ESRF	**Experiment title:** Vibrational density of states in ice probed by inelastic X-ray scattering	**Experiment number**: **HS-2908**
Beamline:	**Date of experiment**: from: 07.09.2005 to: 16.09.2005	**Date of report**: 18.04.2206
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Report:

Water and water solutions have been studied intensively for many decades because of their central importance in many disciplines of science as well as for the existence of life in general. The many unusual properties, which distinguish water from other liquids are commonly believed to be linked with the existence of a dynamical hydrogen-bonded network throughout the liquid.

Dynamical information on atomic length scales has been obtained mainly by neutron techniques, such as coherent and incoherent inelastic scattering. A coherent explanation of the phenomena observed in water/ice is often hampered due to the fact that INS spectra of H_2O contain exclusively information about hydrogen due to its anomalously large incoherent cross-section. This problem can be partially overcome by studying D_2O, but even in this case only generalized density of states can be obtained. On the other hand, the vibrational density of states measured by inelastic X-ray scattering (IXS) will correspond closely to the pure oxygen partial DOS due to the much stronger X-ray scattering power of oxygen with respect to hydrogen.

The formalism and the experimental conditions under which coherent inelastic X-ray scattering from phonons can be utilized to determine the vibrational density of states has been established very recently [1].

The different ice samples (II, V, VI, XII) were prepared, following well established procedures, using equipment, available at the ILL, which has already been successfully used to produce the various recovered phases of ice [2, 3]. The samples were characterized by powder diffraction and stored at liquid nitrogen temperatures. For the experiment, the samples were transferred to the cold finger of a pre-cooled closed-cycle refrigerator. The spectra were recorded at 70 K for two angular settings of the spectrometer arm, thus covering a *Q*-range of about 15 nm^{-1} and yielding ten IXS spectra. The exact angular positions were chosen to have a reasonably good sampling for the X-VDOS reconstruction, and to avoid Bragg peaks. The spectra were recorded with a *Q*-resolution of 0.7 nm^{-1} for the individual analysers, and an energy resolutions of 3.0 meV. The summed spectra were partially deconvoluted with the instrumental function as in [4], but without subtraction of multiphonon contributions. The resulting generalized VDOS are represented in Fig. 1. The VDOS measurements were complemented by low-Q measurements in order to determine the orientationally averaged dispersion of longitudinal acoustic phonons and the averaged longitudinal sound velocity.

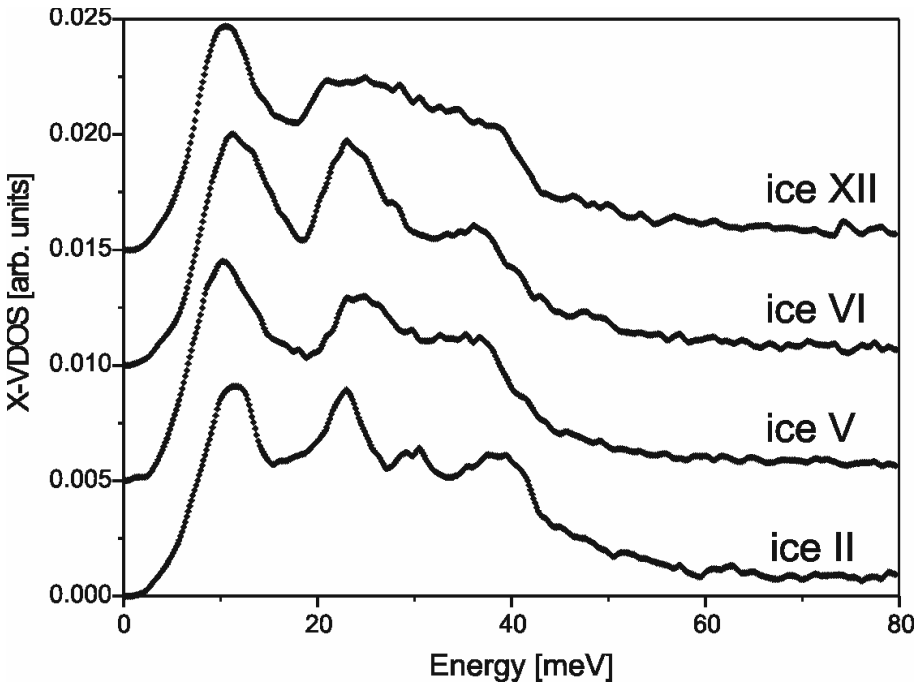

Figure 1. X-ray weighted vibrational DOS of different ice polymorphs

In conclusion, we have successfully obtained the X-ray weighted VDOS of ice II, V, VI, XII in the energy range below 80 meV. The structure of the O-projected DOS (IXS) is quite similar to the structure of the H-projected DOS (INS) for ice II, V, VI [5]. For ice XII the blurring of features in the range 20-40 meV could be interpreted as a consequence of complete hydrogen disorder [2].

[1] A. Bossak, M. Krisch, *Phys. Rev. B* 72 (2005) 224305
[2] M.M. Koza, H. Shober, T, Hansen, A. Tölle, F. Fujara, *Phys. Rev. Lett.* 84 (2000) 4112
[3] H. Schober, M. Koza, A. Toelle, F. Fujara, C.A. Angell, R. Boehmer *Physica* 897 (1998) 241B
[4] V.G. Kohn, A.I. Chumakov *Hyperfine Interactions* 125 (2000) 205
[5] J. Li *J. Chem. Phys.* 105 (1996) 6733