Experimental report

26/04/2020

Proposal: **CRG-2548**

Council: 4/2018

Title: Transport of water in softconfinement

Research area:

This proposal is a new proposal

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Samples: PIM-1

Instrument	Requested days	Allocated days	From	To
IN6-SHARP	3	3	21/09/2018	24/09/2018

Abstract:

Experimental report on the experiment CRG-2548
21-24/09/2018

Context

The present experiment is part of a project that aims at developing a unifying framework for water transport in soft porous materials accounting for coupling between adsorption, deformation, and transport. Our strategy combines well-established experimental, molecular simulation, and theoretical tools to reach this ambitious objective at all relevant length and time scales. We intent at gaining insights into the fundamental microscopic mechanisms while understanding how each scale (from the nm scale to the macroscopic scale) affects water transport in soft porous environments, neutron scattering enabling the investigation of the microscopic scale.

The experiment

In this experiment, we used a well-defined prototypical polymeric materials used for membranes: Polymers with Intrinsic Microporosity (PIM).

This first experiment enabled to characterize the dynamics of water under static hydrolic pressure. A high-pressure cell (Liquid Pressure Cell 19PL10AL6) with aluminium insert enabled to have a rectangular sample of 50*5*0.3 mm^3. A separator was used on top of the stick, so that fluorinert was used as pressurinzing liquid while the sample was soaked into water.

Measurements

We could measured QENS spectra on the dry sample, and on the sample at a pressure of 1, 88 and 400 bars. Bulk water, vanadium and empty cell were measured in the same conditions.

Difficulties were encoutered to measure the empty cell without water because of a leak of the circuit into the cell.

Results. The QENS signal was measured on the dry sample to check for the quasi-elastic signal of the matrix, which is negligible as expected. Although the first analysis in terms of jump diffusion (parameters shown in Fig. 1 below) has to be taken with care, the measurement of the translational diffusion coefficient of water exhibits an increase when confined in the hydrophobic matrix. Although the reliability of this result may be questioned, the disturbance of water dynamics in a different way than in hydrophilic matrices[8] is certain. Further increase of the pressure up to 400 bars, however, does not have any strong effect on the signal, which could be explained by the fact that when pores are already filled with water, the matrix does not deform more and diffusion is not further affected by hydrostatic pressure. The temperature dependence may give another insight into the interaction between water and matrix, and will be the goal of our next experiment.

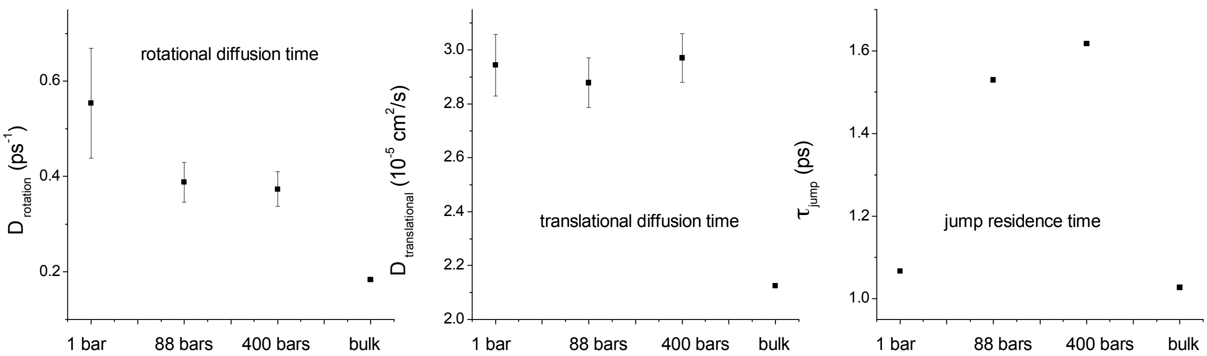

Fig. 1: Parameters extracted from the QENS signal analysis in terms of jump diffusion model at 300 K.