Experimental report

16/09/2018

Proposal: 6-07-27 **Council:** 4/2017

Title: Bonded and confined water along monodisperse hydrophilic and hydrophobic INT channels.

Research area: Materials

This proposal is a continuation of 7-04-155

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Samples: (OH)3Al2O3SixGe1-x(CH3)
(OH)3Al2O3SixGe1-x(OH)

Instrument	Requested days	Allocated days	From	To
IN16B	4	3	07/09/2018	10/09/2018
IN1 LAG	2	0		

Abstract:

Imogolite nanotubes (INT) with the general formula (OH)3Al2O3SixGe1-x(OH) are formed by a curved gibbsite Al(OH)3 layer whose vacancies are bonded at the upright by isolated [(OH)Si(Ge)O3] tetrahedral units on the internal surface, forming aluminosilicate Si(Ge)-INT nanotubes. Functionality of the inner surface of the INT by soft chemistry provides them of hydrophobic (OH)3Al2O3SixGe1-x(OH) or hydrophylic (OH)3Al2O3SixGe1-x(CH3) properties and monodispersity makes INT good candidates for storage of water or other molecules or as filters

Experiment #6-07-27
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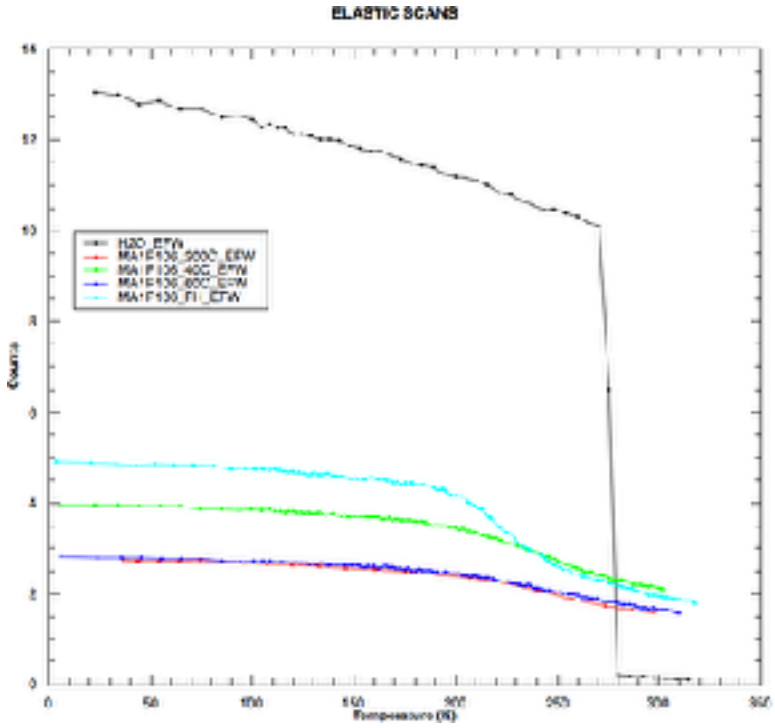
The experiment took place on IN16B on 07-10/09/18, *i.e.* a week before the autumn proposal round 2018 deadline. This explains why the data are still under process.

A single sample, referred as MA1P106 was measured at four hydration states: Fully hydrated, after desorption at 40°C, after desorption at 60°C and in the dry state (after desorption at 200°C). This sample is composed of Single Walled Imogolites Nanotubes (SWINT) of formula $(OH)_3Al_2O_3Ge(OH)$

It was shown from neutron spectroscopy investigations (IN4C and LAGRANGE) that water confined into these channels can be separated in two categories: *confined water* molecules populate the inner channel of the tube and are in interaction via H-bonds with a water layer in stronger interaction with the OH groups at the inner surface of the nanotubes.



The goal of the IN16B investigation is to understand the diffusion of water molecules in direct interaction with the Nanotube, i.e. the bonded layer. The layer water lattice can be rationalised a as triangular lattice, each water molecule being in interaction with three germinal groups. The idea is to detect any quasi elastic (QENS) broadening associated with these molecules and analyse this signal based on different models (jump diffusion, continuous 2D etc…) and Molecular Dynamics simulations.
Fixed window scans were performed (elastic and at 2 microeV) at all hydrations states. A QENS study was performed on the 60°C treated sample as a function of temperatures: (100 K,150 K, 225K, 250 K and 340 K).