Behaviour and Nanostructure of Polymer/Fullerene Bulk-Heterojunction Blends

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The most promising structure for organic photovoltaic (OPV) materials presented to date is the ‘bulk heterojunction’, whereby an electron-donor and -acceptor are intimately blended. Usually, a conjugated polymer is paired with a small-molecular compound such as a fullerene derivative. The reported strong composition- and thermal-treatment dependence of the power-conversion efficiency of such binaries suggests that phase behaviour, processing conditions and the resulting microstructure play a dominant role in the performance of devices based on these systems. A common approach to realise the required fine-grained but relatively pure donor and acceptor domains is to employ (semi-)crystalline materials. We demonstrate that their blends can undergo eutectic solidification, which readily permits formation of the desired nanostructures. A disadvantage is the low photovoltage achievable with these systems. Instead, careful selection of less ordered materials can yield open-circuit voltages above one volt. Unfortunately, non-crystalline semiconductors have the tendency to be at least partially miscible and thus suffer from more pronounced geminate recombination loss mechanisms. Gratifyingly, the solubility of the fullerene derivative in the polymer phase is found to decrease if a higher molecular-weight polymer fraction is employed, which offers routes towards improving the photovoltaic performance of non-crystalline OPV blends. Thus, we argue that it is possible to design eutectic-like binary systems without compromising on photovoltage.