Experimental report

09/02/2016

Proposal:	**7-05-452**	**Council:**	4/2015

Title: Self-Diffusion of pentacene on graphite in the sub-monolayer regime studied with quasi-elastic neutron scattering (QENS).

Research area: Other...

This proposal is a new proposal

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Samples: $C_{22}H_{14}/C$

Instrument	Requested days	Allocated days	From	To
IN6	7	7	09/11/2015	16/11/2015

Abstract:

Organic thin films such as pentacene ($C_{22}H_{14}$) films are promising systems for the development of novel electronic devices. However, the electrical properties of the resulting devices are limited by the quality of the films, which strongly depends on the growth process. Thus, understanding the mechanisms which govern diffusion is essential to set the most favorable conditions for growing well-ordered epitaxial organic thin films on technologically relevant substrates. Quasi-elastic neutron scattering is an excellent tool to investigate both the self- and the collective diffusion of polyclyclic aromatic hydrocarbons (PAH) such as pentacene. We aim to survey the self-diffusion of pentacene molecules adsorbed on exfoliated graphite to complement the measurements of the collective diffusion to be carried out on deuterated pentacene ($C_{22}D_{14}$) with neutron spin-echo (the spin-echo beam time has already been allocated on IN11). The goal is to identify the physical mechanisms, which drive the first layer formation, at the atomic scale, in a weakly physisorbed phase.

Diffusion of pentacene molecules on exfoliated graphite in the sub-monolayer regime studied with neutron time-of-flight.

Organic thin films such as pentacene ($C_{22}H_{14}$) films are promising systems for the development of novel electronic devices. However, the electrical properties of the resulting devices are limited by the quality of the films, which strongly depends on the growth process. Diffusion favours layer-by-layer growth since dissipative motion with frictional forces is an effective mechanism leading to the nucleation of stable islands. However the number of studies on pentacene diffusion on different technologically relevant substrates is very small if compared to structural studies. *In order to fill this gap we have carried out comprehensive measurements of the dynamics of pentacene on exfoliated graphite substrates in the sub-monolayer regime. We have measured the self-diffusion of pentacene on exfoliated graphite substrates, as a function of temperature in the sub-monolayer regime (from 0.1 ML up to 0.5 ML).*

Measurements and experimental set-up:

We have prepared three samples of pentacene ($C_{22}H_{14}$) adsorbed on graphite: 0.1 ML, 0.2 ML and 0.5 ML. The preparation of the samples consists into two steps. First of all we have cleaned the exfoliated graphite substrate, by heating under vacuum conditions in a pyrolytic oven for 24 hours at 350 C. Secondly, we have dosed a known amount of pentacene (powder) which corresponds to a certain surface coverage of the exfoliated graphite substrate in the sample. Finally, we have heated the sample up to 550 K in order to evaporate the powder and promote its adsorption uniformly on the whole volume of the sample.

The measurements have been performed with the cryofurnace set-up which allows us to cover a wide thermal range from 10 K up to 550 K. We measured at 5 K (resolution function), 100 K, 250 K, 350 K. In order to extract the scattering function corresponding to the diffusion of the adsorbates, we perform a first measurement of the clean graphite substrate. Then, we perform a second measurement with a given surface coverage of pentacene adsorbed on the substrate. Finally, in the post-processing of the data, we subtract the signal measured for clean graphite to the signal measured for pentacene/graphite.

The measurement have been carried out in the IN6 time of flight spectrometer, with an incoming wavelength of 5.12 $Å^{-1}$.

Experimental Results

We observe a consistency between the structural studies of pentacene islands performed in D20, the coherent dynamics observed with IN11 and the self-diffusion measured in IN6. Very little dynamics was observed in deuterated pentacene (IN11), while strong diffraction peaks were measured in D20. This means that the coherent part of the scattering function is sensitive to the strong spatial correlation which exists between molecules.In the case of h-pentacene studied in IN6, we are sensitive to the incoherent part of the scattering function. Therefore we monitor the self-diffusion of the molecules and its internal degrees of freedom. Since no quasi-elastic broadening is visible (Fig. 1), we conclude that pentacene is trapped in the molecular islands and has little room to move within the cluster. Molecular rotations seem to be also frozen and no self-diffusion is observed. A possible explanation is that pentacene molecules interact very strongly with each other, forming cluster even at very low coverages (0.1 ML), which are trapped around defects of the substrate. Therefore, pentacene molecules are anchored to the substrate and form very stable islands on the surface in the whole thermal range up to the desorption temperature (between 400 K - 425 K).

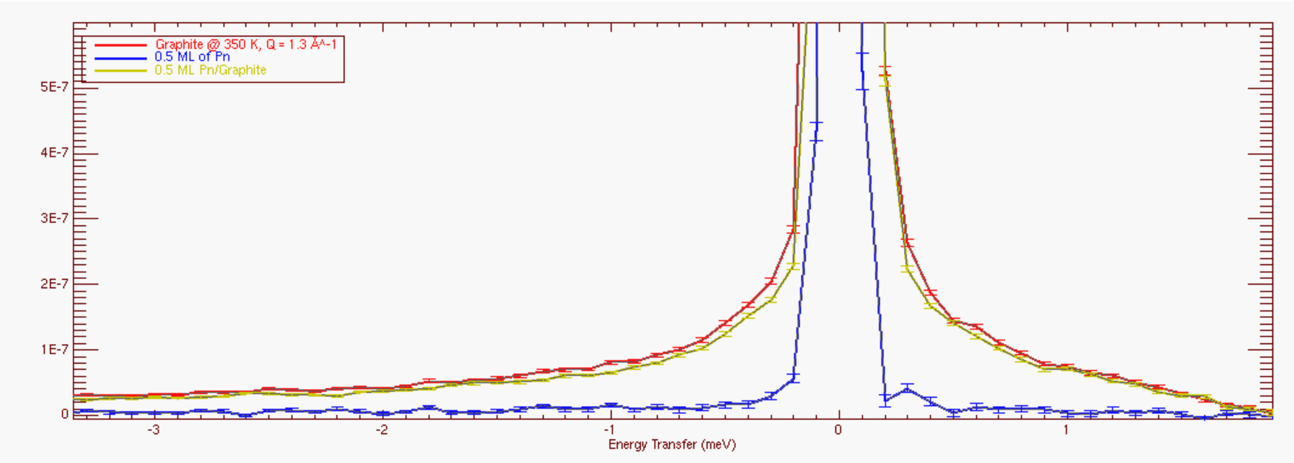

Figure 1: Comparison between the scattering function of graphite (red), 0.5 ML of pentacene (blue) and 0.5 ML of pentacene/graphite (yellow) at 350 K for a momentum transfer value of Q = 1.3 Å^{-1}.