Local structure of semicrystalline P3HT films probed by nanofocused coherent x-rays†

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1 Supplementary information

1.1 Average structural characteristics of a pristine P3HT film

Scattering data ($M = 1000$ diffraction patterns) from pristine P3HT films were analyzed similar to those from P3HT/AuNPs blend. The ensemble averaged radial intensity $\langle\langle I(q,\varphi)\rangle_\varphi\rangle_M$ profile and the difference Fourier components $\langle\widetilde{C}_n(q)\rangle_M$ were determined in the same way as in Ref.[1]. As compared to P3HT/AuNPs blend, the ensemble-averaged Fourier spectrum $\langle\widetilde{C}_n(q)\rangle_M$ does not show any pronounced q-dependence for any of the determined Fourier components. As one can see, the Fourier components in Fig. 1(b) have randomly fluctuating vanishing values, indicating the absence of any orientational order in the system.

1.2 Spatially resolved analysis of diffraction data

Spatially resolved analysis of the diffraction data can be performed directly by applying Eq. (1) (from the main text) to the measured diffraction patterns, as well as using CCFs and the relation $|I_n(q)| = [C_n(q)]^{1/2}$. The first approach is less accurate if detector gaps are present although enables direct calculation of the phases of $I_n(q)$. The second approach allows more accurate determination of the amplitudes $|I_n(q)|$ since detector gaps can be eliminated from the analysis, although phases can not be accessed. In either case, the spectra $I_n(q)$ calculated for a single diffraction pattern may contain nonzero contributions for different n. In this paper only $n = 0, 2, 4$ and 6 were considered, that remain in the spectrum of CCFs after statistical averaging [see the results of XCCA in Ref.[1]].

1.3 Average P3HT domain size

Analysis of the (200) peak fits on the $|I_0(q)|$ profile shows [see Fig. 2], that the average positional correlation length $\xi = 2\pi/\gamma_0$ is of the order of 10 nm.

References

1 R. P. Kurta, L. Grodd, E. Mikayelyan, O. Y. Gorobtsov, I. Fratoddi, I. Venditti, M. Sprung, S. Grigorian and I. A. Vartanyants, *J.Phys: Conf.Series*, 2014, **499**, 012021.

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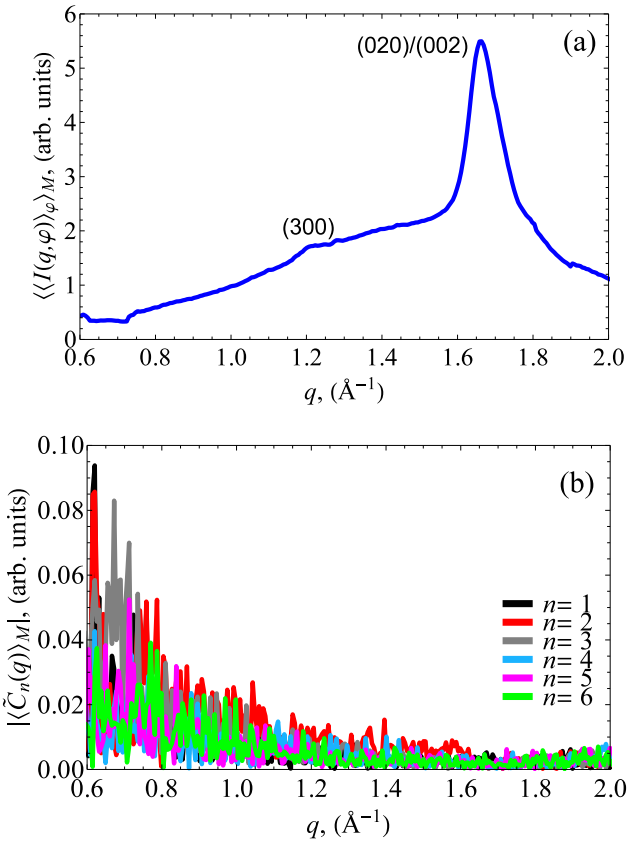

Fig. 1 Average structural characteristics of a pristine P3HT film. (a) Ensemble averaged radial intensity $\langle\langle I(q,\varphi)\rangle_\varphi\rangle_M$. (b) The difference Fourier components $\langle\tilde{C}_n(q)\rangle_M$ as a function of q. Only the first six Fourier components are shown in (b).

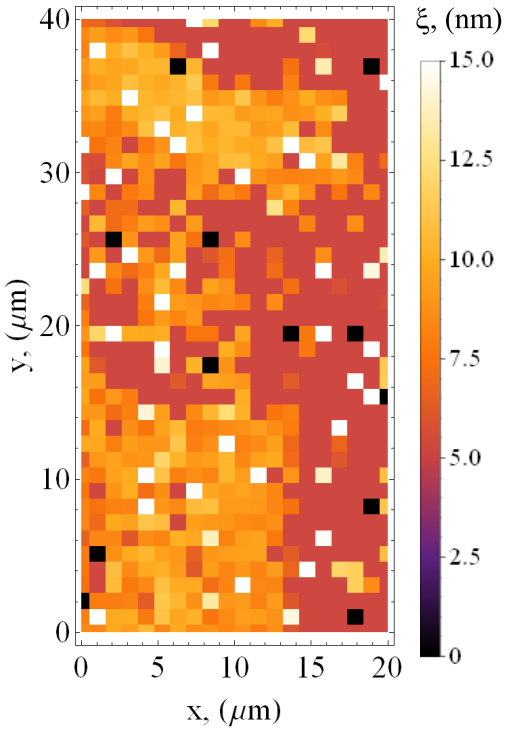

Fig. 2 Spatially resolved 2D map of the positional correlation length $\xi = 2\pi/\gamma_0$ determined from the Lorentzian fit of the (200) peak on the $|I_0(q)|$ profile (see main text).