ESRF	**Experiment title:** X-ray-weighted vibrational density of states in icosahedral MgZnY Quasicrystal	**Experiment number**:
Beamline: IN22N	**Date of experiment**: from: 28. Nov. 2001 to: 4.Dec. 2001	**Date of report**: 2/28/2002 *Received at ESRF:*
Shifts: 18	**Local contact(s)**: A. Chumakov	

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Report:

The vibrational density of states g(E) in icosahedral MgZnY quasicrystals was studied using inelastic x-ray scattering on Beamline ID22N. The energy resolution of ca. 1meV was provided by using nuclear-resonant scattering on the 57Fe in the detector system. The sample was powdered i-MgZnY quasicrystal and the measurements were taken at room temperature. Because of the low countrate in this type of experiment it was decided to measure only the quasicrystaline phase rather than the approximants as well. Since the last experiment (HS1322), we have improved the sample holder to suppress the signal of the Be foil holding the sample.

The aim of the experiment was to determine the x-ray weighted g(E) in this quasicrystal and to compare the result with previous inelastic neutron measurements. The calculation of g(E) from the experimental spectrum assumed a model spectrum is described as a superposition of a delta-function from elastic scattering plus Stokes and antiStokes single phonon contributions as well as multiphonon contributions. To calculate g(E) we used the one phonon approximation. The g(E) resulting from our measurements compared to that from inelastic neutron scattering can be seen in figure 1. The specific heat can be calculated from the VDOS using the following expression:

$$c_v = 3 * k_B \int_0^\infty g(E) * \left(\frac{\beta * E}{e^{\beta E} - 1} \right)^2 e^{\beta E} dE,$$

where all symbols have their conventional meaning.

We have compared as well the lattice specific heat calculated from the velocity of sound and from the phonon dispersion curves measured in MgZnY [from experiment HS1500, Brand et al., to be published] to compare as many as possible different experimental techniques with our results (see figure 2). For temperatures above 11K the neutron data and the x-ray data are in a good agreement. The obvious differences between the neutron scattering data and the inelastic x-ray scattering data in the low temperature region below 10K (in g(E) as well as in the specific heat) can be due to a problem with the deconvolution of the instrumental function from the experimental spectrum which has to be done before calculating g(E). This problem has yet do be solved.

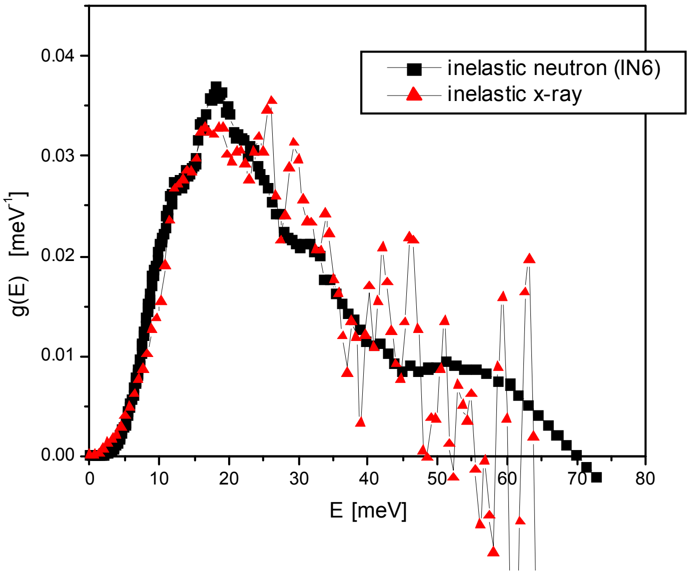

Figure 1. g(E) as calculated from the inelastic x-ray scattering compared to that from inelastic neutron scattering.

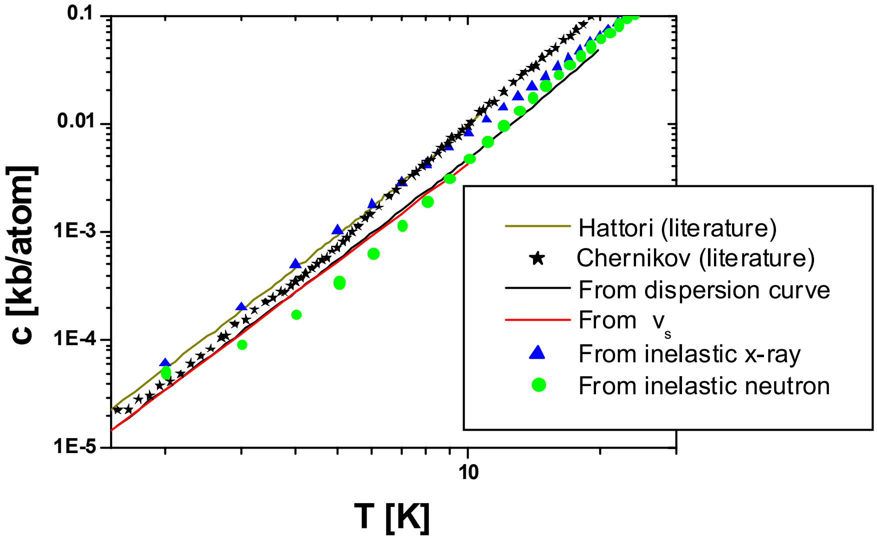

Figure 2. Lattice specific heat calculated from the above compared with two literature results (Hattori and Chernikov) as well as other predictions from the measured dispersions curve – HS1500 – and from the measured sound velocity.