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

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal ("relevant report")

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a *"preliminary report"),*
- even for experiments whose scientific area is different form the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as "relevant report(s)" in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

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.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number 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.

	Experiment title: GIWAXS study on hybrid organic electronics for NIR photodetection: Molecular alignment and In-operando studies of device degradation	Experiment number: A28-1-1307
Beamline: BM28	**Date of experiment**: from: 28 Jun 2022 to: 04 Jul 2022	**Date of report**:
Shifts: 15	**Local contact(s)**: Oier Bikondoa	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Oier Bikondoa*, XMaS UK CRG Beamline, ESRF, France and University of Warwick, UK

Matti Knaapila*, Norwegian University of Science and Technology, Norway

Jakob Kjelstrup-Hansen*, University of Southern Denmark, Denmark

Report:

Article published: Fynbo, C., Huss-Hansen, M. K., Bikondoa, O., Gangadharappa, C., Filho, D. A. D. S., Patil, S., Knaapila, M. & Kjelstrup-Hansen, J., " Structural Study of Diketopyrrolopyrrole Derivative Thin Films: Influence of Deposition Method, Substrate Surface, and Aging", Langmuir, 2023, 39, 12099-12109, DOI: 10.1021/acs.langmuir.3c01378

Abstract

We report the morphology and microstructure of n-dialkyl side-chain-substituted thiophene DPP end-capped with phenyl groups (Ph-TDPP-Ph) thin films and compare the influence of deposition method and substrate surface using thermally oxidized Si and graphene substrates as well as monolayer graphene surfaces with an underlying self-assembled octadecyltrichlorosilane monolayer, complemented by an aging study of spin-coated films over a 2 weeks aging period. A distinct difference in morphology was observed between spin-coated and vacuum-deposited thin films, which formed a fiber-like morphology and a continuous layer of terraced grains, respectively. After an initial film evolution, all combinations of deposition method and substrate type result in well-ordered thin films with almost identical crystalline phases with slight variations in crystallinity and mosaicity. These findings point toward strong intermolecular forces dominating during growth, and the templating effect observed for other oligomer films formed on graphene is consequently ineffective for this material type. Upon aging of spin-coated films, a noticeable evolution involving two different morphologies and crystalline phases were observed. After several days, the thin film evolved into a more stable crystal phase and a fiber-like morphology. Moreover, slight variation in optical spectra were elucidated on the basis on density functional theory calculations. These results demonstrate that thin-film properties of DPP derivatives can be tailored by manipulating the film formation process.