



	Experiment title: Phonon spectrum of the unconventional superconductor PuCoGa ₅	Experiment number: HS - 2695
Beamline: ID28	Date of experiment: from: 17 / 06 / 2005 to: 27 / 06 / 2005	Date of report: 18 / 08 / 2005
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Report:

The phonon spectrum of the unconventional superconductor PuCoGa₅ ($T_c=18$ K) was investigated on the three axis spectrometer ID28 using the Si [11, 11, 11] monochromator reflection. This compound crystallizes in the tetragonal P4/mmm space group with the lattice parameters $a=b=4.232$ Å and $c=6.786$ Å. Single crystalline samples were grown and encapsulated at the ITU-Karlsruhe with chosen orientations that were carefully kept within a few degrees during the encapsulation process. To collect data along different high symmetry directions (namely in the basal plane and along the c-axis), several samples are needed due to experimental limitations of the scattering geometry or/and of the optical opening of the capsule. Four samples were made available (two in reflection geometry and two in transmission geometry) and three of them were measured.

The reflection geometry with [001] normal to the beam has allowed to measure the branches LA[001] and LO [001] (2 branches with significant intensity). However such a geometry was not optimal due to the reduced opening of the capsule which precludes the measurement of transverse modes. Most of the measurements were subsequently realized in transmission geometry with two platelet-shaped samples of thickness 40 µm and 20 µm. The first sample with [001] normal to the platelet has allowed to measure the LA[100], TA[001]a and TO[001]a (3 branches) modes. The second sample with [100] normal to the platelet was measured for 3 different scattering geometries with the following scattering planes a) ([100],[001]), b) ([110],[001]) and c) ([100],[010]). The corresponding measured modes were a) LA[001], LO[001], TA[100]c and TO[100]c (3 branches) b) LA[001], TA[110]c, TO[110]c (3 branches) and c) LA[110], TA[100]b, TO[100]b, (2 branches), LO [110] (3 branches) TA[110]₁₋₁₀ and TO[110]₁₋₁₀ (2 branches) . Representative scans are shown in Fig. 1 for the LA[100] branch.

Ab-initio calculation was made prior to the experiment (P. Piekarz et al., Phys. Rev. B 72 (2005) 014521) and this has allowed to select the needed intensity zones in order to optimize the contrast between

the different phonon branches. The modes were then assigned “on-line” for a better efficiency. This calculation was made for several Coulomb interaction parameters $U=0$ and $U=3$ eV. A better agreement is found for the calculation with $U=3$ eV as seen in particular on the lowest energy TO modes and higher energy LO modes. The comparison between the measured frequencies and the calculation with $U=3$ eV is shown in Fig.2 for the three directions [100], [110] and [001] . While the agreement is already good, work is in progress for a better description of the data.

This experimental study of the lattice dynamics of PuCoGa_5 is a first step in view of further measurements to be performed in the superconducting phase and aimed to address the question of the mechanism of superconductivity in this system. Attention will be paid to electron-phonon coupling. However, the present exhaustive mapping of the phonon spectrum of PuCoGa_5 is of crucial interest by itself in view of recent developments in band structure calculation of actinide compounds. It validates new advances in ab-initio lattice dynamic calculation.

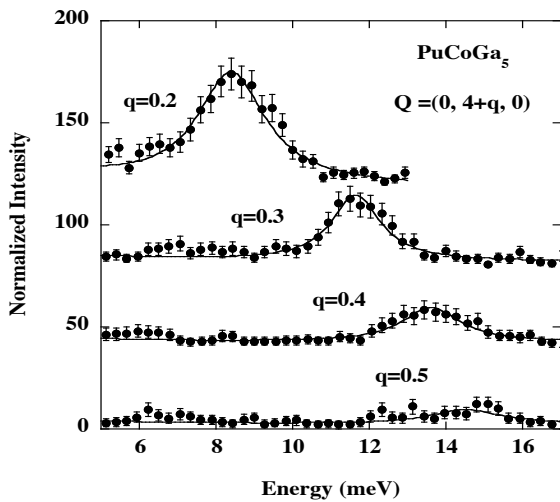


Fig 1 : Phonon spectra of PuCoGa_5 for $\mathbf{Q}=(0, 4+q, 0)$ corresponding to the LA[100] mode.

Fig 2 : Experimental data obtained for the three principal directions [100], [110] and [001] compared with ab-initio theoretical calculation.

