Soft Matter, Polymers, Composites

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Characterization of codeposited pentacene/perfluoropentacene on different substrates by transmission electron microscopy

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Over the last several years organic semiconductor materials gain more and more importance. Two examples for such materials are pentacene (PEN) and perfluoropentacene (PFP). PEN is a polycyclic aromatic hydrocarbon ($C_{22}H_{14}$) with a HOMO-LUMO gap of approximately 2.1eV. Because of its high hole mobility it acts as an p-type semiconductor. The unit cell of PEN crystals contains two nonequivalent PEN molecules and crystallization takes always place in a triclinic crystal structure. The different phases, like for example the Campbell [1] and the thin film [2] phase, that have been observed for PEN differ in the parameters of the triclinic unit cell.

In case of PFP ($C_{22}F_{14}$) the hydrogen atoms are replaced by fluorine atoms. The strong electronegativity of fluorine results in an inverted quadrupole moment of PFP from PEN. PFP acts as a n-type semiconductor and crystallizes in a monoclinic crystal structure. Also for PFP different polymorphs exist [3],[4]. The strong structural relation of PFP to PEN makes these two materials promising for p-n-junctions because high quality interfaces are expected in between.

Transmission electron microscopy (TEM) is a quite useful method to investigate such structures at a high resolution level und thus to analyse the quality of PFP:PEN composite materials.

In our work we investigated PFP:PEN codeposited films that have been grown on different substrates like alkali halides (sodium fluoride (NaF), potassium chloride (KCl)) and silicon oxide via organic molecular beam deposition (OMBD). Overview TEM images as well as atomic force microscopy images show that the samples grown on alkali halogenides consist of organic fibers lying on an organic background layer.

In the TEM we used electron diffraction to get information on the crystal orientation of submicrometer-sized regions. This gives indication of local orientation correlations that cannot be investigated by X-ray diffraction because of the spatial averaging.

Besides electron diffraction also high resolution TEM imaging is a method to identify and to distinguish between separated PEN or PFP films and mixed PFP:PEN phases. Figure 1 shows a high resolution TEM image of PEN:PFP grown on NaF substrate. During the preparation process the substrate was removed and should not contribute to the signals in TEM. Generating a linescan along the turquoise area in the high resolution image a lattice plane spacing of 3.76Å was determined. This corresponds well to the (020) PEN thin film planes. Figure 2 shows a high resolution TEM image of the same sample. In this case a lattice plane spacing of 3.61Å was determined. This spacing does not fit to PEN, PFP or residues of the NaF substrate. Thus, it is attributed to the mixed phase.

High resolution TEM of one of the fibers that developed in a PEN:PFP sample grown on KCl is shown in Figure 3 (a). The lattice plane spacing was again determined from a line scan (b) along the turquoise area in (a). The spacing of 13.1Å is quite large and may be related to one of the lattice constants of the mixed phase. In Figure 3 (c) another part of the fiber is displayed, showing that the orientation does not change along the fiber.

The presentation will summarize the influence of different substrates on the growth of codeposited PFP/PEN and discuss its implications on the understanding of the film formation.

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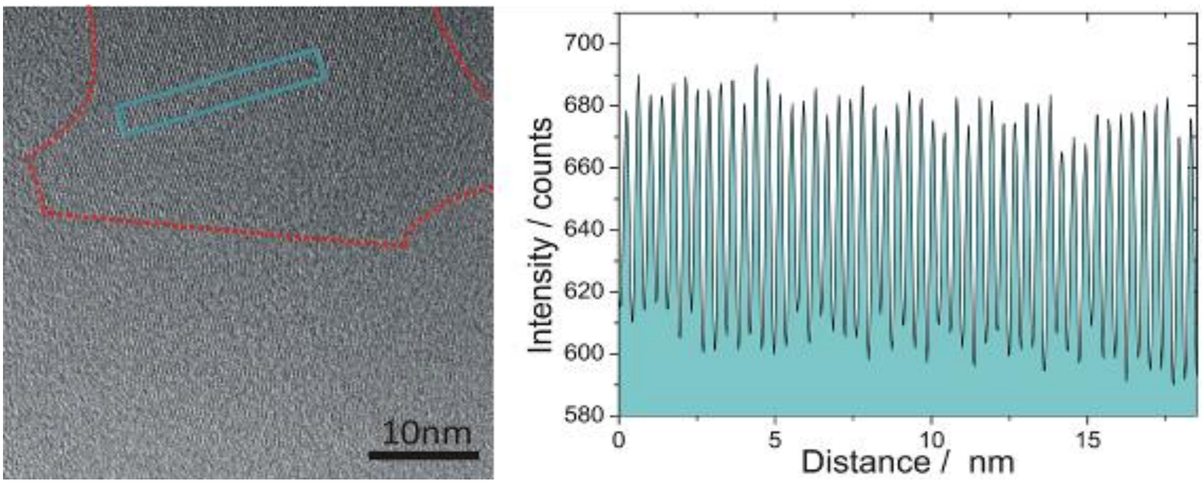

Figure 1. High resolution TEM image of a PEN:PFP/NaF sample. From the linescan along the turquoise area a lattice plane spacing of 3.76Å can be determined. This corresponds well to the (020) PEN thin film planes.

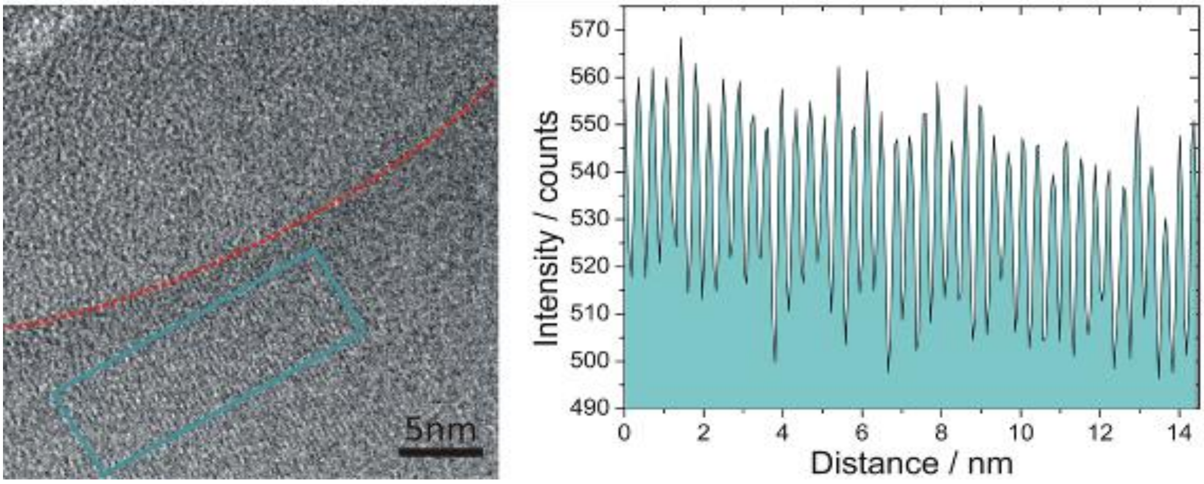

Figure 2. High resolution TEM image of a PEN:PFP/NaF sample. From the linescan along the turquoise area a lattice plane spacing of 3.61Å can be determined. This spacing does not fit to PEN or PFP and is attributed to the mixed phase.

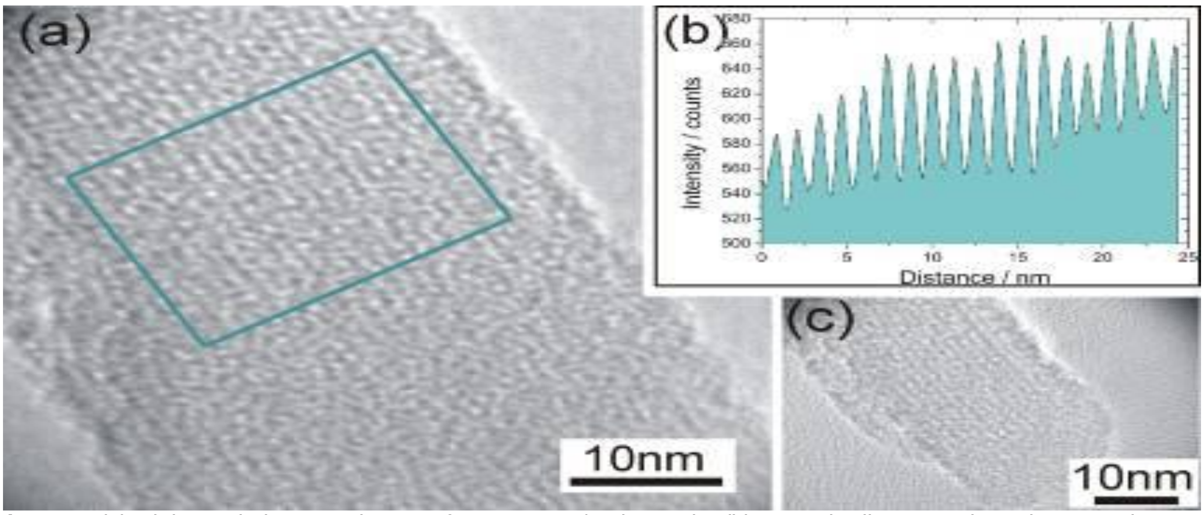

Figure 3. (a) High resolution TEM image of a PEN:PFP/KCl sample. (b) From the linescan along the turquoise area in (a) a lattice plane spacing of approximately 13.1Å can be determined. (c) A high resolution TEM image of another part of the fiber shows that the orientation does not change along the fiber.