ESRF	**Experiment title:** Optical phonon branch in the quasicrystal i-AlCuFe	**Experiment number**: HS-3459
Beamline: ID28	**Date of experiment**: from: 29.08.2007 to: 1.09.2007	**Date of report**: 28.09.2009
Shifts: 9	**Local contact(s)**: Dr. Alexei Bossak	*Received at ESRF:*

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Report:

In the previous experiment we studied a single-grain icosahedral quasicrystal i-AlCuFe sample and measured both the LA and TA acoustic branches but were unable to study the optical branch due to a lack of time.

This present experiment concentrates on the high energy region between 20 and 60 meV. The sample was studied in reflection geometry with only one of the detectors in proper theta-2theta geometry (detector #2). In order to maximize the counting rate we used the analyzer reflection Si(999), which means less resolution.

Previously we found at high resolution the LA and TA modes given in black and red in the second figure. These agree well with the known sound velocities at low Q, also given in figure 2.

In this new experiment we measured up to higher energies but with lower resolution. What we found was a broad band of states above the acoustic mode found before. This is shown in the first graph (for reduced q = 3.13 nm-1), giving the measured counts and a fit to the central elastic line with a Voigt profile. The difference between the Voigt line and the measured curve shows the acoustic excitation found before, and excess counts in a broad region up to about 30 to 50 meV on the average. Similar spectra were mesaured for Q values ranging from 1.5 to 6.5 nm-1. The upper energy value at which excess counts can be detected is shown on the second figure as the navy blue squares as a

function of Q . Assuming little or no dispersion, the average upper limit is about at 40 meV over a the whole Q range. We conclude that the optical branch is very broad and poorly defined in i-AlCuFe.

We also have used all detectors to average over the reciprocal space. This cannot be used to deduce the dispersion curve (only one detector being in proper theta-2theta geometry) but can be used for the vibrational density of states g(E). This is shown as the light pink line (E vertical, g(E) at the top). The major peak agrees with the flattening of the acoustic branches, and the tail with the upper limit of the excess states.

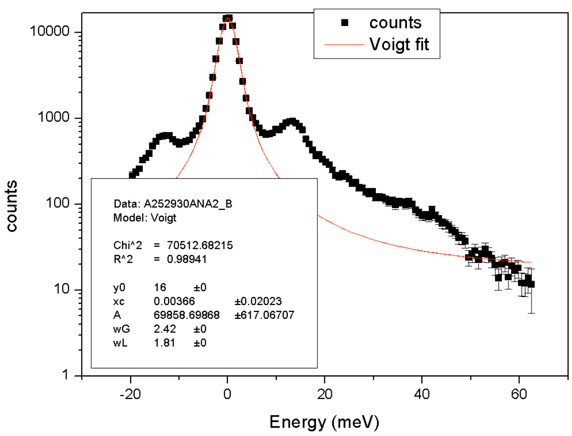

Figure 1.

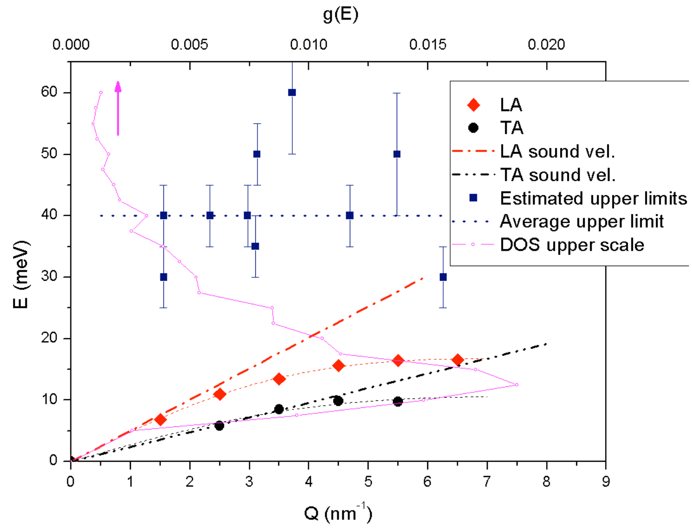

Figure 2.