EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

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:** In situ real-time investigation of substrate templating effect on the phase separation in organic molecular thin films of pentacene and cyanoperylenediimide	**Experiment number**: SC 4535
Beamline: ID10	**Date of experiment**: from: 03 May 2017 to: 09 May 2017	**Date of report**: 29.08.2017
Shifts: 18	**Local contact(s)**: Andrei Chumakov	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Alexander Gerlach[1], Frank Schreiber[1], Valentina Belova[1]*, Alexander Hinderhofer[1]*, Jakub Rozbořil[2]*, Clemens Zeiser[1]*

[1]Institut für Angewandte Physik - Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

[2]Central European Institute of Technology - Masaryk University, Kamenice 5, CZ-62500 Brno, Czech Republic

Report:

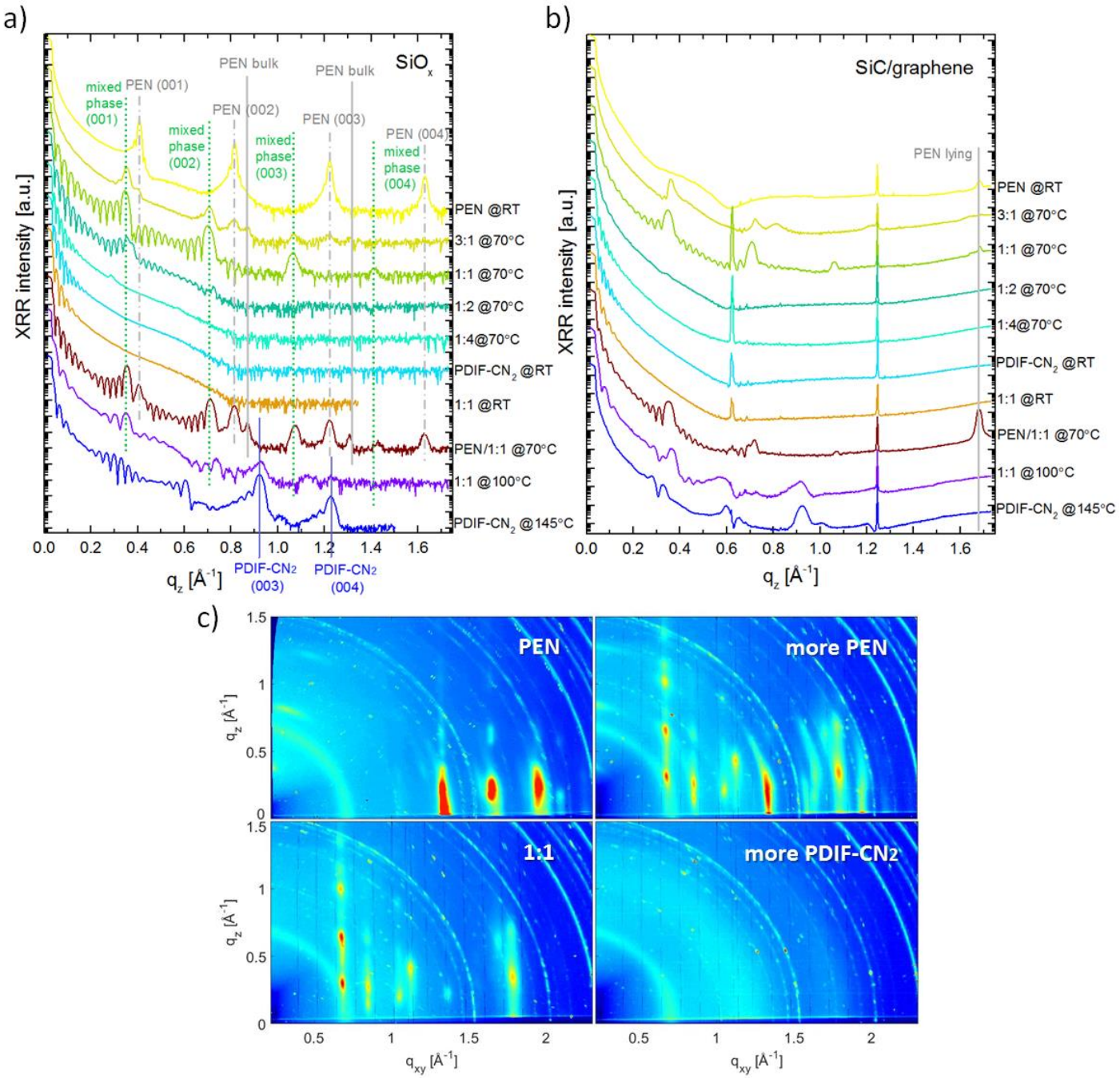
1. Abstract

We report an *in situ* and real-time investigation on growth kinetics and mixing behavior of binary co-deposited small-molecule organic semiconductor thin films by organic molecular beam deposition as a function of mixing ratio, growth temperature and substrate material using X-Ray Diffraction techniques. We use pentacene (PEN) as a donor component and N,N0-1H,1H-perfluorobutyl-cyanoperylenediimide (PDIF-CN_2) as an acceptor component revealing different growth behavior. We observed a strong tendency to a mixed crystal formation between the donor and the acceptor molecules governed by intermolecular interaction.

2. Experimental Results

We performed monitoring of thin films growth in an Ultra high Vacuum mobile chamber in real time using two detectors: a 2D PILATUS 300k and a point detector. The films were simultaneously grown on two different substrates: a non-interacting silicon wafer with a native oxide and a SiC wafer with an interacting graphene monolayer on top (Figures a and b). When grown on SiO_x both compounds (PEN and PDIF-CN_2) prefer a standing up-right molecule orientation as well as their mixed phase obtained by equimolar co-evaporation. In contrast, on graphene PEN is adsorbing in lying down manner, however, the acceptor molecules and the mixed phase maintain the unit cells observed on SiO_x, that confirms the stronger π-π intermolecular interaction in face-on stacks in comparison with the herringbone lattice of PEN. The substrate temperature affects the crystallinity of PDIF-CN_2 films so that PDIF-CN_2 and 1:1 films are almost amorphous at room temperature. When deposited at 70 °C the 1:1 film reveals a well-ordered mixed crystal (Figure c). By changing the mixing ratio the growth behavior varies from phase separation between the crystalline PEN and the mixed crystal in a film with PEN excess to unstructured

intermixing in a film with disordered PDIF-CN_2 excess. In films with dominating PEN its bulk phase was observed.



Figures. Postgrowth XRR scans of all prepared films on silicon (a) and graphene (b) substrates. (c) Reciprocal space maps of sample series with changing molar mixing ratio.

3. Remarks on quality of measurements

We found the ID10 beamline particularly suited for our real-time experiments with weakly scattering organic materials. We used two kinds of the detectors (PILATUS 300K and point detector) which allowed obtaining excellent results in the framework of our study, although a detector with a larger amount of pixels could reduce the measurement time.

4. Status and progress of data evaluation

We aim to include these data in a publication concerning intermolecular interactions in small-molecule donor-acceptor systems grown by vacuum molecular deposition, once the dataset is fully analyzed.

We thank Andrey Chumakov and Karim Lhoste for the valuable support during the beamtime.