	Experiment title: Inelastic scattering in icosahedral i-MgZnYi quasicrystal: phonon density of states	**Experiment number**: HS-1322
Beamline: ID22N	**Date of experiment**: from: 06.09.2000 to: 11.09.2000	**Date of report**: 28 August 2001 *Received at ESRF:*
Shifts: 15	**Local contact(s)**: A. Chumakov	

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Report:

This experiment was to study the x-ray-weighted vibrational density of states of the icosahedral quasicrystalline system i-Mg-Zn-Y. We measured the inelastic scattering of 14.4keV gamma rays at the ID22N beamline using time-resolved APD detectors. They were covered with foils of 57Fe to provide the energy resolution of the detection. This indirect method measures any inelastic channel in the sample + sample holder. It was decided due to the rather low count rate to study the icosahedral quasicrystal and one (rather than two) periodic hexagonal phase(s) as a comparison. The measurements were also only at room temperature. The raw results for the icosahedral sample are shown in Figure 1. This data has been treated in the following way. First the background countrate was subtracted, and a central line fitted and stripped from the data. The positive energy part (down-scattering for the gamma ray: it creates a phonon in the sample and loses energy) is used in the further analysis. This is shown in Figure 2. We see a large maximum the 40 to 80meV range, unexpected for such a heavy material. In addition we have in the meantime some data for inelastic neutron scattering showing most of the weight below 50 meV. This difference is (unfortunately) explained by the presence of a signal due to the Beryllium sample holder. A thin (125 micron) foil of Be

was used to hold the sample powder, and the geometry was such that the incoming gamma beam first struck the Be foil, then the sample. Also shown in Figure 2 is the density of states of Be as found in the literature. While there is certainly a discrepancy at higher energies, the main peak is fairly well explained by a Be signal. We subtracted these two signals, paying attention to normalise the data a consistent way. The result is shown in Figure 3. Here a comparison is made with the data from ILL IN6. Clearly we have an idea of the x-ray-weighted DOS. However our goal is to detect the differences between this and the neutron-weighted DOS measured by INS. The data is not reliable enough in the important ranges of low (below 15 meV) and higher (above 35 meV) ranges. A second goal was to compare the icosahedral phase to the hexagonal one in order to provide input for the theoretical modelling of the icosahedral structure and force constants.

Therefore we plan to re-submit this experiment including a re-build of the sample holder. The main idea is that the radiation exiting the thick sample is many orders of magnitude weaker than that entering. Thus a simple mount such that the gamma ray first strikes the sample, and then after exiting the sample meets the Be foil is sufficient to eliminate completely the signal due to the Be. This will give data which is very reliable in the whole energy range, with no real problems. Such a sample holder has already been discussed with the beamline staff.

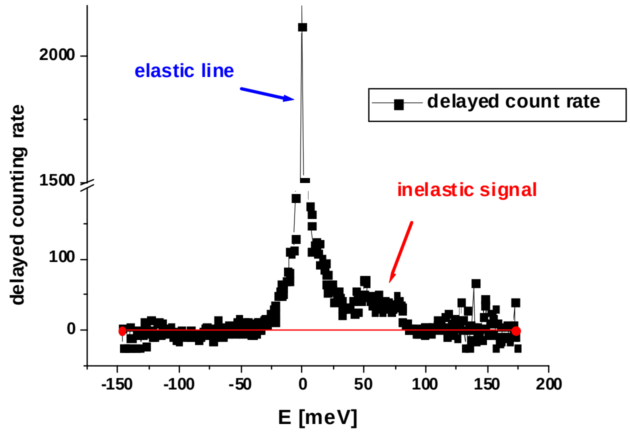

Figure 1.: shown is the inelastic counting rate as a function of energy offset between the high resolution monochromator and the 57Fe nuclear resonance. The zero-point is found from the large central elastic peak. Note the broaken vertical axis. The baseline is shown as a solid line.

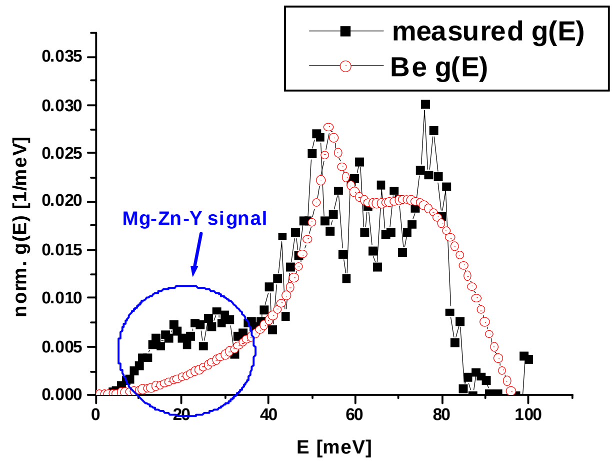

Figure 2: shown is the resulting experimental DOS from the inelastic signal (only the down-scattering part) up to 100 meV. Shown as well is a result from the literature for the DOS of Be.

The region inside the circle shows the “extra” part due to the sample.

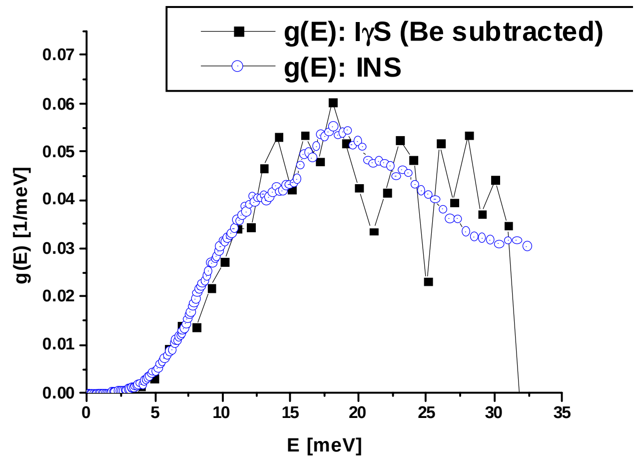

Figure 3: shown as solid squares is the resulting difference between the experimental DOS and the Be DOS. This is compared with the inelastic neutron DOS (open circles).