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Tuning edge-on oriented ordering of solution-aged poly(3-hexylthiophene) thin films

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Information of P3HT nanofibers from AFM images

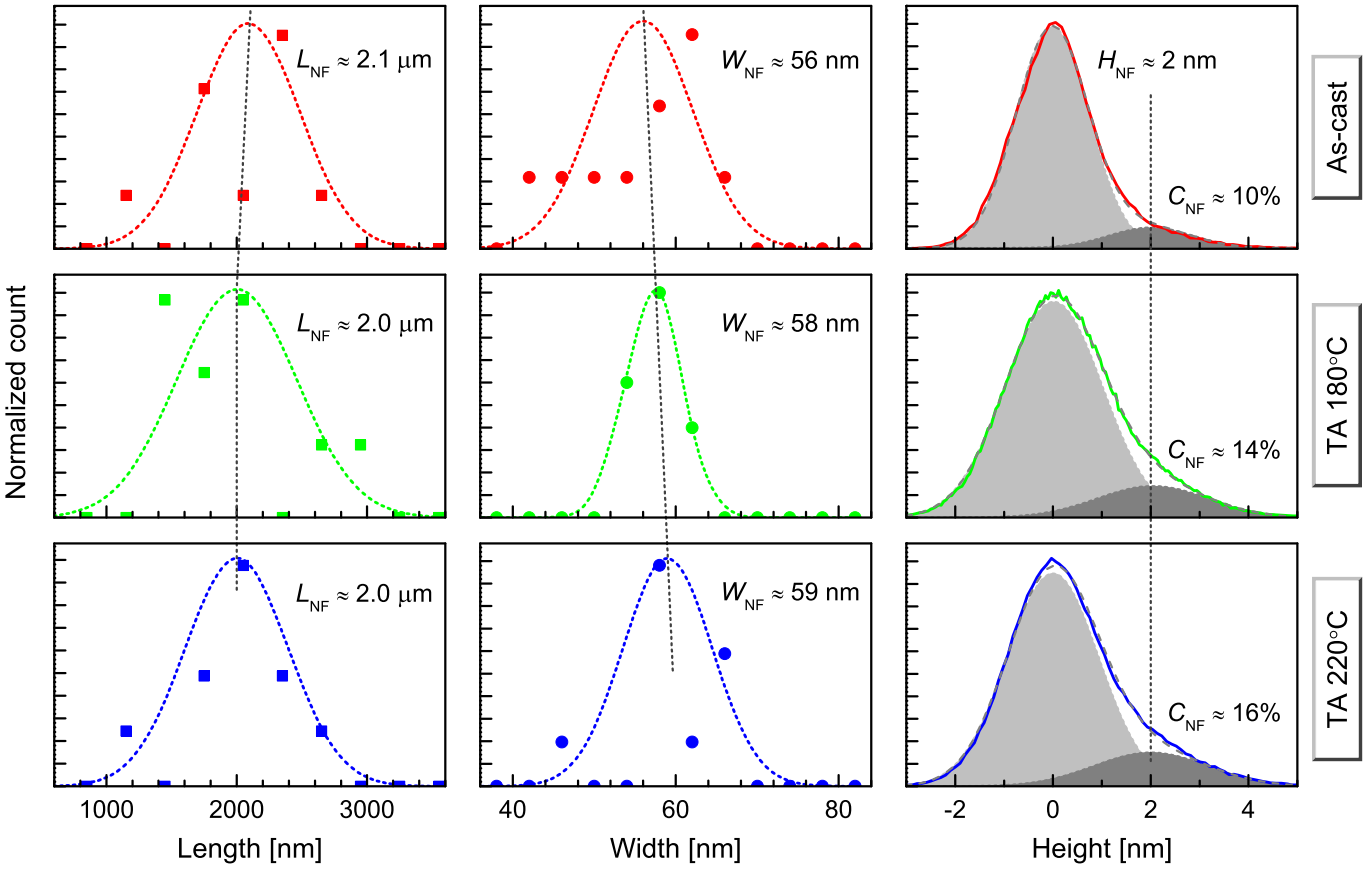

Fig. S1 Length and width distribution of nanofibers and surface height distribution of the solution-aged P3HT thin film ($S1_A$) for the as-cast and after TA at different temperatures, as obtained from the analysis of the AFM images and Gaussian distribution of the length and width of nanofibres and deconvoluted Gaussian distribution of the height of nanofibers with respect to the average surface. Corresponding average length (L_{NF}), width (W_{NF}), height (H_{NF}) and coverage (C_{NF}) of the nanofibers on the surface are indicated.

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Information of P3HT nanofibers from VU-Vis spectra

The intensity of optical absorption spectra of the solution-aged P3HT thin film can be considered as a combination of two parts:

$$I(\lambda) = I_a(\lambda) + I_c(\lambda), \tag{S1}$$

where $I_a(\lambda)$ is the contribution due to the amorphous or disordered (coil-like) polymer chains and $I_c(\lambda)$ is the contribution due to the crystalline aggregates or nanofibers. The contribution of rod-like polymer chains, if any, are not considered separately. Further it is assumed that $I_a(\lambda)$ can be expressed using a broad Gaussian peak, associated with the intrachain π–π^* transition, while $I_a(\lambda)$ can be expressed using a series of Gaussian peaks, associated with the transitions between weakly interacting H-aggerate states:

$$I_a(\lambda) = I_{a,0} \exp\left[-\left(\frac{\lambda - \lambda_a}{\sigma_a}\right)^2\right] \tag{S2a}$$

and

$$I_c(\lambda) = \sum_j I_{0-j} \exp\left[-\left(\frac{\lambda - \lambda_{0-j}}{\sigma_c}\right)^2\right], \tag{S2b}$$

where $I_{a,0}$ is the peak-intensity, λ_a is the peak-position and σ_a is the peak-width related term of the Gaussian peak of the amorphous part, while I_{0-j} is the peak-intensity, λ_{0-j} is the peak-position and σ_c is the peak-width related term of the jth Gaussian peak of the crystalline part. For the calculation of the latter part four peaks are considered. The optical absorption spectra, thus simulated considering Eqs. S1 and S2, are shown in Fig. S2. The relative amount of amorphous and crystalline parts can be estimated considering areas (A_a and A_c) under that curves expressed by Eqs. S2a and S2b, respectively. Such areas under the curves (considering Gaussian functional form) can be expressed as:

$$A_a = \sqrt{\pi}\sigma_a I_a \tag{S3a}$$

and

$$A_c = \sqrt{\pi}\sigma_c \sum_j I_{0-j}. \tag{S3a}$$

Here, for the calculation of the crystalline part, four peaks were considered. The optical absorption spectra, thus simulated considering Eqs. S1 and S2, are shown in Fig. S2. The values of A_a and A_c, obtained from such simulated curves using Eqs. S3a and S3b, were then used to estimate the percentage [namely $A_a/(A_a+A_c)$ and $A_c/(A_a+A_c)$] of the disordered polymer chains and the crystalline nanofibers.

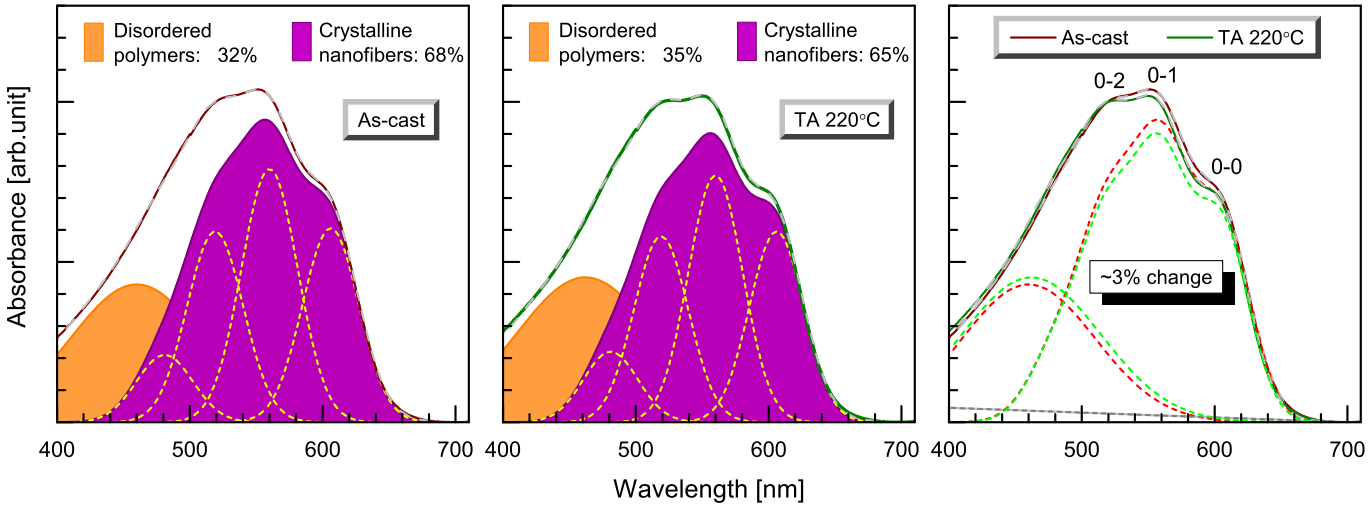

Fig. S2 Optical absorption spectra and their deconvolution (using Eqs. S1 and S2) of the solution-aged P3HT thin film (G1) for the as-cast and after TA at 220°C. Contribution of the disordered polymer chains and the crystalline nanofibers are indicated by different filled colors. Corresponding percentages are indicated. Small change in the percentage with TA is evident from the values and also from the comparative curves.