



Experiment title:
Structural and optical evolution of PEN:PFP mixtures during temperature driven phase transitions

Experiment number:
SC3170 + SI2220

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|---------------------------|---|--------------------------------------|
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Report:

As stated in the proposal, we have grown mixed organic thin films by coevaporation of the molecules Pentacene (PEN, C₂₂H₁₄) and its fluorinated counterpart Perfluoropentacene (PFP, C₂₂F₁₄). In order to characterize these mixtures, the study was complemented by a temperature dependent series of three pure PFP-films. A MARCCD was used to measure X-ray diffraction during growth, *in situ* in real-time. After each growth run, post growth scans were applied to measure a large range in q-space, for the pure PFP- and each coevaporated thin film, respectively. Since the analysis of the data is still in progress we can present only some preliminary findings.

In Fig. 1 the reflectivity data of three 50 nm PFP-films, which were grown at 333K, 253K and 153K, is shown. For 333K and 253K Bragg reflections can be observed until the 4th order, indicating a good out-of-plane crystallinity for both temperatures. The lattice spacing of 15.6 Å is attributed to the phase of upright standing molecules and agrees well with the literature. In addition, a new peak at $q_z = 1.55 \text{ \AA}^{-1}$ was found for 253 K. This corresponds to a lattice spacing of 4.01 Å, which indicates the existence of a phase with lying down molecules at low temperatures. For 153K, no Bragg reflections can be observed, thus suggesting an amorphous film growth, which is also confirmed by postgrowth GIXD and MARCCD measurements.

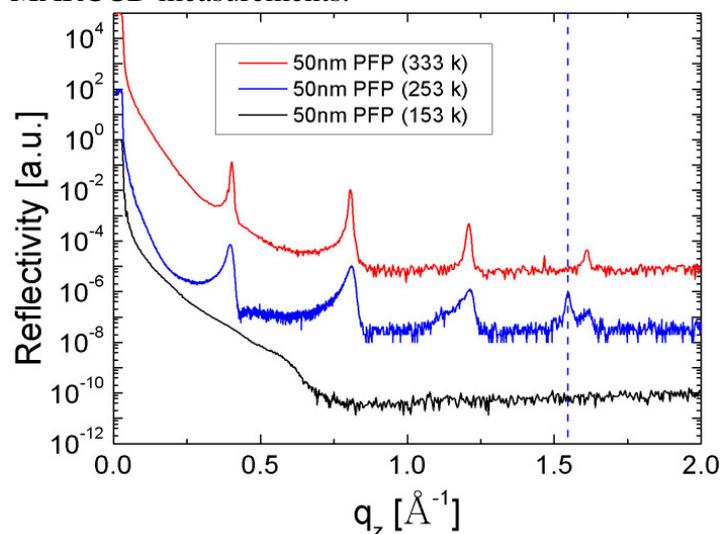


Figure 1: Out-of-plane post growth scan of 50nm PFP films at three substrate temperatures.

Figure 2 shows a postgrowth Reciprocal Space Map (RSM) of a 50nm PFP-film, which was grown at a substrate temperature of 333K. At $Q_{\parallel} = 1.09 \text{ \AA}^{-1}$ and $Q_{\parallel} = 1.76 \text{ \AA}^{-1}$ Bragg reflections until the second order can be observed along the Q_z direction. The positions were previously reported in the literature and assigned to the PFP thin film phase with a monoclinic unit cell. However, our measurements reveal a strong temperature dependence of the film texture, which is most intense at 333K and almost vanishes for 253K.

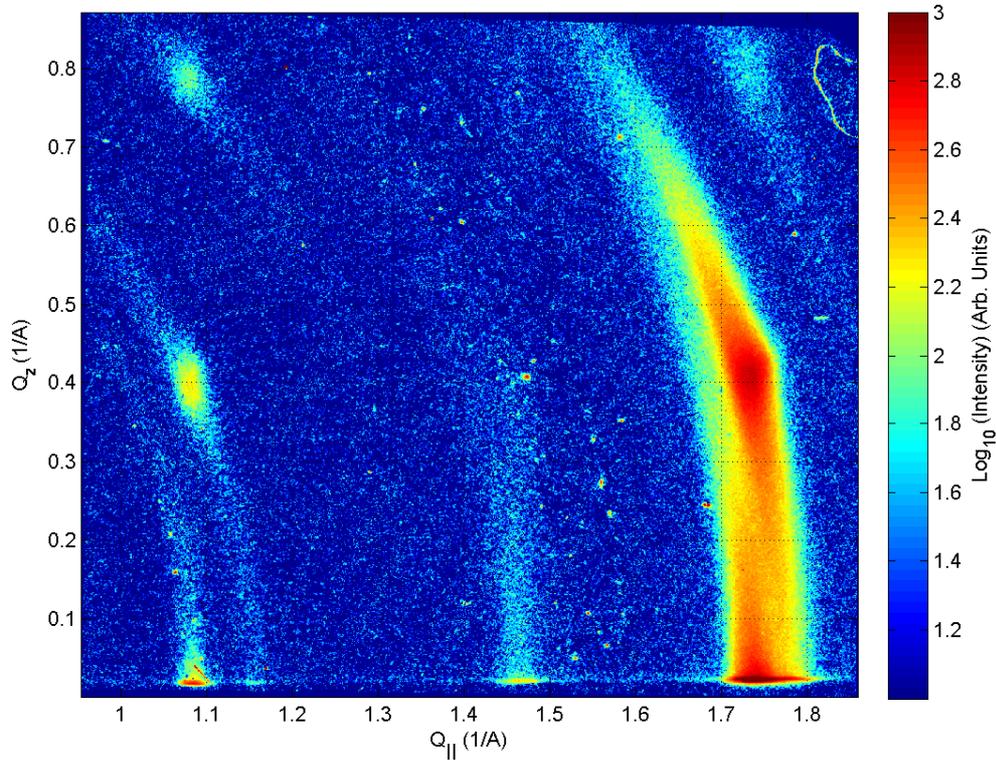


Figure 2: RSM of 50nm PFP at 333K substrate temperature.

We wish to acknowledge the excellent collaboration with the local contact Roberto Nervo which made this challenging experiment a success.