Supporting Information

Gaining further insight into the solvent additive-driven crystallization of bulk-heterojunction solar cells by in-situ x-ray scattering and optical reflectometry

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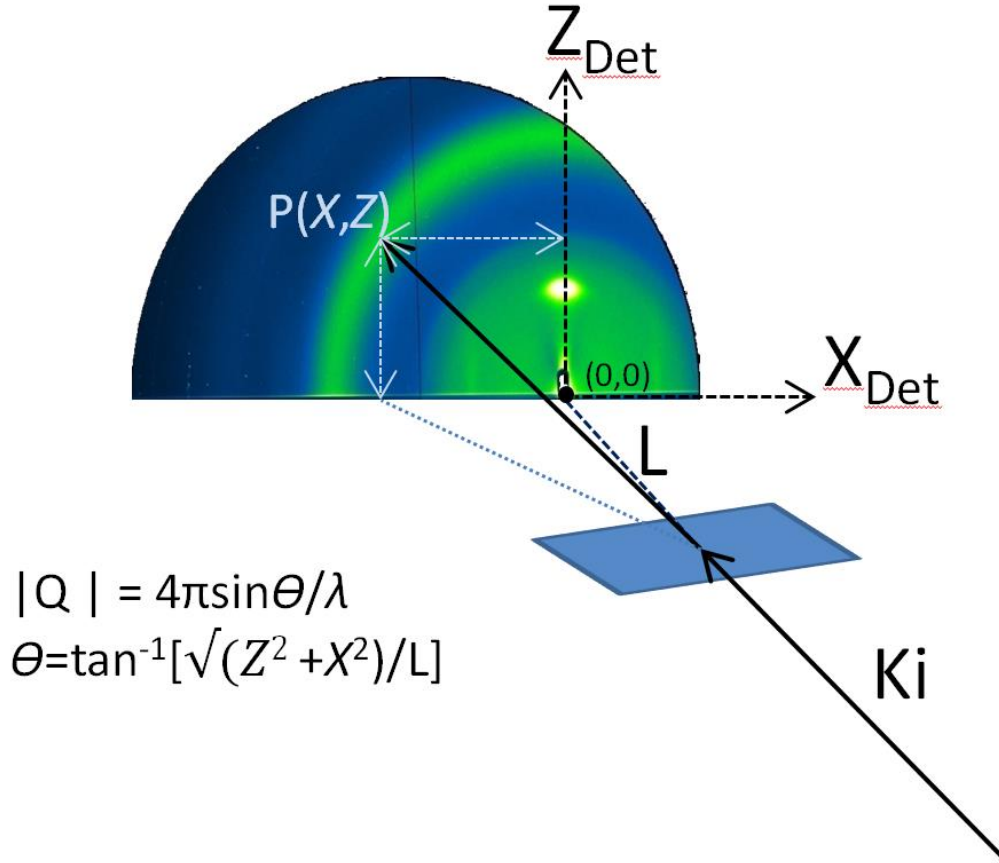
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$$|Q| = 4\pi \sin\Theta / \lambda$$
$$\Theta = \tan^{-1}[\sqrt{(Z^2 + X^2)}/L]$$

Figure SI.1. Scheme of the grazing incidence wide angle x-ray scattering (GIWAXS). X_{DET}, Z_{DET} indicate the coordinates on the detector frame. The absolute value of the scattering vector, Q, is determined from the total scattering angle derived from the pixel position on the detector. Because in GIWAXS the Bragg specular condition is not met, a line scan along Z_{DET} do not correspond to a specular scan (i.e. that direction deviates from Q_Z in the sample reference frame). A 2D MARCCD camera was used with a diameter of 133 mm (2048 pixels). The sample-detector distance was 26.6 cm (calculated from detector scans, moving the detector vertically and horizontally).
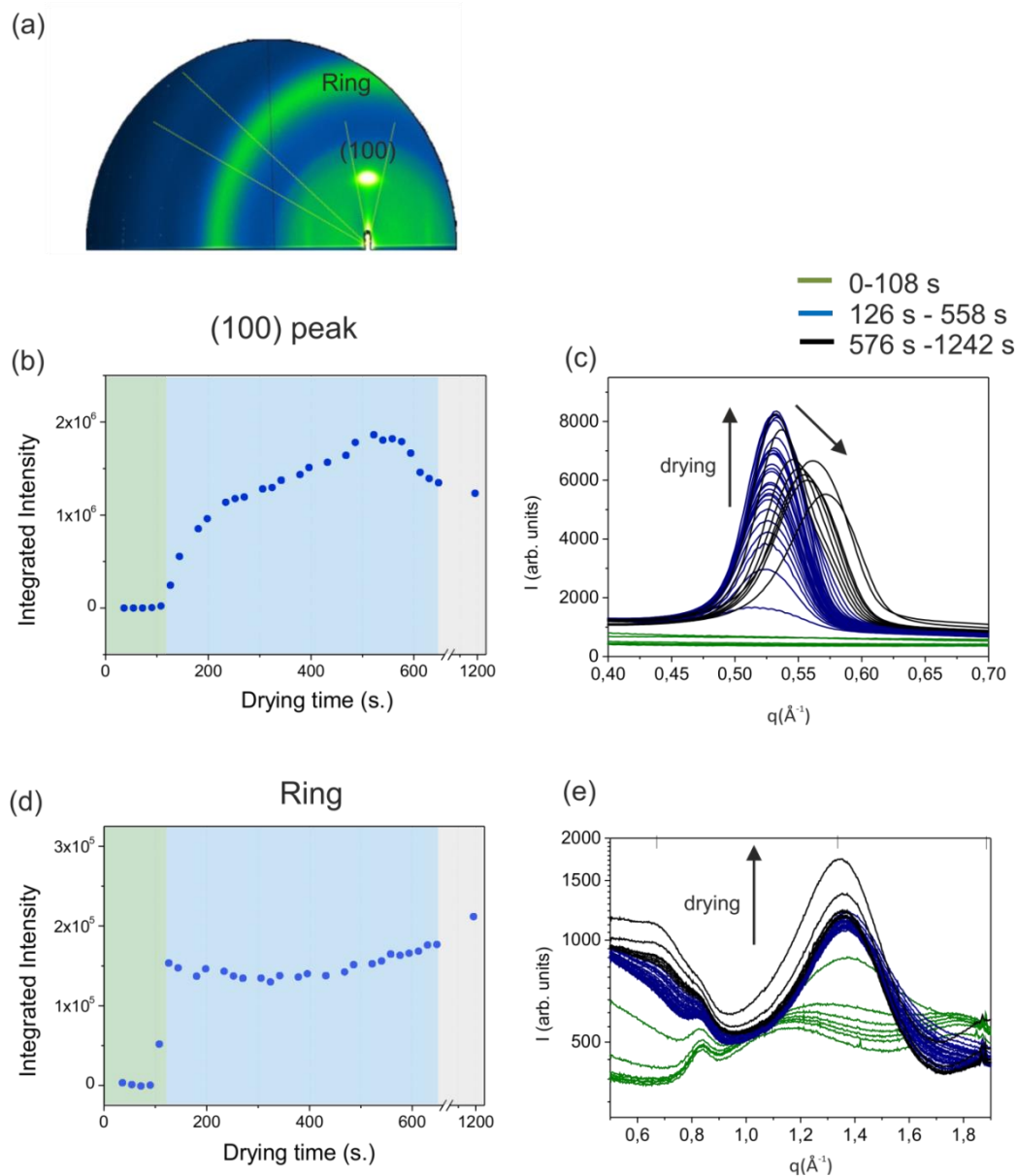
Figure SI.2. Time evolution of radial profiles for PCPDTBT:PC$_{71}$BM cast from DCB/ODT over extended drying time. a) Illustration of the radial cuts used for 0° and 45° in part b and d. b), d) Continuation of integrated intensities in Fig3d over extended drying times. Polymer:Fullerene demixing due to PC$_{71}$BM aggregation in part d at the late stages of drying is accompanied by a decrease in intensity for the polymer peak in part b. c) Shift of the (100) peak from q=0.53 Å^{-1} to q= 0.575 Å^{-1} due to alkyl chain interspace reduction. e) Build up of a broad plateau from q = 0.5-0.7 Å^{-1} and shift of amorphous polymer peak q = 1.37 Å^{-1} to q = 1.34 Å^{-1} due to PC$_{71}$BM aggregation.
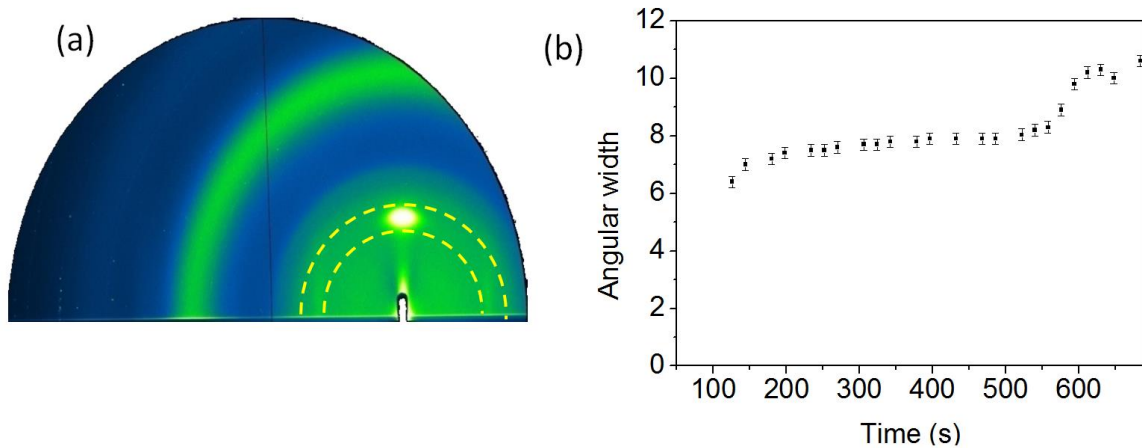
Figure SI.3. a) Scheme showing the angular width profile**.** b) The X-ray intensity was integrated between two concentric semi-circles in the 2D GIWAXS frames containing the (100) peak to account for the orientation distribution of PCPDTBT and plotted as a function of drying time.