ESRF	**Experiment title:** Pressure induced changes in hot dense water dynamics	**Experiment number**: HC1693
Beamline: ID28	**Date of experiment**: from: 19/11/2014 to: 25/11/2014	**Date of report**: 08/01/2016
Shifts: 18	**Local contacts**: L. Paolasini, T. Forrest	*Received at ESRF:*

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Report:

We have measured the dynamic structure factor of liquid water in the 0.3-2.5 GPa range along the 450 K isotherm on the three-axes x-ray spectrometer ID28. We employed the silicon (999) configuration, associated with an instrumental energy resolution of about 3 meV. Pressure was generated by a diamond anvil cell (DAC) of membrane type, equipped with ultralow-fluorescence high-quality IIA synthetic diamonds. We used rhenium as gasket material and, to prevent corrosion of the gasket and contamination of the sample, we isolated the latter from the gasket by using a gold ring. To minimize the parasitic elastic contribution at low momentum transfer Q, the DAC was placed in a furnace specially designed for low-scattering angle IXS measurements [1]. Pressure was measured by means of the ruby fluorescence with a precision better than 0.05 GPa. Temperature was measured close to the sample by a thermocouple and its stability was better than 0.5 K. We collected good quality data (see Figure1) within approx. 16h of data acquisition per pressure point. In the assigned 6 days we measured 4 pressure points and an energy resolution measurement run with same statistics on a 50 μm-thin amorphous diamond sample at 15 K.

The recorded spectra were analyzed within a viscoelastic model based on the memory function formalism [2] and revealed a viscoelastic transition of the sound velocity from its known adiabatic value c_0 to its high-frequency one c_∞ upon increasing the excitation energy. The high-frequency sound velocity was so estimated for each pressure point. Its density dependence is well-described by a linear law which extrapolates very well to the existing literature point [2] at 0.15 GPa (see Figure2).
These new results, combined with the ones from previous beamtime HC1112, provide new and interesting insights [3] on the effect of GPa pressures on the hydrogen bond relaxation in hot dense water, to be compared with the recent findings on water self-dynamics provided by QENS measurements [4].

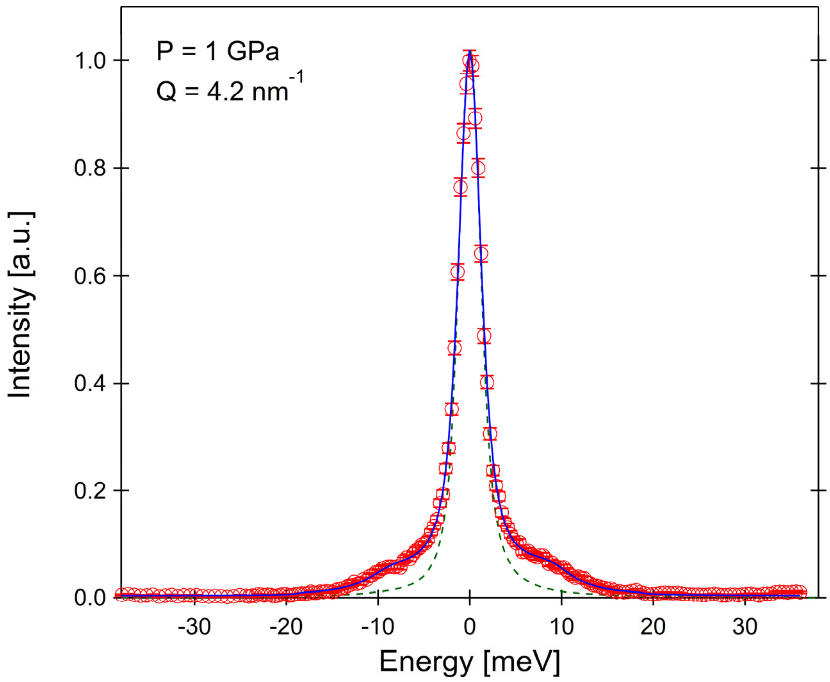

Figure1: *Example of IXS spectrum of water at 450K at the pressure and Q values indicated as measured on ID28 during the HC1693 beamtime. Normalized experimental data (empty red circles) are compared to the best fit (blue line) as obtained within the viscoelastic model and to the instrumental resolution function (broken green line).*

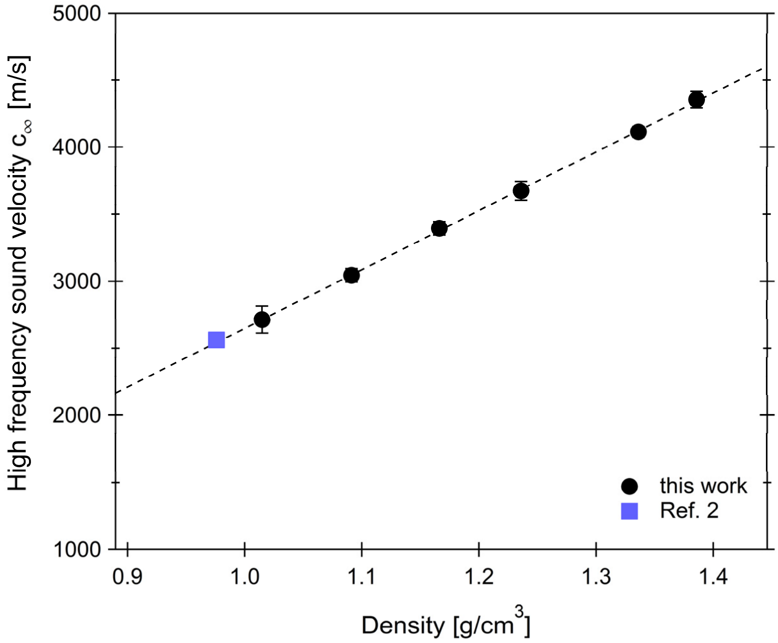

Figure2: *Density dependence of the high-frequency sound velocity c_∞ of water at 450 K, as determined during beamtimes HC1112 and HC1693, together with its best linear fit.*

References:

[1] F. A. Gorelli et al., *Inelastic X-Ray Scattering From High Pressure Fluids in a Diamond Anvil Cell*. Appl. Phys. Lett. 2009, 94, 074102.

[2] G. Monaco et al., *Viscoelastic Behaviour of Water in the Terahertz-Frequency Range: An Inelastic X-Ray Scattering Study*. Phys. Rev. E 1999, 60, 5505-5521.

[3] U. Ranieri et al., submitted (2015).

[4] L. E. Bove et al., *Translational and Rotational Diffusion in Water in the Gigapascal Range*. Phys. Rev. Lett. 2013, 111, 185901.