



ESRF	Experiment title: Structural and Dynamical Transitions in Molecular Ultra-Thin Films for Charge Transport	Experiment number: SI1001
	Beamline: ID03	Date of experiment: from: 28 April 2004 to: 06 May 2004
Shifts: 21	Local contact(s): Ioana POPA	<i>Received at ESRF:</i>
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Report:

Experiment SI-1001 dealt with the study of organic semi conductor (OSC) thin film growth. The aim of the experiment was to elucidate the structure of the very first monolayers of sexithiophene (T6) films grown by high vacuum (HV) sublimation, as well as to get insights on the growth mode (layer by layer or 3D) of these films. Two types of time resolved measurements were performed during deposition of T6 on SiO₂ and H terminated silicon substrates: GIXD was used to determine the in plane organization and specular reflectometry was used to follow the evolution of the density profile in the out of plane direction. Specular reflectometry (fig. 1 and 2) spectra were analyzed following the Parratt model. This analysis showed that the 5-10 first monolayers of T6 films are formed of molecules standing exactly normal to the substrate (periodicity 24 Å equal to the molecular length of T6); further growth leads to the observation of the well known bulk structure formed of molecules tilted by 23 degrees with respect to the substrate normal. The evolution of the density profile with time was analysed in terms of individual monolayer coverage (fig. 3) and it was observed that, in the range of temperatures studied, growth followed a 3D mode. GIXD data have shown (fig. 4) that on SiO₂ as well as SiH and for the whole range of temperature studied (RT to 90C), crystals are already formed for sub monolayer coverage. The observed diffraction peaks could be indexed as (0kl) on the basis of a unit cell which is contracted with respect to the bulk one ($b_{thin\,film}=7.70\text{ Å}$ $c_{thin\,film}=5.52\text{ Å}$, $b_{bulk}=7.851\text{ Å}$ $c_{bulk}=6.029\text{ Å}$). For thicknesses larger than 6 monolayers, the bulk structure starts being observed.

These observations show that the region of T6 thin films which is responsible for charge transport in field effect transistors is formed by a thin film phase different of the bulk structure. The intermolecular distances in this phase are smaller than in the bulk and the molecular orientation is normal to the substrate. These results are extremely important for an accurate description of the charge transport phenomena in these technologically relevant systems. The information gathered during this experiment will also provide a very valuable input for our next proposal that deals with template growth of organic semiconductors on substrates that were patterned at the meso/nano scale in order to promote oriented growth and control grain size.

Figure 1
Specular Reflectometry

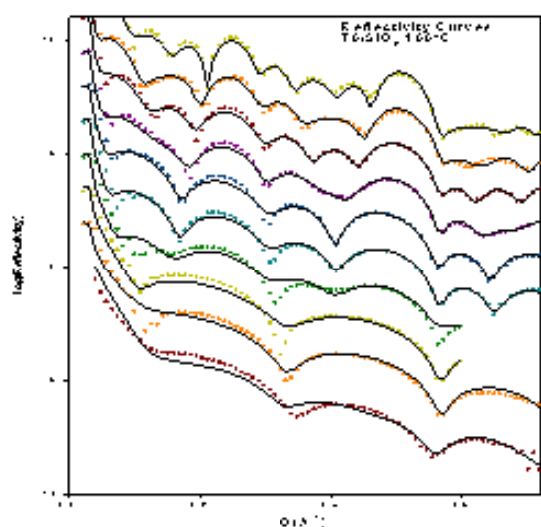


Figure 2
Out-of-Plane Density Profile

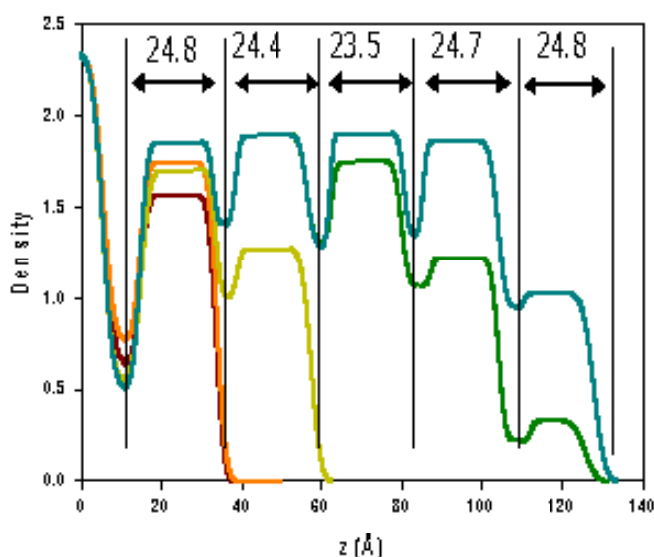


Figure 3
Evolution of Coverage

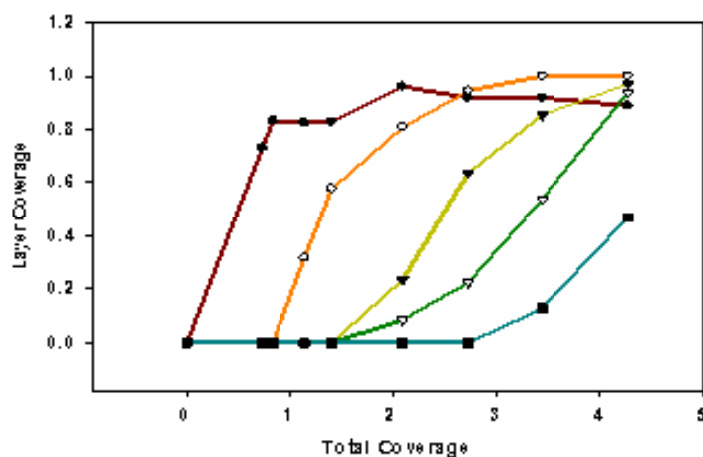


Figure 4
GIXD In-Plane Scans

