ESRF	**Experiment title:** **In-situ real-time GI-SAXS/WAXS investigation of diindenoperylene orientation and growth kinetics on monolayer MoS_2**	**Experiment number**: SC-4814
Beamline: ID10	**Date of experiment**: from: 02.03.2018 to: 06.03.2018	**Date of report**: 3.3.2020
Shifts: 12	**Local contact(s)**: Andrei Chumakov	*Received at ESRF:*

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Report:

1. Abstract

During this beamtime we performed in-situ real-time GI-SAXS/WAXS experiments of diindenoperylene (DIP) growing on monolayer MoS_2 and few-layer MoS_2 with different alignment of atomic layers [1]. We studied the intra-island molecular orientation of the DIP molecules during growth on MoS_2 with different alignment. In-situ real-time GIWAXS was employed to verify the *lying-down* or *standing-up* DIP phase in thin film [2].

2. Experimental Results

Our setup consisted of organic molecular beam deposition (OMBD) chamber [3] and 2D detector: Pilatus in 0.36m sample-detector distance to record GIWAXS data. We deposited in total eight samples with different substrates and substrate temperatures. In real-time GIWAXS measurements we tracked the 001 integral intensity and diffraction peak width along q_z and q_{xy} directions in reciprocal space maps (RSMs). The total deposition time was 90 minutes with the integration time of 60 s for single frame. The fitted change of unit cell's c axis as a function of effective thickness (nm) for *lying-down* and *standing-up* DIP are given in Fig. 2. We found out that the orientation of the MoS_2 layers subsequently influences the orientation of DIP molecules. Fig. 1 shows the 001 diffraction peak positions of DIP layers ($q \approx 0.39$ Å^{-1}) grown on 3 and 9 nm thick MoS_2 films (left and right RSM). On the horizontally aligned MoS_2, we also detected the 110 diffraction peak ($q \approx 1.15$ Å^{-1}), see Fig. 1 (left). More diffraction spots were observed for DIP thin films on a MoS_2 monolayer, which were used to calculate the full set of unit cell parameters and the molecular orientation within the unit cell.

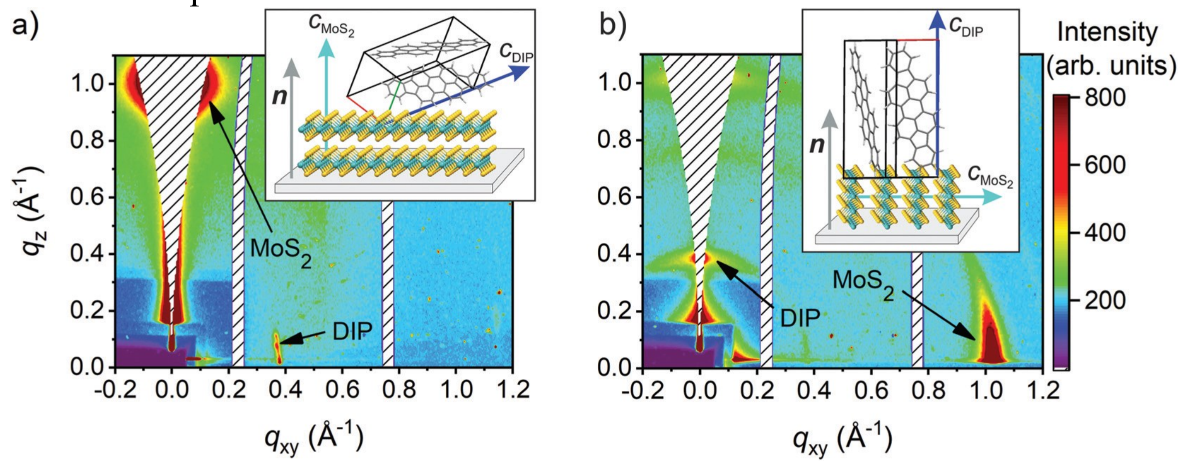

Fig. 1 reciprocal space maps of MoS_2 with different alignment and deposited DIP layers. Inset shows schematic of mutual orientations of the c-axes of DIP and MoS_2

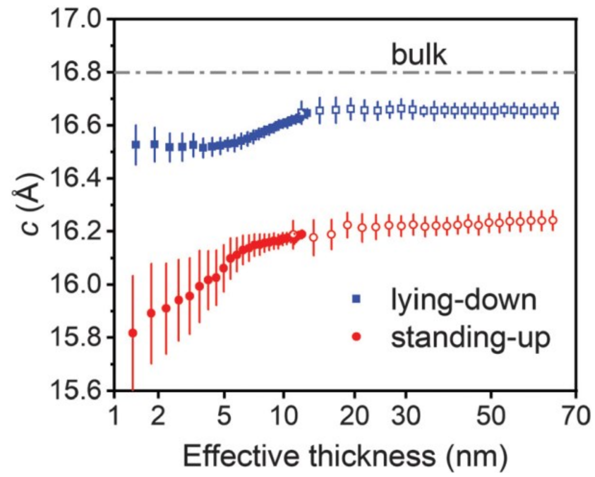

Fig. 2 Temporal evolution of unit cell's *c* axis as a function of effective thickness (nm) for *lying-down* and *standing-up* DIP

3. Remarks on quality of measurements

We found the ID10 beamline particularly suited for our in-situ real-time GI-SAXS/WAXS experiments with weakly scattering organic materials. Although we had to take some precautions in order to avoid beam damage on our samples, we consider the obtained signal very good.

4. Status and progress of data evaluation

We fully analyzed the data and published two articles out of this experiment.

- N. Mrkyvkova *et al.*, Appl. Phys. Lett. 114 (**2019**), 251906
- J. Hagara *et al.*, Phys. Chem. Chem. Phys. 22 (**2020**), 3097-3104

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5. References

1. M. Sojkova *et al.*, RSC Adv. 9 (**2019**), 29645-29651
2. M. Hodas *et al.*, ACS Appl. Nano Mater. 1 (**2018**), 2819−2826
3. K. A. Ritley *et al.*, Rev. Sci. Instr. 72 (**2000**), 1453