Experimental report

08/09/2015

Proposal: 7-04-134 **Council:** 4/2014

Title: Molecular dynamics of a discotic liquid crystal confined to unidirectional pores with low nanometer dimensions

Research area: Soft condensed matter

This proposal is a resubmission of 7-04-92

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Local contacts: Bernhard FRICK

Samples: C54_H84_O6
Anodic Aluminium Membrane, Al2O3

Instrument	Requested days	Allocated days	From	To
IN16B	3	2	14/10/2014	16/10/2014

Abstract:

Discotic liquid crystals (DLC) are soft-matter materials which organize into columns that further assemble into two-dimensional arrays with a hexagonal mesophase. Highly ordered columnar structures were found to be very promising as active semiconductors in organic field-effect transistors and photovoltaic devices. The charge transport in these systems is controlled by their molecular mobility. Confining DLCs to the unidirectional channels of nanoporous anodic aluminium (AAO) can be regarded as model system for nanoscaled wires. To get an overview about the molecular mobility of a triphenylene based DLC confined to the 25 nm wide pores of AAO at a time scale of ca. 2 ns it is proposed to carry out elastic scans on a backscattering instrument.

EXPERIMENTAL REPORT

EXPERIMENT N°7-04-134 INSTRUMENT IN16B

DATES OF EXPERIMENT 14/10/2014-16/10/2014

TITLE

Molecular dynamics of a discotic liquid crystal confined to unidirectional pores with low nanometer dimensions

EXPERIMENTAL TEAM

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Date of report 07/09/2015

Discotic liquid crystals (DLC) are self-assembled materials where self-assembly is driven by noncovalent intermolecular interactions [1]. DLCs consist of a flat and rigid aromatic core substituted by flexible aliphatic side chains. The former is responsible for the π-stacking and the latter for the increased solubility, processability, and rich thermotropic behavior. The disc-shaped molecules organize into columns that further assemble into two-dimensional arrays with a hexagonal mesophase. The alkyl chains fill the intercolumnar space giving rise to a nanophase separated state.

To have an overview about the influence of a nanoscale confinement on the molecular dynamics incoherent quasielastic neutron scattering experiments are carried out at IN16B for Hexakis [n-hexaoxy]triphenylene (HAT6) embedded to the pores of commercial available anodic aluminum membranes (AAO, Smart Membranes) with a pore diameter of 25nm. For preparation, the empty aluminium membrans were treated in vacuum to remove impurities and after that transfered in vacuum into a glove box filled with Argon. The pores were filled by melting the DLC on the top of the membrane at a temperature above the clearing temperature by capillary wetting. The filling degree was estimated by TGA measurements. The experiments were done on IN16B (λ=6.271Å)in the elastic scan mode. The phase-space transformer was used but at a reduced speed of 2366 rpm. All spectra were corrected for the scattering of the empty host membrane sealed under Argon and the empty can. Because of the high incoherent scattering cross section of protons the scattering is dominated by the dynamics of the material in the intercolumnar space of the DCL where most of the hydrogen atoms are located.

Figure 1 depicts the normalized elastic scattered intensity of bulk HAT6 with that for HAT6 confined to nanoporous channels with a pore diameter of 25 nm. Compared to bulk HAT6, for the confined material the phase transitions are semeared out.

In order to probe the effect of the pore orientation with respect to the q vector, HAT6 confined to pores with a diameter of 25 nm was measured in two orientations of the pore axis parallel and perpendicular to the q vector. Figure 2 shows that there seems to be no influence of the orientation of the pore axis with respect to the q vector of the incident beam. From this one can conlude that there is no anisotropy of the dynamics on the length and time scale of the backscattering experiment.

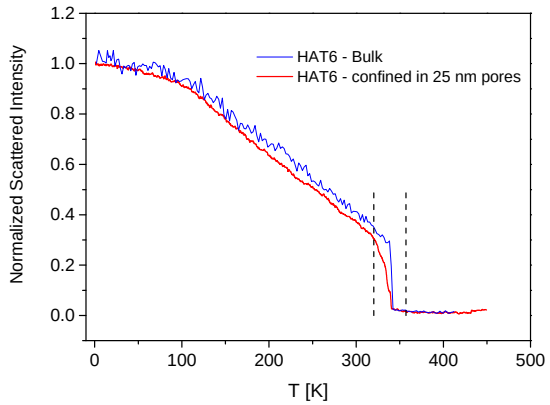

Fig. 1: Normalized elastic scattered intensity for bulk HAT6 and confined to cannels with a pore diameter of 25 nm. The averaged angle was 91.6°. The data for bulk HAT6 were measured with IN10. The dashed lines indicate the phase transition temperatures measured by DSC.

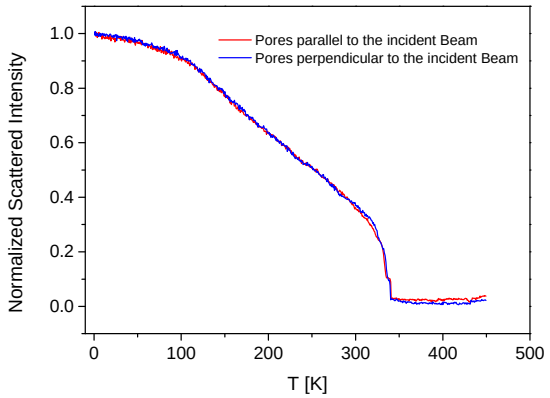

Fig. 2: Normalized elastic scattered intensity of HAT6 confined to self-ordered AAO membranes with a pore sizes of 25 nm with parallel) and perpendicular orientation of the pore axis with respect to the q vector of the incident beam as indicated**.**

[1] J. Wu, W. Pisula, and K. Müllen, Chem. Rev. **107**, 718 (2007)