EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON



	Experiment title: Fondamental study of ionics in single-digit nanoconfinement	Experiment number:
ESRF		A32-2-853 A32-2-846
Beamline:	Date of experiment:	Date of report:
ID02	from:05/10/2022 to: 12/10/2022	
Shifts: 20	Local contact(s): Samuel Tardif	Received at ESRF:

Names and affiliations of applicants (* indicates experimentalists):

Dr. Diane Rebiscoul*

Dr Hassan Khoder

The results presented in this experimental report correspond to the experiments performed in april 2022 (A32-2-846) and october 2022 (A32-2-853).

The goal of these experiments were to study the filling kinetics by hard X-ray reflectometry in confinement of 2, 3 and 4 nm nanochannels with electrolytes having ions presenting various size and solubility in order to highlight ion specific effect. Today, only KCl, NaCl, RbCl, CsCl at 1M presented in Table 1 were studied.

Table 1: Comparison of salt solubility in water at 20°C, and ions hydrated radii from Nightinga et al **Erreur! Source** du renvoi introuvable..

Salts	Solubility in water [M]	Cations	Hydrated radii [nm]
KCl	4.6	\mathbf{K}^{+}	3.3
NaCl	6.1	Na ⁺	3.6
RbCl	7.5	Rb ⁺	3.3
CsCl	11	Cs ⁺	3.3

Two types of kinetics study were done. The first one consists in the study of the filling of the nanochannels of 2 and 4 nm with the electrolyte solution. An example of X-ray reflectivity curve evolutions during the filling of the nanochannels with RbCl 1M is presented on Figure 1.

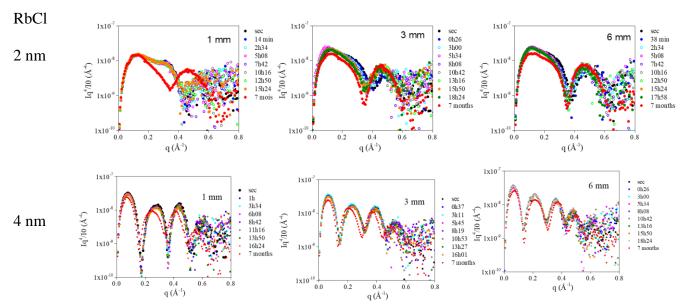


Figure 1: Example of the evolution of X-ray reflectivity during the filling of 2 and 4 nm nanochannels with RbCl 1M solution.

The second experiment consists in the study of the transport of ions in already water filled nanochannels of 3 nm. The results are presented Figure 2. An example of electron density profile in the nanochannel is also presented.

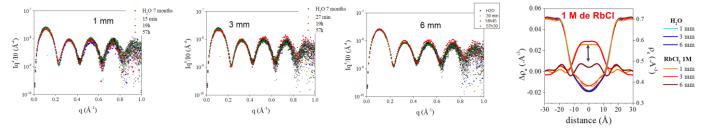


Figure 2: Example of the evolution of X-ray reflectivity when nanochannels of 3 nm already filled with water are in contact with a RbCl 1M solution. The electron density profile evolution in the nanochannels is also presented.

The results obtained are now under treatment to calculated the electron density profile as a function of the time as in 10.1016/j.jcis.2022.01.128 and the same systems at the equilibrium are simulating using molecular dynamics and PMF calulation.

Next proposal we will focus on the behavior of lanthanide elements in confinement as a function of their conter-ions.