EUROPEAN SYNCHROTRON RADIATION FACILITY

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ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Structural investigation of the organic-organic interface in planar heterojunctions of C_{60} buckminster fullerene and diindenoidperylene for organic photovoltaics	**Experiment number**: SC-3597
Beamline: ID10	**Date of experiment**: from: 2013-06-26 to: 2013-07-02	**Date of report**: 2014-03-04
Shifts: 18	**Local contact(s)**: Giovanni Li Destri, Federico Zontone	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Christopher Lorch*, Heiko Frank*, Dr. Rupak Banerjee*, Dr. Alexander Gerlach*, Prof. Frank Schreiber

all Universtät Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, D-72076 Tübingen, Germany

Report:

Overview

During this experiment the material combination diindenoperylene (DIP) and C_{60} buckminster fullerene was investigated using real-time *in situ* X-ray diffraction methods. The samples were prepared in a portable ultra-high vacuum chamber equipped with a beryllium window mounted on the diffractometer of the ID10. Film thicknesses and growth rates were controlled with a quartz crystal microbalance, calibrated via X-ray reflectivity (XRR) measurements.
The preparation conditions were systematically varied during the growth in a wide range. The substrate temperature was kept constant at 240 K, 278 K, 308 K and 373 K, respectively. Furthermore, the chosen growth rate was between 0.2 nm/min and 1.5 nm/min. Additionally, films were prepared by interrupting the growth repeatedly for a short period of time after a certain amount of material was deposited in order to give the molecules time to diffuse.
During the allocated 18 shifts we were able to prepare all the proposed films and performed grazing incidence X-ray diffraction (GIXD) scans during the growth using the provided 2D Pilatus detector. For all the prepared samples, we did a detailed post-growth characterization including wide-range, high-resolution GIXD and XRR scans with corresponding diffuse and rocking scans. Furthermore, we mapped the reciprocal space using the Pilatus detector and checked for beam-damage on the films by repeating selected measurements at different spots of the sample.

Quality of measurement and data

All real-time scans could be performed uninterruptedly due to the availability of a reliable beam.
For the real-time measurements we aimed for a good balance between time resolution, spatial resolution and q-range of the scans. The resulting time-resolution was 40 seconds. Compared to the total growth time, which was between 14 and 100 minutes per film, we have obtained a detailed picture of the growth process.

Status and progress of evaluation

All the datasets were categorized and compared to each other. The post-growth scans were converted to q-space and background-corrected (Fig. 1). The X-ray reflectivity data was fitted via the Parratt formalism. The crystal structure of the material was identified using known crystallographic information files and the observed Bragg reflections. The datasets obtained under different growth conditions were compared to each other (Fig 1).
The data evaluation is in a mature state and we expect to publish the results in due course of time.

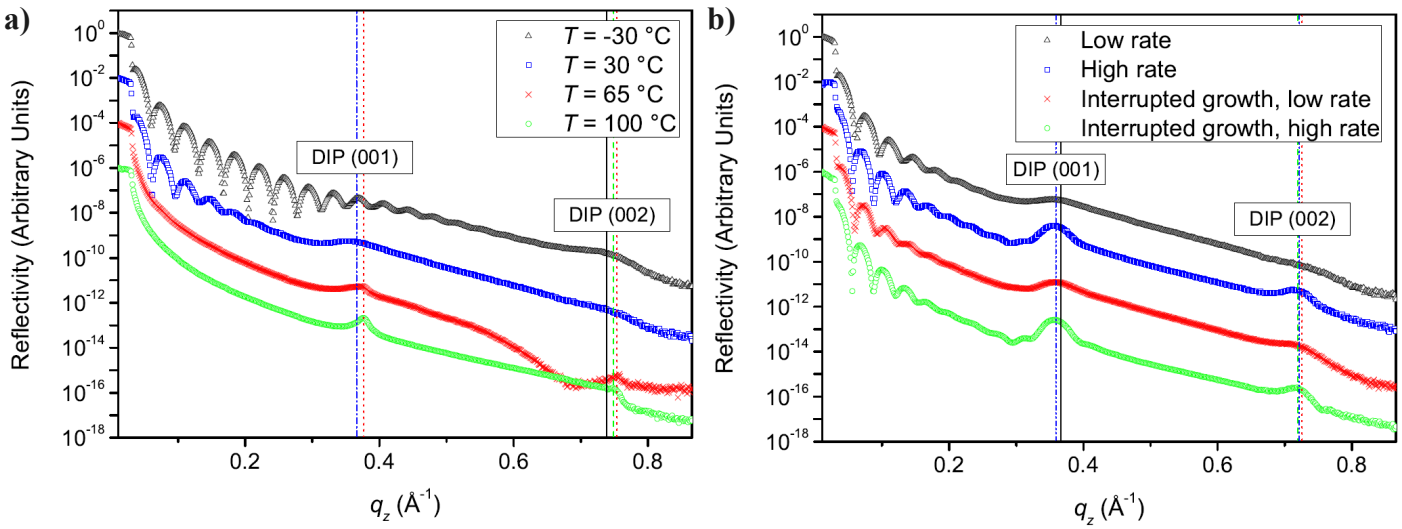

Fig. 1: XRR data of thin films consisting of DIP and C_{60} in equimolar composition compared for different substrate temperatures T (**a**) and for different growth conditions (**b**). The datasets were fitted to extract the roughnesses of the films.

Preliminary results

We have observed that different preparation conditions of the films can lead to relatively similar crystal structures and morphologies. For example, a decrease of the substrate temperature or a high deposition rate lead to a smoother film, compared to higher substrate temperatures or low deposition rates, respectively. These observations can be explained by a consistent interpretation in terms of the diffusion length scales of the molecules with strong dependence on preparation conditions. Detailed understanding of the diffusion process provides key insights into the growth processes of organic thin films.

We want to thank the ESRF for granting us beamtime and our local contacts for their help and their excellent support.