	Experiment title: Grazing-incidence x-ray diffraction from semiconducting polymer films	Experiment number: 28-01-26
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Report:

Electroluminescence from ultrathin layers of organic materials have been explored for several decades. Much of the initial development was not of polymers but of small molecules made up of a series of rings, such as aluminium quinolate (Alq). Conjugated polymers promise an attractive alternative in view of their robustness and processability - interest in these light emitting polymers has mushroomed since 1989 when Richard Friend, Andrew Holmes and colleagues generated yellow-green light from a poly (phenylene vinylene) (PPV) light emitting diode. Both technologies rely on charge conduction via delocalised π-electrons along a molecular framework of alternating single and multiple bonds. PPV is formed by thermal conversion from precursors. After conversion and annealing, there is little scope for control of the chain microstructure and alignment. A recently developed alternative, poly (9,9-dioctylfluorene) (PFO), is a conjugated liquid crystalline polymer made up of an aromatic backbone of repeated linked benzene rings with long aliphatic side-chains (fig.1) [1]. It emits light in the blue region of the spectrum. Its structure can be controlled to an extent by thermal processing offering a potential advantage over PPV.   The main aim of this experiment was to investigate the surface structure of PPV, since the interfacial conformation is likely to affect the electrical behaviour of a p-n junction and to investigate the structural properties of PFO regarding which relatively little is known.

Two scattering geometries were employed each with a grazing angle of incidence β. In geometry A, the diffracted beam and the scattering vector **Q** are in the plane defined by the incident beam and the surface normal: this geometry is most sensitive to correlations normal to the surface with an additional in-plane component. In geometry B, the diffracted beam also subtends a grazing angle to

the surface for $\beta, \beta' \leq \beta_c$, where β_c is the critical angle, sensitive to correlations in the plane of the surface. The PPV samples were found to be not fully converted from the precursors and the measurements were curtailed. PFO samples annealed at 130°C and 180-200°C, known from calorimetric measurements to have different liquid crystalline states, were investigated (fig 1).
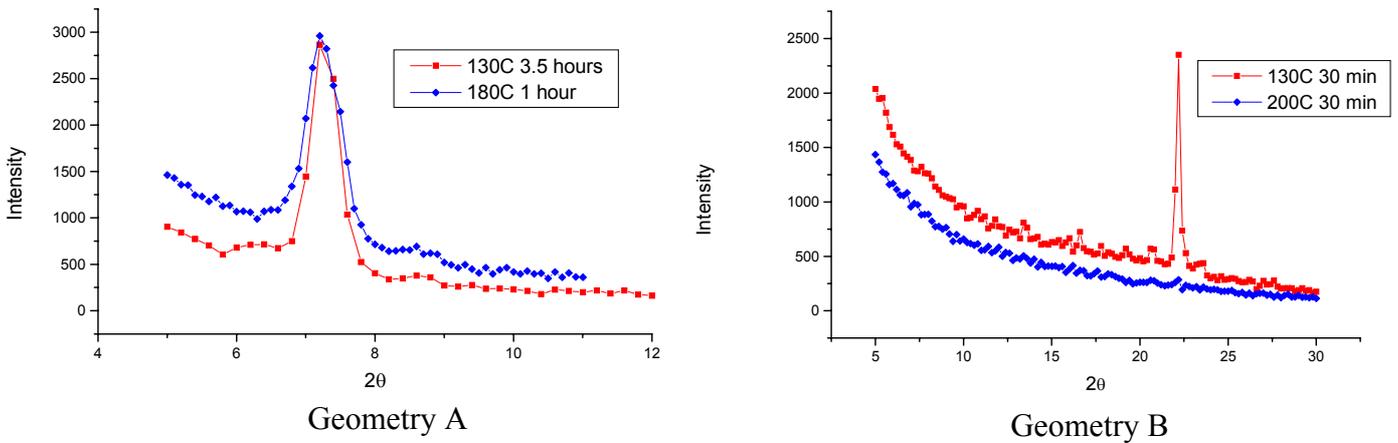

Geometry A

Geometry B

Fig. 1 Grazing incidence scans in geometries A and B for samples in the two liquid crystalline phases of PFO. The higher temperature phase shows nematic ordering whereas the lower temperature phase is smectic.

By varying the angle of incidence the relative order in the surface and bulk regions could be probed. The data indicate that the surface is more ordered in the nematic phase than in the crystalline phase. However, the bulk structure is more ordered in the crystalline phase. This apparent effect needs further investigation, particularly in view of the important role of the interface in potential electronic applications. Scans of the angle of incidence through the diffraction peaks appear to contain much information (fig. 2) and we are currently attempting to fit these to gain some information about the degree of order as a function of depth.
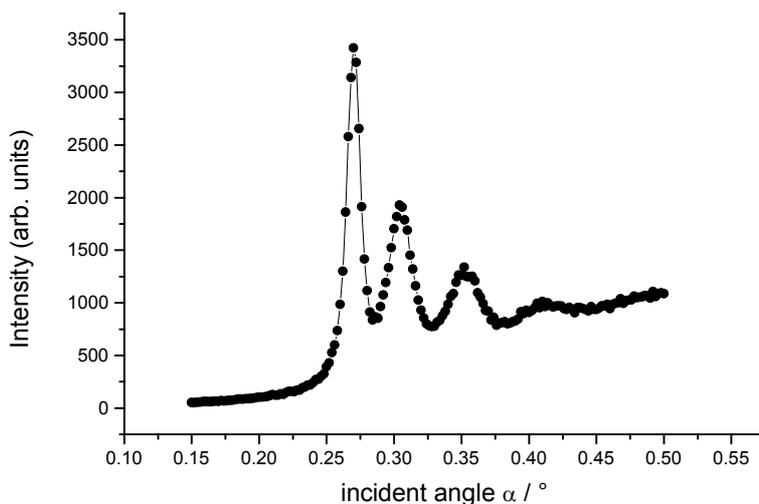

Fig. 2 Variation of peak intensity with angle of incidence for the peak at 7.2° (geometry A) in fig. 1. The oscillations arise from the film thickness and the overall intensity distribution depends on the depth of the ordered region relative to the surface.