Supplementary Information - Morphological and structural investigation of sexithiophene growth on KCl (100)

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Experimental Results

Morphological Investigation

As presented in the manuscript we have investigated the morphology of sexithiophene (6T) deposited on KCl substrates by means of scanning force microscopy (SFM). The samples have been prepared at substrate temperatures ranging from 60 °C to 135 °C and we have found significant differences as visible in figure 1. With increasing substrate temperature we observe a reduction in the number of islands and an increase in the cross-sectional dimensions of the needles.

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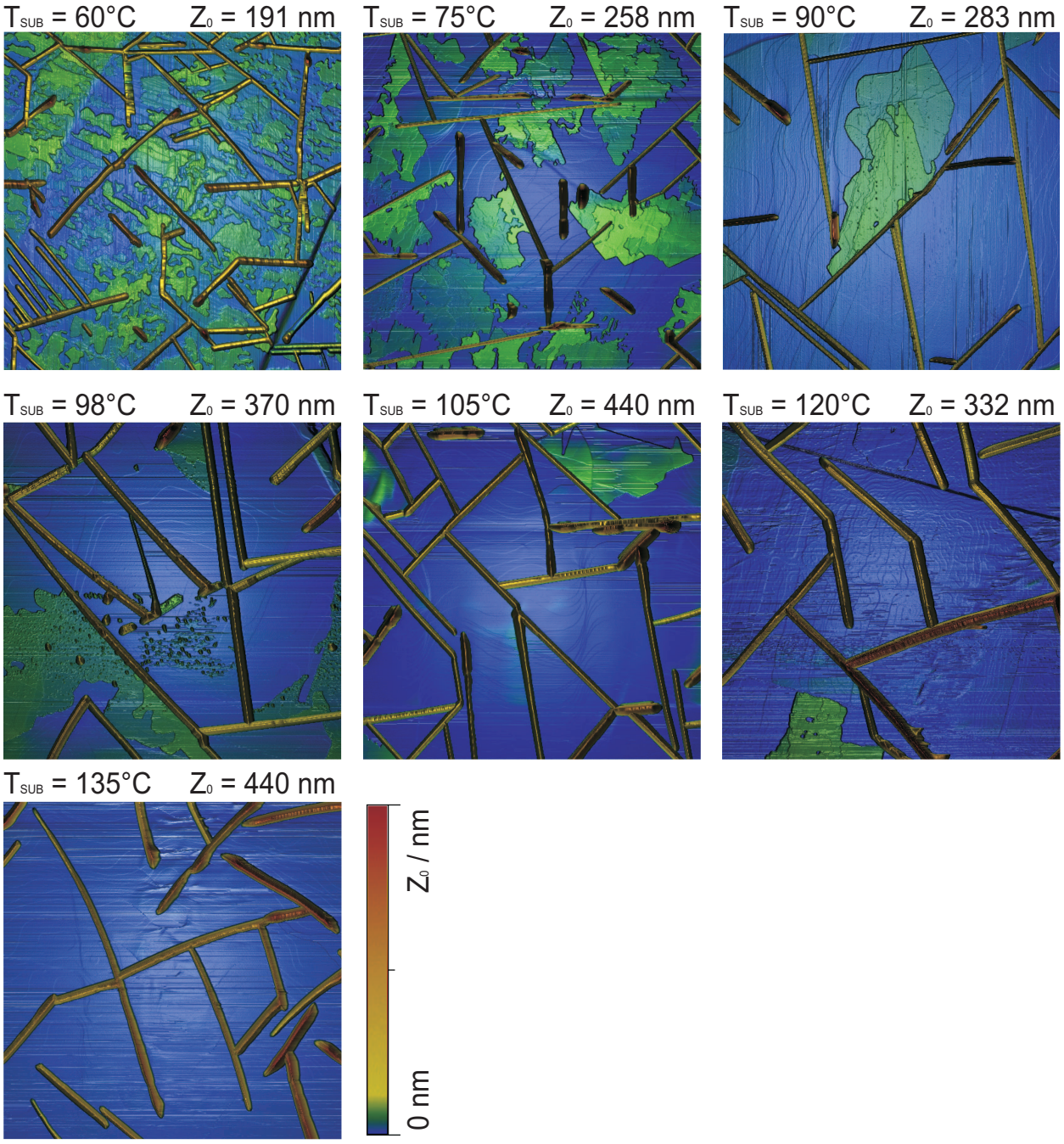

Figure 1: Scanning force microscopy investigation of sexithiophene on KCl prepared at substrate temperatures (T_{SUB}) ranging from 60 °C to 135 °C. The area of the scans is $10 \times 10\,\mu m^2$ and the maximum height (Z_0) is given for each image.

Azimuthal Alignment of Crystallites

By performing specular XRD scans it was demonstrated in the manuscript, that three distinct structures are present on the samples:

- needle-like crystals of type A with a (010) contact plane (lying molecules)
- needle-like crystals of type B with a $(\bar{4}11)$ contact plane (lying molecules)
- island-like crystals of type S with a (100) contact plane (standing molecules)

In order to clarify not only the contact plane, but also the azimuthal orientation of the crystals on the KCl surface, XRD pole figures have been collected for the $\{\bar{4}11\}$, $\{\bar{3}11\}$ and $\{\bar{2}11\}$ net planes. This allowed us to conclude, that all types of crystals are in an epitaxial alignment with the surface.

To further substantiate this results we have also taken pole figures for the $\{120\}$ and $\{011\}$ net planes as shown in figure 2 (a) and (b). The simulated peaks positions depicted in the right panel are based on the assumption that crystals of type A, B and S are present on the samples and the simulation nicely resembles the measurement results. Please note that reflections originating from crystals exhibiting different contact planes are expected to appear in the same pole figure, if the scanned net planes have equal lattice spacing.

FFT analysis of optical micrograph images

The azimuthal alignment of the needle-like crystallites was further analyzed by optical microscopy. In figure 3, a complete series of images and their respective Fourier transformations are depicted. It is visible that the average length of the 6T crystallites is increasing with increasing substrate temperature. Consequently the quality of the Fourier transformed images is better for samples prepared at higher temperatures. In some cases it is even possible to distinguish between the long needle axis (LNAs) of crystals of type A and B, that differ by only 8.6° as evaluated by XRD.

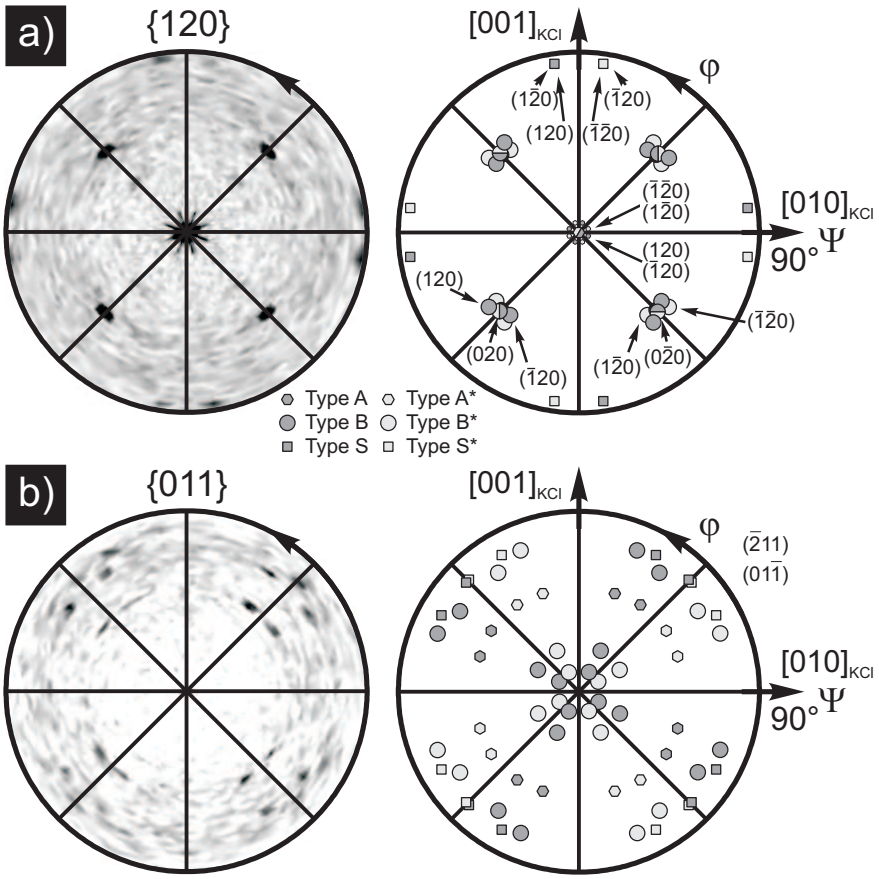

Figure 2: Measured (left) and simulated (right) X-ray diffraction pole figures of the (a) $\{120\}$ and (c) $\{011\}$ net plane normals (poles). Reflections of crystal type A, B and S are indexed with hexagons, circles and rectangles respectively. Symmetry equivalent crystals denoted by A*, B* and S* exhibiting contact planes of $\{0\bar{1}0\}$, $\{4\bar{1}\bar{1}\}$ and $\{\bar{1}00\}$ respectively, are formed due to mirror axis of the substrate surface (black lines). The measurements were performed on a sexithiophene layer deposited at a substrate temperature of 90 °C.

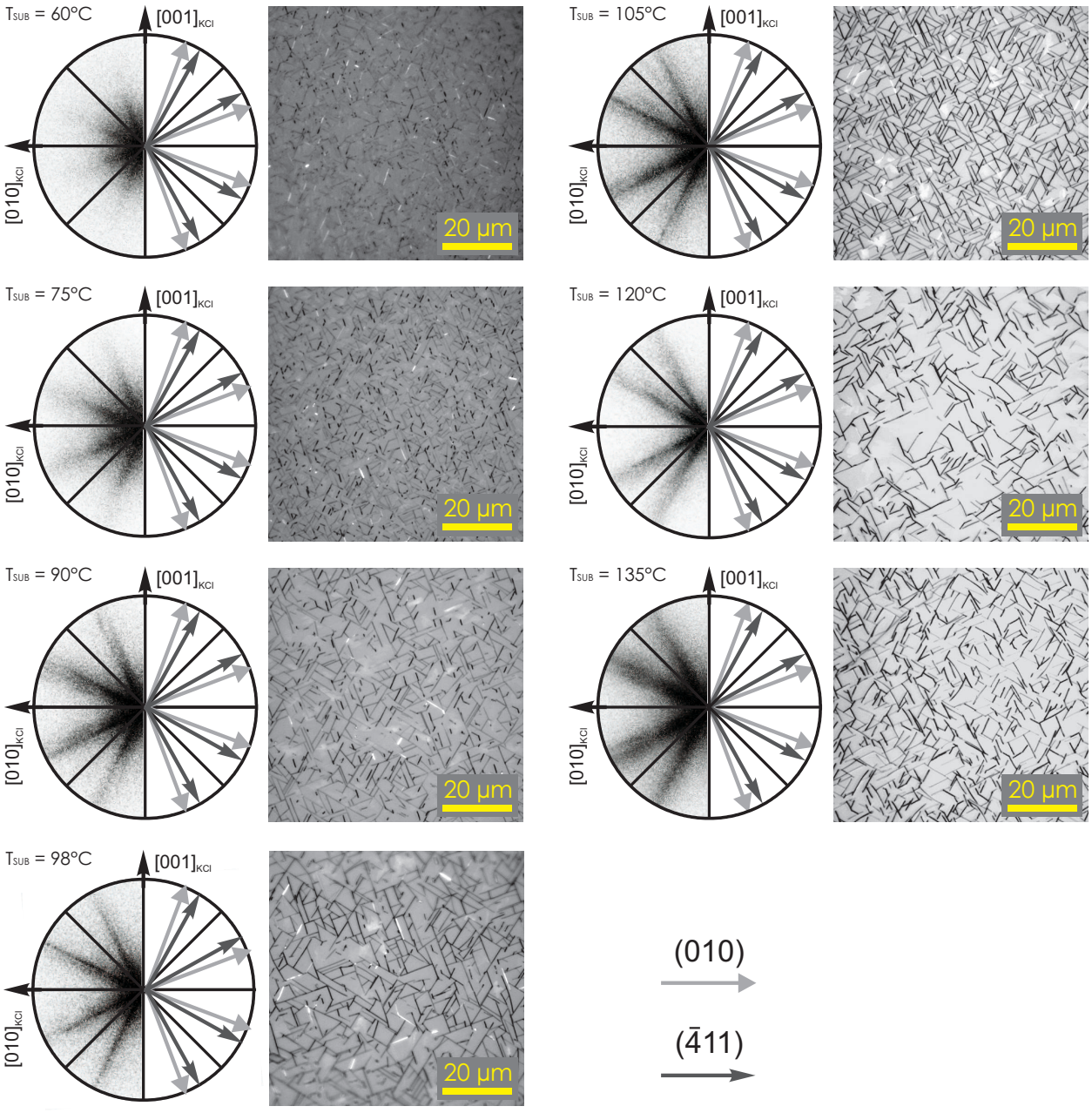

Figure 3: Optical microscope image of sexithiophene deposited on KCl (100) at substrate temperatures of 60 °C to 135 °C and their respective Fourier transformations revealing the long needle axis (LNAs) present in the image. The different orientations of LNAs for needles of type A (010) and type B $(\bar{4}11)$ are sketched as deduced from X-ray diffraction pole figure analysis.