EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:
https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal ("relevant report")

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a *"preliminary report"),*
- even for experiments whose scientific area is different form the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as "relevant report(s)" in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** High-pressure dependence of the low-frequency mode in liquid water	**Experiment number**: HC3686
Beamline: ID28	**Date of experiment**: from: 08/02/2018 to: 15/02/2018	**Date of report**: 01/11/2020
Shifts: 18	**Local contact(s)**: L. Paolasini	*Received at ESRF:*

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Report:

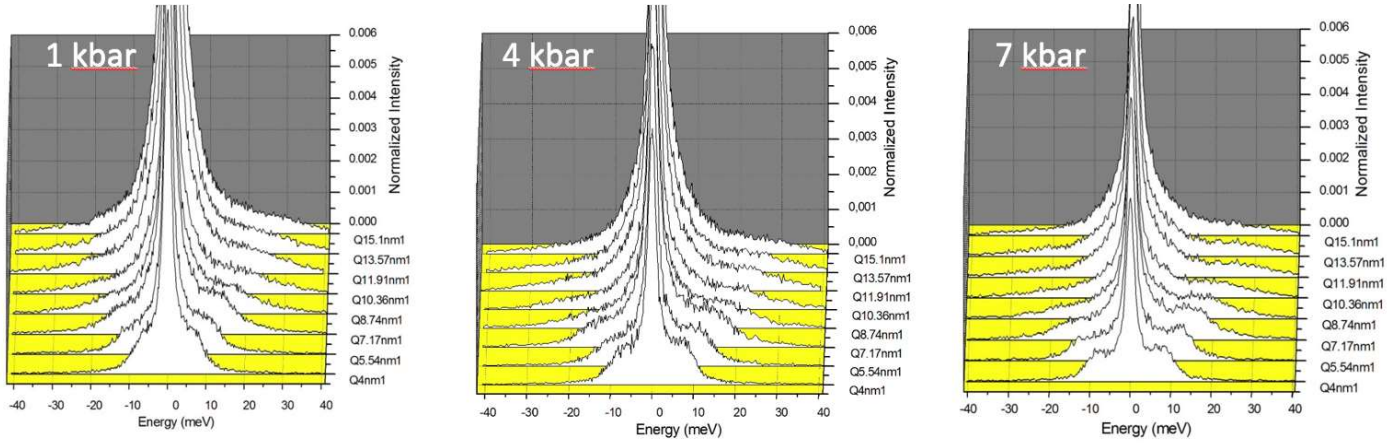
The existence of a low-frequency and weakly-dispersing mode in the THz spectrum of liquid water is known since the seventy's but its origin is still controversial [1-4]. The goal of our experiment was to determine how the low-frequency mode of water would be affected by the application of high pressure. To do that, we developed a novel CuBe large-volume piston-cylinder clamp with panoramic diamond windows. This allowed us to measure inelastic x-ray scattering spectra of liquid water as a function of pressure up to the crystallization point at room temperature.

Experimental method

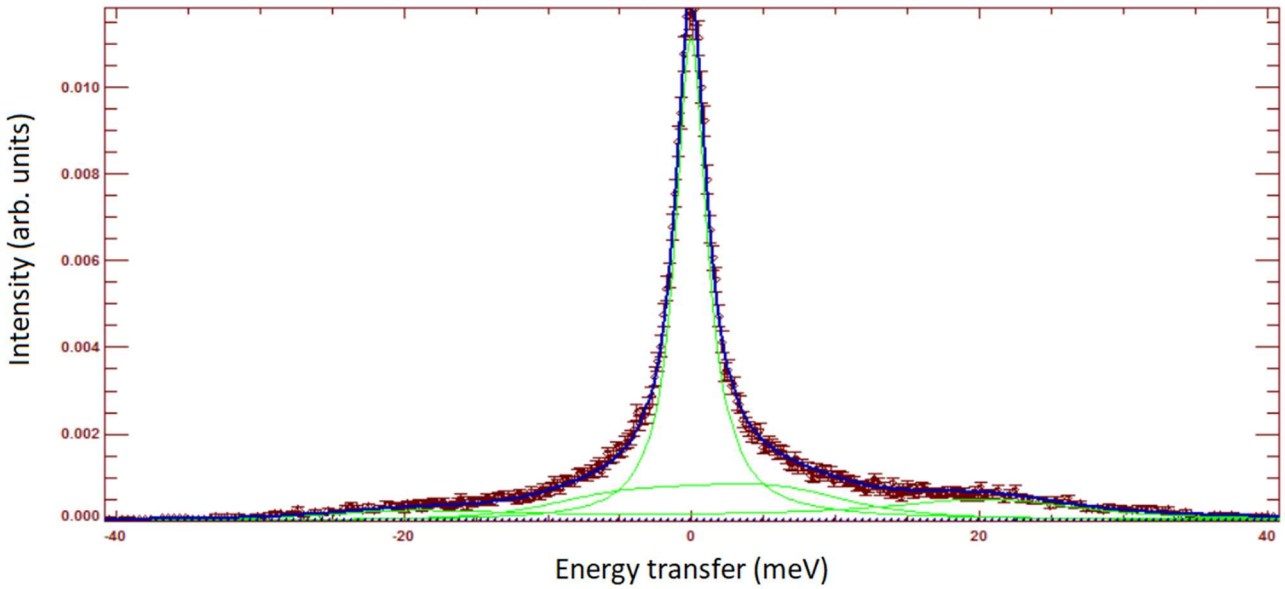
Deuterated water was chosen as the sample because of the lower crystallization pressure. The sample was loaded into the CuBe large-volume clamp and the clamp was inserted into a vacuum chamber specially designed for IXS measurements. We employed the silicon (11 11 11) configuration, resulting in an instrumental energy resolution of about 1.5 meV. Data were collected at the constant temperature of 300 K and eight pressures ranging from 1 to 10 kbar. For each pressure point, eight energy scans were simultaneously recorded at eight momentum transfer values in the 4−15 nm^{-1} range. At the highest investigated pressure (10 kbar), the sample was found to have crystallized into ice (phase VI).

Obtained results

The following figure reports examples of experimental spectra of water at three selected pressures.



Spectra have been fitted using a Lorentzian function (for the elastic peak) and two DHO functions (for the acoustic longitudinal mode and the low-frequency mode). An example of fit is shown below (4 kbar, 10.4 nm^{-1}):



The relative intensity of the low-frequency mode was found to increase as a function of pressure as water approaches its solid phase. This finding seems consistent with a transverse character of the mode. However, the observed increase is very weak and does not follow the behaviour of the shear viscosity along the same isotherm. Re-analysis of the data using the viscoelastic model based on the memory function formalism is ongoing.

References

[1] A. Rahman and F. H. Stillinger, Phys. Rev. A 10, 368–378 (1974).
[2] M. Sampoli et al., Phys. Rev. Lett. 79, 1678 (1997).
[3] A. Cunsolo et al., Phys. Rev. B 85, 174305 (2012).
[4] K. Amann-Winkel et al., Chem. Rev., 116 (13), pp 7570–7589 (2016).