ESRF	Experiment title: Crystalline Order and Epitaxy of PTCDA molecules on Ag(111)	Experiment number: SC-562
Beamline: ID 10 B	Date of experiment: from: April 14, 1999 to: April 19, 1999	Date of report: August 23, 1999
Shifts: 18	Local contact(s): D. Smilgies	Received at ESRF: 31 AOUT 1999

Names and affiliations of applicants (* indicates experimentalists):

*Frank Schreiber, *Kenneth A. Ritley, *Bärbel Krause, *Arndt Dürr
Björn Edinger, Helmut Dosch
(all Max-Planck-Insitut für Metallforschung, D-70569 Stuttgart)
Detlef Smilgies (ESRF)

Report:

As proposed, the experiment was performed doing GIXD on crystalline organic thin films of PTCDA (3,4,9,10 perylene-tetracarboxylic dianhydride) on Ag(111) substrates.

Due to the expectedly complex structure, the analysis of the data is not trivial and still in progress. Here we provide an overview of the most important findings, but we emphasize that they are preliminary in nature.

1) The epitaxial relationship of the aromatic molecules on the Ag(111) substrate could be determined from GIXD at high resolution. The structure of the PTCDA film is monoclinic with several symmetry-equivalent domains. From the location of the in-plane diffraction peaks not only the epitaxial relationship but also the structural phase could be determined as a function of thickness (compares to the beta-Phase of bulk PTCDA, although the alpha-Phase is the equilibrium phase at room temperature).
2) The out-of-plane structure was determined from scans along the specular rod, evidencing a coherent structure thoughout the entire film. The bulk cleavage plane (102) was found to by exactly parallel to the substrate plane. The rocking width is essentially determined by the substrate (about 0.2 degrees). Laue oscillations were detected. From their attenuation, a static Debye-Waller-like term can be determined, which changes with preparation temperature.
3) From the analysis of the position and width (radial and transverse) of different in-plane peaks the evolution of disorder can be analyzed (rotational and positional).
4) From growth under different conditions (temperature and rate), the transition from high strain to low strain can be determined.
5) From real-time detection of the intensity oscillations at the anti-Bragg-point (to some extent, but not entirely similar to RHEED oscillations, see Figure), we could determine the growth mode for different conditions (we believe it is Stranski-Krastanov at high temperature).
6) From high-resolution measurements of the lattice parameter as a function of temperature, we could determine the thermal expansion and a possible high-temperature anomaly.