ESRF	**Experiment title:** Anomalous temperature dependence of thermal conductivity in Xe hydrate investigated by nuclear inelastic scattering	**Experiment number**: HS-4634
Beamline: ID18	**Date of experiment**: from: 06.06.2011 to: 12.06.2011	**Date of report**: 23.08.2012
Shifts: 18	**Local contact(s)**: Aleksander Chumakov (email: chumakov@esrf.fr)	*Received at ESRF:*

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Report:

Within the beam time allocated for proposal HS 4634 the Mössbauer resonance of Xe-129 was accessed for the first time by means of nuclear inelastic scattering (NIS) using the experimental facilities provided at beamline ID18.

The resonance was found using three different reflections, i.e. (19 9 28), (2 13 70) and (5 17 54) of the sapphire backscattering crystal [1], while only the last one was used for actual measurements. Using high precision measurements of the sapphire lattice constants [2], the Xe-129 resonance energy was determined to be 39581.3(2) eV, which is in good agreement with the value of 39578(4) eV reported within the nuclear data sheets [3], but adds accuracy. The lifetime of this specific nuclear level was determined to be 1.465(72) ns (yielding a half-life of 1.015(49) ns) using solely the time-resolved signal of the inelastic decay channel. It is in rough agreement with the weighted average of 1.399 ns reported in [3].

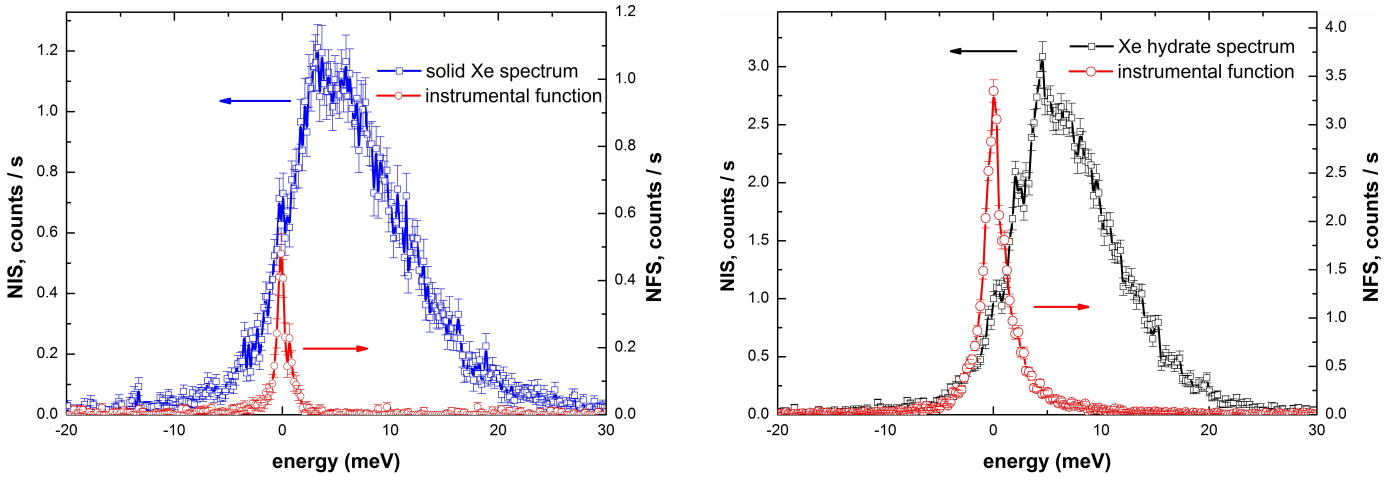

Fig. 1: Experimental NIS spectra obtained for crystalline Xe and Xe hydrate including the corresponding experimental resolution functions.

During beam time two different samples could be investigated with respect to their Xe specific densities of phonon states (DPS), i.e. crystalline Xe (25% natural abundance of Xe-129) at 20K and an enriched (90% Xe-129) Xe hydrate at 16K. Raw NIS spectra including the corresponding instrumental resolution functions are shown in Fig. 1. The instrumental function obtained during measurements of solid Xe is shown in more detail in Fig. 2. A full width of half maximum of slightly less than 1 meV could be achieved.

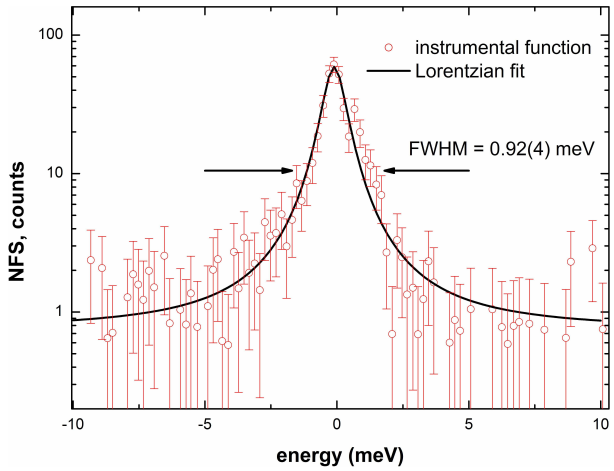

Fig. 2: Experimental resolution function obtained during measurements of the crystalline Xe sample including Lorentzian fit yielding a FWHM of 0.92(4) meV. The FWHM during measurements of the Xe hydrate was about 1.3 meV.

Since spectra of both samples exhibit an enormous contribution of multi-phonons, the Xe specific DPS were obtained using a modified version of DOS [4], in which the Lamb-Mössbauer factor is introduced as a fixed rather than a free parameter. The results of this procedure are shown in Fig. 3.

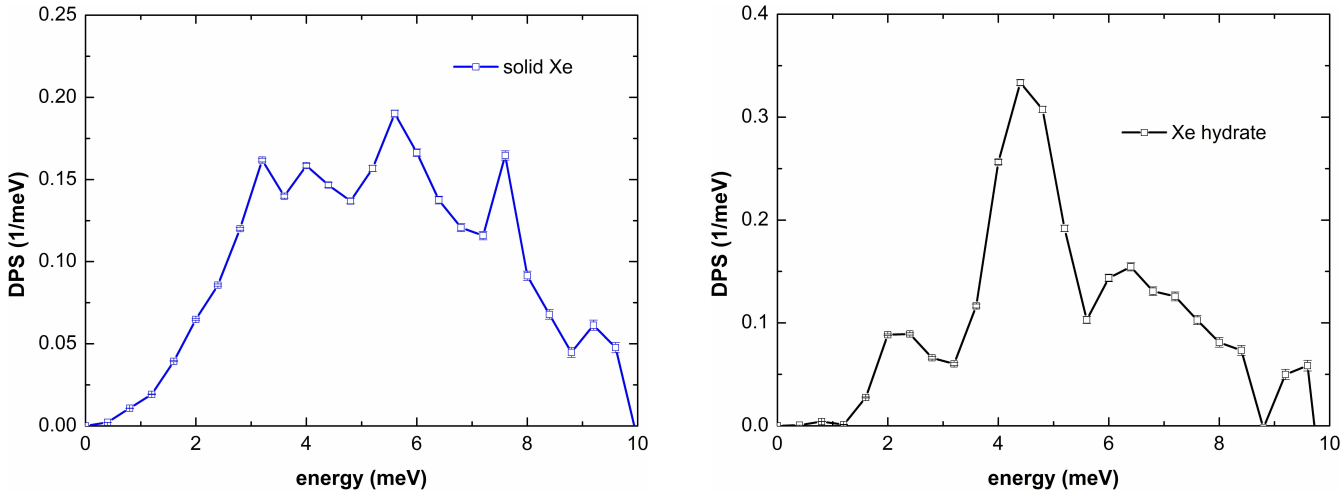

Fig. 3: Xe-specific phonon densities of state for crystalline Xe and a Xe hydrate. In both cases the energy cut-off is at about 10 meV at most.

In the case of solid Xe the mode energies up to 6 meV are in agreement with neutron inelastic scattering data [5], though there no higher modes are reported. In the case of the Xe hydrate the Xe-specific DOS clearly proves that the low lying modes, which were also detected using neutron scattering [6], are to be attributed to the Xe guest and not to the hydrate cage. Due to the low Lamb-Mössbauer factors of 0.1 and 0.19 for Xe and Xe hydrate respectively, measurements at higher temperatures were not feasible.

References:
[1] I. Sergueev et al., J. Synchrotron Rad. 18 (2011) 802.
[2] Yu. V. Shvyd'ko et al., J. Synchrotron Rad. 9 (2002) 17.
[3] Y. Tendow, Nuclear Data Sheets 77 (1996) 631.
[4] V. G. Kohn and A. I. Chumakov, Hyperfine Interact. 1-4 (2000) 205.
[5] B. J. Palmer et al., J. Phys. C: Solid State Phys. 6 (1973) L313.
[6] C. Gutt et al., J. Chem. Phys. 116 (2002) 3795.