ESRF	<b>Experiment title:</b> Inelastic scattering on Al-Pd-Mn single-grain quasicrystals: phonon structure	Experiment number: HS-1001
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## **Report**:

We have studied the phonon dispersion curves of the icosahedral i-AlPdMn using inelastic coherent scattering. This sample studied was a single grain cut with a 2-fold axis perpendicular to the surface. The (52,84) reflection was chosen as the starting point as it lies conveniently on a 2-fold axis, and is the strongest reflection at this large scattering vector G. In contradistinction to almost all previous studies (using inelastic neutron scattering), we chose to scan along the 2-fold direction rather than the 5-fold one. We denote the deviation from this reflection as q = Q - G, where Q is the true scattering vector. We have studied both the longitudinal (LA) as well as the transverse acoustic (TA) modes up to  $q = 5 \text{ nm}^{-1}$ . We have obtained the following results: (1) Both TA and LA branches agree well in the  $q \rightarrow 0$  limit given by the sound velocity. (2) Both branched deviate from this result at very low q: at ca. 2 (LA) to 3 (TA) nm<sup>-1</sup>. This is significantly lower than previously measured along the 5-fold direction (see for example [1]). (3) Some evidence was found for non-acoustic, probably dispersionless, modes around the LA and TA branches. Although these are difficult to quantify, there is definitely evidence for such modes. The thermal and vibrational properties of quasicrystals have remained difficult to understand. It has been noted that specific heat measurements do not agree with the experimental sound velocity and vibrational density of states (DOS).

To explain these discrepancies, non-acoustic localized states have been postulated but never really directly observed. Interesting from this point of view, we observe firstly a deviation from linearity (speed of sound limit) at low energy as compared to previous studies along the 5-fold axis [1]. However this result does not seem sufficient to explain the specific heat results [2] since new inelastic studies indicate [3] that these low energy non-acoustic vibrational states must exist distributed in the energy range from 0 to ca. 10 meV. Thus our observation of bands of inelastic signal outside the LA and TA branches is very important. These signals must be further studied in order to finally determine their nature. The very high resolution for inelastic coherent scattering of this beamline makes such studies possible. (They are for example not possible to observe by inelastic neutron scattering due to the lower intrinsic resolution.)



Left: Typical scan result along the 2-fold axis. The phonon creation and annhilation peaks have been fitted with a damped harmonic oscillator model. Some signal is observed between these and the central elasticline as well as near ca.  $\pm$  10 meV. These may signal non-acoustic excitations.

Right: The results for the average energy (found from the damped oscillator model) for different scattering vector q = Q-G. At the point where the dispersion curve deviates from the linear velocity-of-sound limit, there is also a dramatic increase in the linewidth (oscillator damping constant) shown for example for the LA branch.

In this first experiment we did not have the time to measure along the 3- and 5-fold axes nor to pursue the newly discovered non-acoustic signals in detail. Since there is sufficient indirect evidence that these should exist in quasicrystals, we would propose following up this experiment with further studies designed to investigate this.

It must also be said that this is the first time that crystalline materials with such heavy elements have been successfully studied on this beamline. This opens new possibilities for studies of crystalline and quasicrystalline materials on this beamline.

[1] M. de Boissieu et al, J.Phys. Conden.Matter 5 (1993) 4945.

[2] M.A. Chernikov et al., Phys. Rev. B 48 (1993) 3058.

[3] R.A.Brand et al, Phys. Rev. B submitted.