	Experiment title: Interface structure in a light-emitting semiconducting polymer	Experiment number:
Beamline: **BM 28**	**Date of experiment:** from: 6 September 2000 to: 12 September 2000	**Date of report:** 29/7/02 *Received at XMaS:*
Shifts: 18	**Local contact(s):** Dr Simon Brown	

Names and affiliations of applicants (* indicates experimentalists):

M Durell*, C Lei*, J E Macdonald*,
Department of Physics and Astronomy, Cardiff University

P Jukes* and R A L Jones
Department of Physics and Astronomy, University of Sheffield

Report:

Semiconducting conjugated-chain polymers are attracting intense current interest for display and electronic applications. The interfacial properties are of particular importance for understanding and optimizing electronic properties at junctions: however little is known about structural properties at the interface which must influence the electronic behaviour. This project is aimed at understanding the structural properties of semiconducting interfaces with a view to understanding, optimising and controlling the electronic properties.

In February 1999, we performed a preliminary experiment to elucidate the thin film structure of poly(9,9-dioctylfluorene) (PFO or F8). This material has come to be considered one of the most promising semiconducting polymer materials, supplanting poly(phenyl vinylene), PPV. The data from our previous experiment enabled us to identify the structure of the liquid crystalline phases and to demonstrate that the presence of the two interfaces governs the orientation of the chains in the bulk of the film. During the current experiment, we aimed to complete *ex-situ* measurements on the previously annealed samples and to undertake a first investigation of *in-situ* grazing-incidence diffraction during annealing.

***Ex-situ* measurements on previously annealed samples**

In order to understand the origin of the previously observed peaks in F8, poly(9,9-dihexilfluorene) (F6), which has the identical structure but with shorter alkyl side-chains of 6 C atoms rather than eight C atoms in PFO, was investigated. Scans with **Q** in the plane of

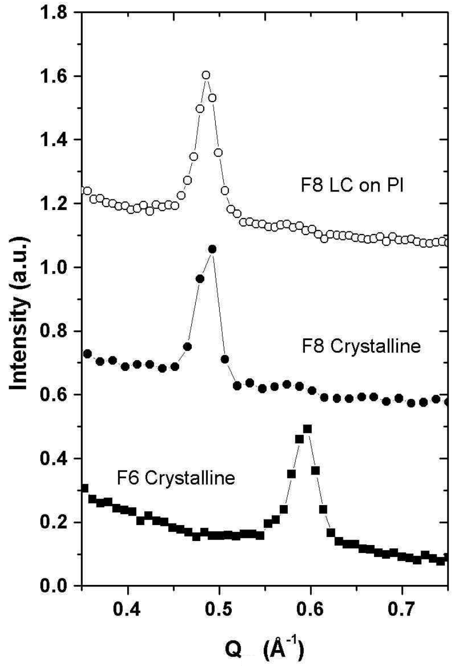

Fig. 1 GIXRD scans with Q in the plane of the surface normal for F8 and F6

the surface normal yielded a main peak at 0.596Å^{-1}, compared to 0.491 Å^{-1} in F8 (fig 1). The component of **Q** normal to the interface $Q_{\perp}$ = 0.490 Å^{-1} and 0.583 Å^{-1} for F8 and F6 correspond to d-spacings normal to the interface of 12.8 Å and 10.8 Å respectively. Scans in the plane of the interface showed Q value for both F6 and F8 at $Q_{//} = 2\pi/d$ = 1.50 Å^{-1}. These peaks can be identified with the benzene ring repeat distance along the polymer chain 4.15 Å. Thus, the molecules are inferred to lie in the plane of the interface with layering in the surface normal direction in both F8 and F6, the repeat distance being governed by the side-chain length. These findings have now been published [1].

In-situ **scans during annealing**

Preliminary reflectivity and GIXRD scans were performed during *in-situ* annealing at a range of temperatures 90-180°C. The reflectivity results show that the polymer surface roughens on entering the crystalline phase as a result of local density changes as the mesoscopic structure changes. On entering the liquid crystalline phase, a smoother surface is restored - but the fringes display a modulation having a period in Q of twice the fringe separation. This puzzling effect needs further investigation.

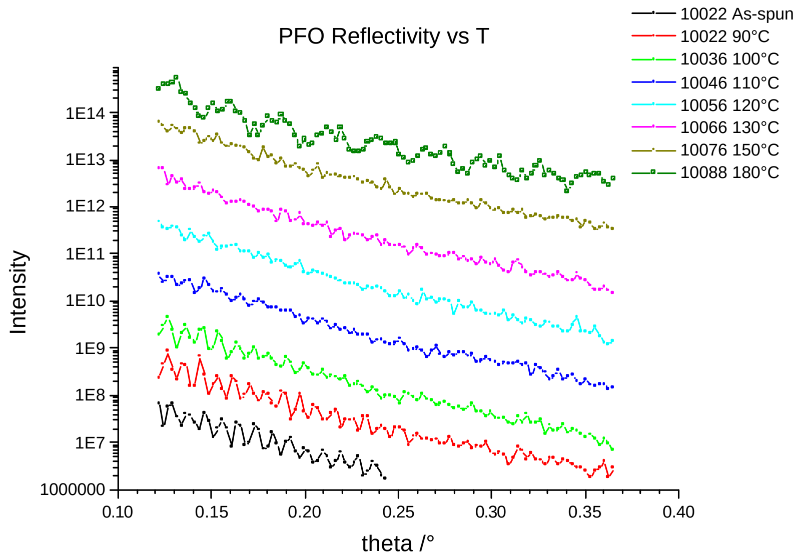

Fig 2 Reflectivity scans of a PFO polymer film at a range of temperatures during in-situ annealing

[1] S. Kawana, M. Durrell, J. Lu, J. E. Macdonald, M. Grell, D. D. C. Bradley, P. Jukes, R. A. L. Jones and S. L. Bennett, Polymer 43 (2002) 1907-1913