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Insights into the stability and thermal degradation of P3HT:C₆₀ blended films for solar cell applications

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Abstract

This paper demonstrates the changes in the nanoscale morphology of the blended films induced by a diffusion of C₆₀ molecules and degradation during longer thermal treatment above the glass transition temperature (130 °C). The results showed that the film morphology, including the size and population of poly(3-hexylthiophene) (P3HT) crystallites, rapidly reduced with annealing time. A large-scale (>1µm) C₆₀ aggregation, demonstrating a bulky phase separation between the polymer and C₆₀, was identified after 5 h annealing, which resulted in a degradation of charge carrier mobility and conductivity. X-ray diffraction verifies that the interchain packing of P3HT within the crystallized phase improved with an increasing in annealing time, but the volume fraction of the P3HT (100) phase normal to substrate increased up to 3 h and decreased at longer annealing times resulting in the ageing of the films. Changes in the infrared spectra of the extended annealed samples were recorded and the oxidation products were identified. A degradation mechanism that accounted for the modifications in the infrared spectra and a detachment of the hexyl chain from P3HT was demonstrated, resulting in chain cutting, conjugation loss and a reduction in the UV-vis absorbance. The morphology change with the annealing time resulted in an abrupt decrease in the PCE of P3HT:C₆₀ solar cells. These findings signify that the stability of P3HT:C₆₀ solar cells cannot be secured for longer annealing period owing to the unsettled morphology.

