Experimental Report Proposal SC-5202

Proposal: Polymorphism in Organic Semiconductors: Understanding the effects of nanoconfinement on molecular packing

Scope of the experiment

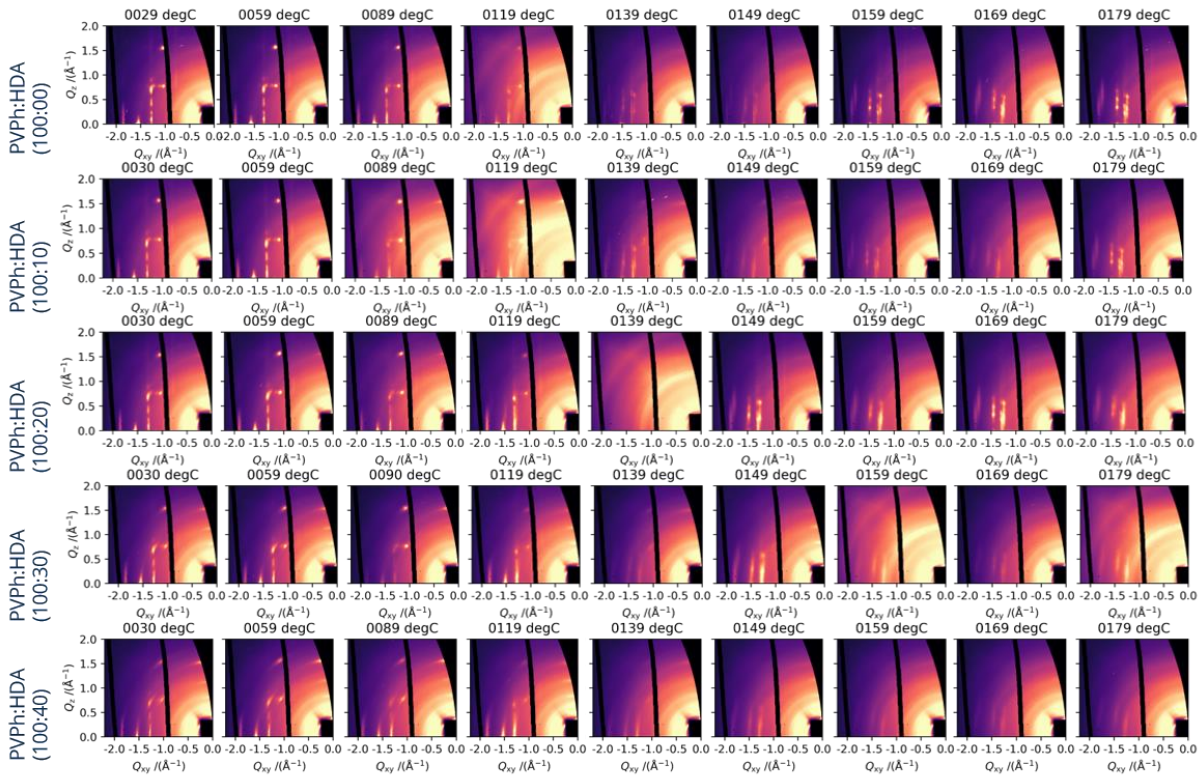
From the proposed study, we expected to gain further information about the effects of confinement on polymorphic transitions in organic semiconductors. To perform the study, we have chosen the benchmark small molecule semiconductor C10-DNTT, for which we have recently reported a polymorphic transition around 120 °C.

In this experiment, we performed in situ heating GIWAXS experiments on C10-DNTT films on top of PVPh layers cross-linked to different degrees with and without an additional capping layer of the same material to study the effects of film thickness and nanoconfinement on the polymorphic transition.

To our fullest satisfaction, we performed these experiments at the ID10 beamline at the ESRF experiments. The local beamline scientist's support was outstanding, and the overall setup of the beamline was good. In the future, upgrading the heating stage and the area detector should be considered.

Experimental results

C10-DNTT on top of different sublayers

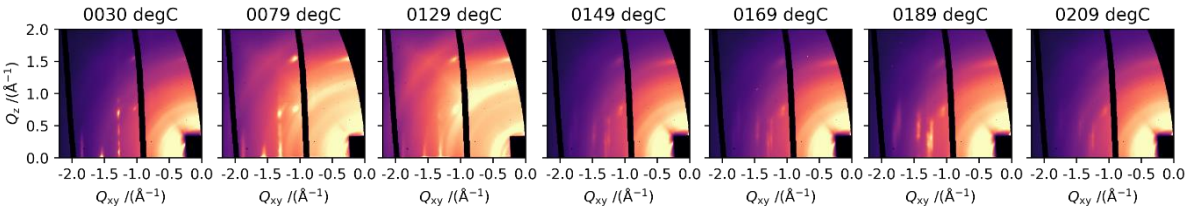


The Figure above shows the heating cycles of C10-DNTT on top of different sub-layers. The sublayers consist of PVPh cross-linked with HDA to different degrees. All films show the phase transition

around 120 °C. The transition temperature is shifted to higher temperatures for the strongly cross-linked layers with ratios of 100:40 and 100:30.

The experiment shows that the existence of the polymorphic transition is not dependent on the sub-layer but can be shifted depending on the layer's stiffness.

C10-DNTT sandwiched between sub- and capping layer



The Figure above shows a C10-DNTT between a PVPh sub-layer and capping layer. The sandwiched layers show the same phase transition, shifting to slightly higher temperatures. The in-depth investigation is still ongoing.

Additional measurements

Additional measurements include thin films of C4-DNTT and C6-DNTT, which share the same DNTT core as C10-DNTT with different alkyl side chains. The transition temperature for these films is significantly shifted towards to higher temperature. Films with different capping layers were measured for the two derivatives as well. Additionally, a DNTT derivative with an s-shaped core was investigated to assess the influence of the core on the polymorphic transition. A detailed investigation of these measurements is still ongoing.

Conclusion and outlook

The experiments at beamline ID10 of the ESRF synchrotron were a success. The obtained data is beneficial to further our understanding of phase transitions in DNTT derivatives. Combined with electrical characterizations of OFET devices employing these materials, more morphological investigations of the thin films, and simulations, the findings will lead to a better understanding of the structure-property relationships of this class of materials. Some detailed investigations of the obtained data is still ongoing. The measurements will be used in upcoming publications.