ESRF	Experiment title: Structural Phase Transitions in Self-Assembled Monolayers	number: SC-634
Beamline: ID 10 B	Date of experiment: from: Sept. 29, 1999 to: Oct. 5, 1999	Date of report: Feb. 28, 2000
Shifts:	Local contact(s): D. Smilgies	Received at ESRF:

Names and affiliations of applicants (* indicates experimentalists):

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

Report:

Phase transitions in reduced dimensions are a very fundamental problem in condensed matter research which has drawn significant theoretical and experimental attention. One of the currently open issues concerns the behavior of systems with internal degrees of freedom. Organic thin films are very suitable for the study of these effects. Moreover, their behavior can be tuned by changing specific functional groups of the molecule. Since the beamtime was not allocated in a period with maximum flux, which is usually needed for organic thin films with their low scattering cross section, we focussed on perylene-derivatives which give still comparatively high Bragg intensities in mono- and multilayers.

The analysis of the data is still in progress. Here we provide an overview of the most important findings, but we emphasize that they are preliminary in nature.

During preparation of the films, the structure evolution was studied in real time, which
gave important insight in the growth mode. At high temperatures, we found a post-growth
re-ordering process, for which we could determine the characteristic time scale. This, in
turn, will allow us to determine the diffusion barriers in this system and correlate these
with theoretical estimations.

- 2) The as-grown structure for different temperatures including the epitaxial relation with the substrate was investigated from GIXD at high resolution, which allows us to determine the phase diagram as a function of temperature and coverage.
- 3) We found evidence for an epitaxy-induced phase transition from the beta- to the alphaphase. The transition appears to be continuous with coverage. The driving force for this transition is apparently the built-up of strain. The threshold for structural changes due to strain seems to be very high, exceeding 5 %.
- 4) The out-of-plane structure was determined from rodscans. From growth under different conditions (temperature and rate), the transition from high strain to low strain was determined.
- 5) In temperature-dependent high-resolution measurements of the out-of-plane structure we found a high-temperature anomaly.
- 6) At temperatures above 150 deg C, we observed a dewetting transition, which we studied in detail as a function of time and temperature. The figure shows the growth of the sharp component of an out-of-plane Bragg reflection due to the built-up of highly coherent islands during the dewetting process. Dewetting transitions are presently an important issue, frequently studied in non-crystalline and polymeric systems. Here we believe to have identified a crystalline organic thin film system which exhibits typical features of dewetting transitions, but compared to polymeric systems, in which capillary waves on the surface can have a strong impact, in this epitaxial system the built-up of strain is suspected to be the driving force. This will be further analyzed.

