

	<b>Experiment title:</b> Phonon dynamics in Al-Cu-Fe quasicrystals	<b>Experiment number:</b> HS-440
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### Report:

This was a test experiment to probe the possibility of studying the Vibrational Density of States (VDOS) of a  $\text{Al}_{62}\text{Cu}_{25.5}^{57}\text{Fe}_{12.5}$  single-phase quasicrystalline powder. The experiment uses the inelastic scattering of T-rays detected by nuclear resonant transitions. The high-resolution spectrometer yielded an energy resolution of 4.4 meV and the ring was in mixed mode. Two samples were studied. The first contained iron enriched to 100 % in  $^{57}\text{Fe}$ , and the other contained natural iron with 2 %  $^{57}\text{Fe}$ . We measured both the foreword and the  $4\pi$  scattered delayed (nuclear) signal in the range of  $\pm 100$  me V energy shift. For the first sample, inelastic scattering on the iron should dominate the  $4\pi$  scattered and energy shifted signal, while for the second sample, inelastic scattering on all atoms contributes. For the second sample, foils of  $^{57}\text{Fe}$  were placed before the detectors.

The results for the first sample are shown in the figure. On the left: inelastic  $4\pi$  as well as foreword signal. On the right: deconvoluted density of states. The deconvolution was performed in the usual way, using the Lipkin sum rule to normalise the spectrum, and stripping off the central elastic peak. Our results are: (1) The Fe-VDOS has a much lower cut-off in energy (ca. 40 meV) than the total-VDOS (60 to 80 meV) as was measured by inelastic neutron scattering. [1,2] This means that the higher-energy phonons measured in the inelastic neutron scattering experiment involve principally the Al atoms. (2) The resolution (4.4 meV) was not sufficient to resolve details of the low-energy portion of the Fe-VDOS, important to resolve discrepancies between specific heat and inelastic neutron scattering data. [3] However, a band of low-frequency modes was shown in the results near 14 meV. This band has also been seen in the inelastic neutron results. [2] (3) We also measured a sample with natural iron, but using resonant detectors, so that the total VDOS (Al, Cu and Fe) should be measured. The statistics (mixed mode) was not sufficient to allow an interpretation of these results but we were able to estimate and test for the best sample thickness for later experiments (preferably in 16-bunch mode).

It must be emphasised that this was a test experiment in order to judge the feasibility of measuring the phonon density of states on a rather dilute sample (only containing 12.5 % iron but including 25.5 % copper, making self-absorption a problem). In addition, the spectrometer resolution was only 4.4 meV rather than the best attainable 1.65 meV. This obviously did not allow sufficient resolution for the low-energy parts of the VDOS and the mixed mode of the ring (*only 2* counting periods per revolution) did not allow sufficient counting rates to accumulate enough statistics in a total of 9 shifts. Our results obtained from this trial experiment are very encouraging. We were able to determine that the experiments are feasible and that quantitative results can be expected with better statistics. In addition, results on a number of different quasicrystals indicate that inelastic neutron scattering misses parts of the low frequency dispersionless modes. The phonon contribution to the specific heat is always higher than that which would be predicted from the inelastic neutron scattering results. It seems that this is a result of the fact that inelastic neutron scattering misses part of the important (w-Q) space for this problem.

### References:

- [1] T. Klein et al. J. Non-Cryst. Solids 153-154 (1993) 562.
- [2] J.-B. Suck J. Non-Cryst. Solids 150 (1992) 231.
- [3] M.A. Chernikov et al. Europhysics Letters 35 (1996) 431.
- [4] M. Quilichini and T. Janssen, Rev. Modern Physics 69 (1997) 277.

Figure: (left) Inelastic signal as well as the foreword signal for the first sample. (right) Deconvoluted density of phonon states. The extra states near 10 to 15 meV are visible. The structure of the low energy side of the curve is reminiscent of the model calculations for quasicrystals. [4]

