



Experiment title: Spatially and time resolved structure formation in conducting discotic liquid crystalline (LC) systems during extrusion.

Experiment number:
ME-1024

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Shifts: 12	Local contact(s): Dr. Richard DAVIES	<i>Received at ESRF:</i>

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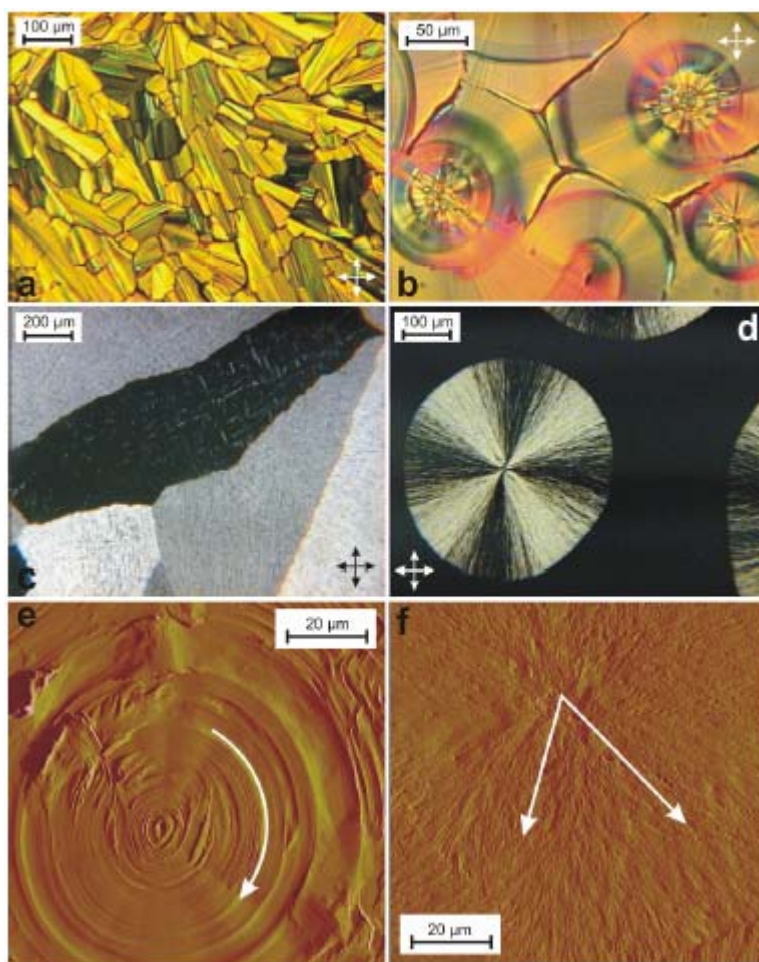
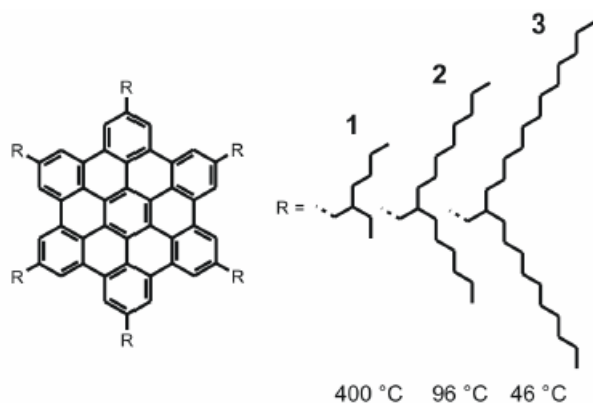
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Report:

Organic electronics are emerging as viable technology options for creating new, improved electrical and optical systems. In this area, two distinct approaches are pursued. One utilizes electron transfer along a covalently bound oligomer or polymer chain. The other aims to exploit extensive non-covalent interactions of low molecular weight molecules to prepare large domains by supramolecular organisation. For this approach, it is a prerequisite to orient the molecules adequately on a substrate with respect to their function in the device and put them in electrical contact with electrodes. Discotic hexa-*peri*-hexabenzocoronenes (HBC), as a mesogen, exhibit some of the highest values of intrinsic charge carrier mobility, which allow their successful implementation in photovoltaic devices and field-effect transistors (FET). Thereby, different device geometries necessitate a specific macroscopic alignment of the molecules with respect to the substrate. In FETs, the charges migrate between source and drain parallel to the substrate, which requires an edge-on arrangement of the molecules. On the other hand, a molecular face-on orientation, which leads to the formation of a homeotropic phase, is thought to improve the efficiency of photovoltaic cells or could be interesting as hole-injection layers for organic LEDs. The control of the molecular orientation and therefore the alignment of the charge carrier pathways constitute a task of major importance for material scientists, because it sensitively determines the performance of the electronic device. However, the mechanism for the self-organisation and orientation of a discotic material on a substrate is not fully understood.

We have investigated the simple melt-processing of three hydrocarbon HBC derivatives (Figure 1), providing control of the columnar structure orientation on a substrate. The morphology has been locally investigated using a synchrotron radiation (SR) microfocussed X-ray beam to probe the local columnar orientation.



To gain a further structural insight, 2D wide-angle X-ray scattering (2D-WAXS) experiments were performed on the obtained films at ID13 using a microfocus X-ray beam with a beam spot size at the focal position of approximately $0.8 \times 0.8 \mu\text{m}^2$. The structure of the morphology was mapped by performing a raster scan over the sample and taking diffractograms. Diffraction data was collected using a “MARCCD” area detector, with an

In the case of compound **1**, the columnar axis lay perpendicular to the substrate surface. Since the material did not pack in a hexagonal unit cell, as has been observed for a wide variety of discotic molecules, the POM image revealed birefringence. The orientation of the unit cells in the recorded diffraction pattern matrix (Figure 3B) was analyzed by determining the orientation vector arrays (Figure 3C), which has been found to correlate well with the optical domain boundaries (Figure 3D).

organisations within the different morphologies of **2** and **3**, which differed only in the length of the attached chains. Surprisingly, the change of the alkyl chain bulkiness influenced the spontaneous molecular organisation and the growth direction with respect to the nucleation centre in the domains. This might be caused by differences in the side-chain packing of the two derivatives.

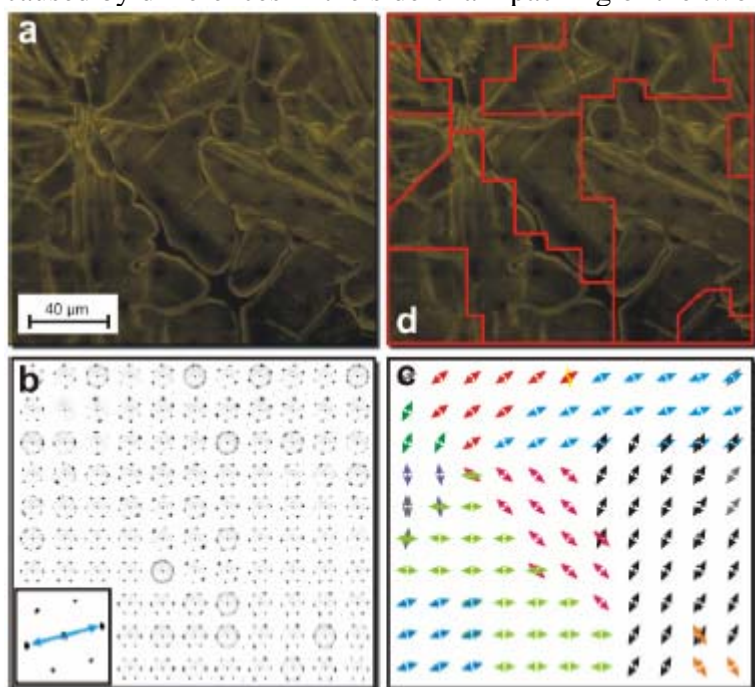


Figure 3. Scanning synchrotron experiments, (a) Reflected light darkfield optical microscopy image of **1**, sandwiched between glass slides, (b) array of transmission diffraction patterns recorded by scanning across the local texture (220 x 200 μm, 20 μm step size), inset: magnification of one X-ray pattern with the orientation vector (c) array of the orientations of the unit cell, (d) domain boundaries detected by X-ray scattering superimposed on the optical microscopy image.

The different molecular orientation with respect to the substrate for **2** and **3** opened the possibility to investigate the charge carrier transport in the crystalline columnar phase, both along and perpendicular to the stacking axis.

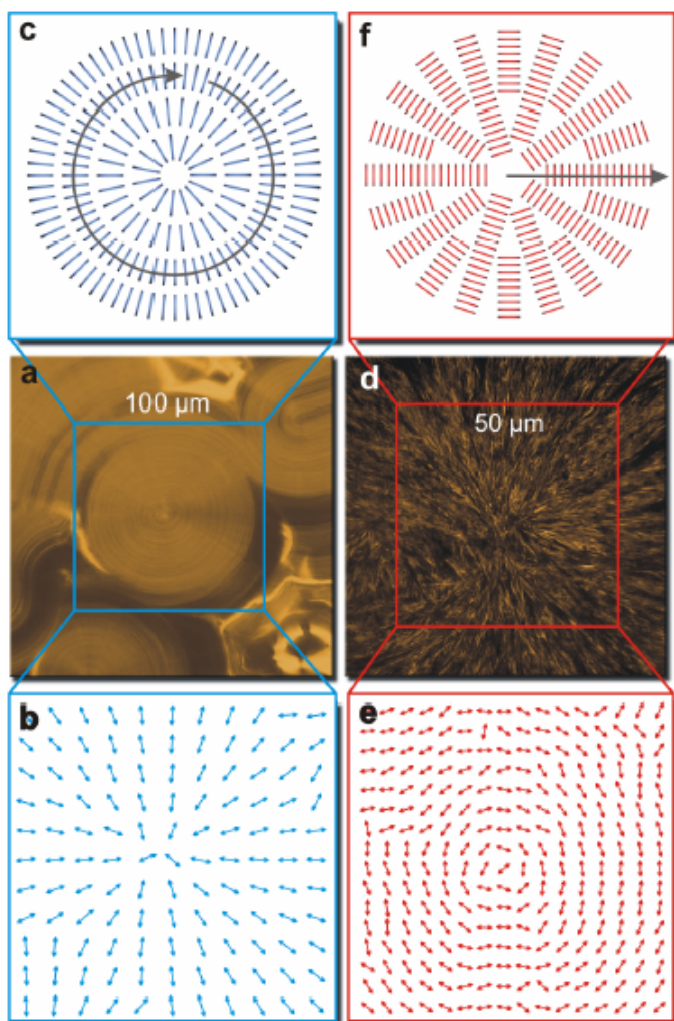


Figure 4. Comparison of the morphologies of **2** and **3**, reflected light dark-field optical microscopy image of (a) **2**, crystallized on one surface and (d) **3**; vector array displaying the orientation of the unit cells in the marked area for (b) **2** (blue) and (e) **3** (red); schematical columnar orientation for (c) **2** and (f) **3**.