ESRF	**Experiment title:** Real-time investigations of structural changes during growth and their influence on the optical properties of equimolar mixtures of organic semiconductors	**Experiment number**: SC-3298
Beamline: ID 10B	**Date of experiment**: from: 21/09/2011 to: 27/09/2011	**Date of report**: 17/02/2012 *Received at ESRF:*
Shifts: 18	**Local contact(s)**: Dr. R. Nervo	

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Report:

1. Introduction

As described in the proposal, the purpose of the experiment at ID10B was to study structural properties of mixtures of organic semiconductors. While many organic semiconducting molecules are well studied in pure films, fundamental issues in mixed systems are still open. These issues include the mixing behavior of the two compounds, that is, whether phase separation occurs or whether the compounds intermix on a molecular level, including the possible formation of a new crystalline structure [1,2]. To address these questions is of high relevance for fundamental research as well as for applications, since mixed systems are part of future optoelectronic devices such as organic photovoltaic cells and organic light-emitting diodes.

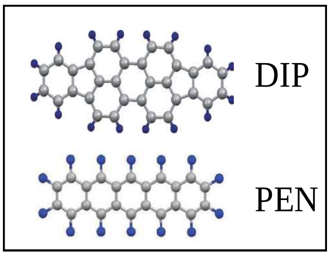

Fig. 1: Chemical structure of diindenoperylene (DIP) and pentacene (PEN).

The experiment was performed using a home-built portable UHV-chamber which allows in situ X-ray measurements during growth. Using this chamber mixed films of Pentacene (PEN, $C_{22}H_{14}$) and Diindenoperylene (DIP, $C_{32}H_{16}$), two organic semiconductors which are well-studied and are promising materials for applications, were grown on SiO_2 at substrate temperatures of 280 K, 300 K and 365 K. In the following we give a summary of the results obtained during the beamtime SC-3298 at ID10B.

2. Real-time and post growth measurements of PEN:DIP 1:1 on SiO_2

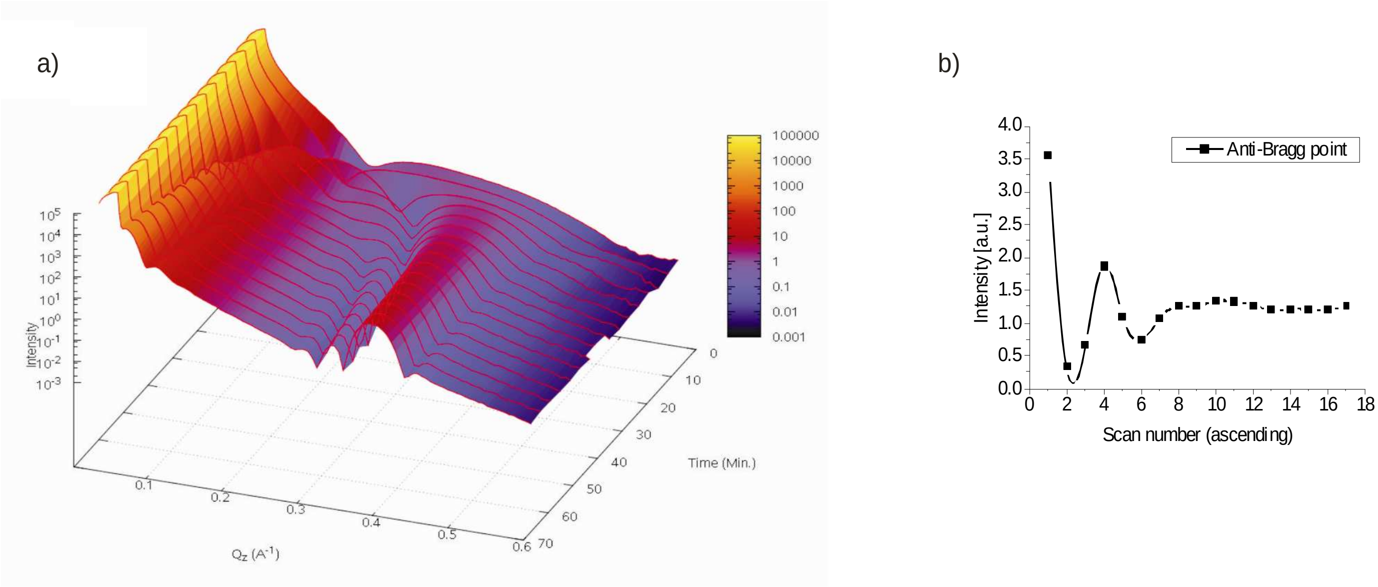

Fig. 2: a) Real-time XRR data of an equimolecular mixture of PEN:DIP grown at 303 K, b) Oscillations at the Anti-Bragg-point

The results of real-time XRR-measurements of an equimolecular mixture of PEN:DIP (mixing ratio 1:1) deposited on SiO_2 at 300 K are shown in Fig 2. We observe in the last XRR-scan in Fig. 2a) a Bragg peak at q_z =0.4 $Å^{-1}$ corresponding to a lattice spacing of 1.57 nm and therefore, almost upright standing molecules. The reflectivity data show pronounced Laue oscillations, indicating a well ordered structure perpendicular to the substrate surface (out-of-plane). From the oscillations at the Anti-Bragg-point (Fig. 2b) one can conclude that island growth starts after the first monolayer is filled. We repeated these measurements for 1:1-mixtures grown at other substrate temperatures (280 K and 360 K) and found also for these films a well-ordered out-of-plane structure and the beginning of island growth from the second monolayer on.

3. Comparison with other mixing ratios

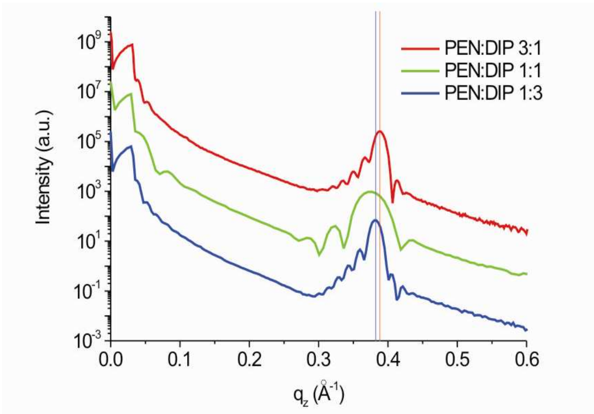

Fig. 3: Comparison of XRR-scans for different mixing ratios of PEN and DIP. Data have been offsetted for clarity.

To study the influence of different volume ratios of PEN and DIP on the film structure we repeated the measurements for two films with mixing ratios PEN:DIP 3:1 and 1:3 (Fig. 3). We observe a shift of the Bragg-peak to higher q_z-values in the film with a higher volume fraction of DIP indicating an decreased lattice spacing and a slightly increased film roughness with increasing DIP-ratio.

4. Summary

We studied mixtures of PEN and DIP grown at three different substrate temperatures and mixing ratios. For a mixing ratio of PEN:DIP 1:1 we found a well-ordered out-of-plane structure and beginning of island growth after the first monolayer. When we varied the mixing ratio we observed a decreased lattice spacing and increased film roughness for films containing more DIP.

A publication with these results is in preparation. – We would like to thank our local contact for the support on ID10B.

5. References

[1] Hinderhofer et al., J. Chem. Phys. **134**, 104702, (2011)
[2] J. Reinhardt et al., submitted