ESRF	**Experiment title:** Temperature dependence of the lattice parameters in the heavy-fermion superconductor $PuCoGa_5$	**Experiment number**: **HC- 1772**
Beamline: ID22	**Date of experiment**: from: 15/05/2015 to: 19/05/2015	**Date of report**: 06/07/2015
Shifts: 9	**Local contact(s)**: Carlotta Giacobbe	*Received at ESRF:*

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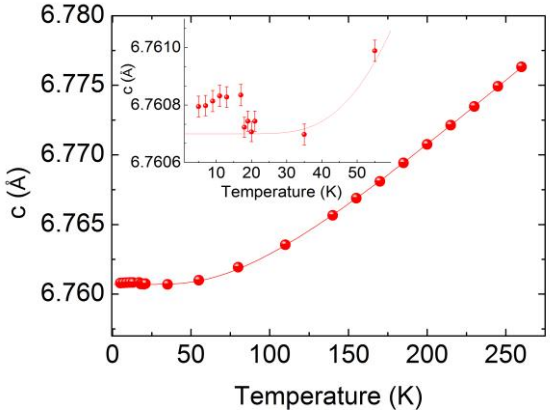
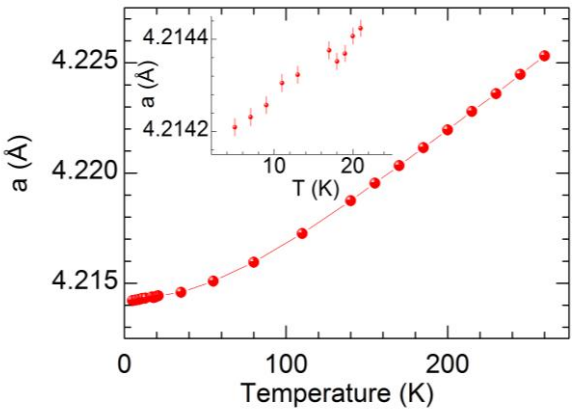
Report:

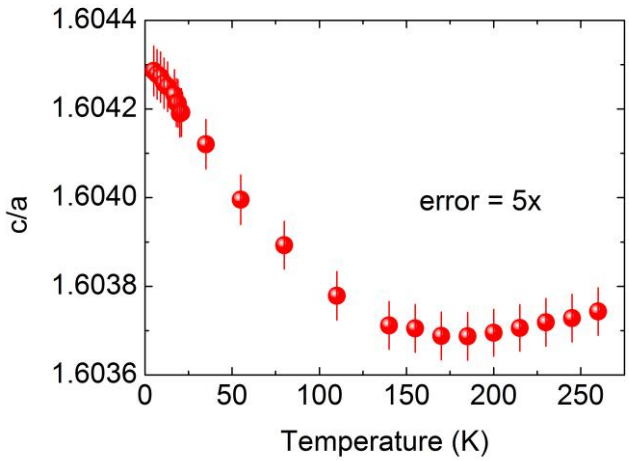
Aims of this experiment on $PuCoGa_5$ were: i) to verify the absence of lattice distortions at the superconducting critical temperature T_c = 18.7 K and ii) to measure with high accuracy the lattice thermal expansion. Data have been collected on a sample obtained by crushing a single crystal grown in a Ga flux using the ^{242}Pu isotope. The total sample mass was 4.90 mg, corresponding to a plutonium mass of 1.81 mg and a total activity of 264 kBq. The powdered sample was put inside a hermetic sample holder providing four levels of containment. For this, we used a kapton capillary (1 mm diameter, ~25 mm in length) half filled with Stycast. The resin was allowed to cure, before a 5 mm mixture of a second resin (Epofix) and the sample was inserted with a pipette. The Epofix was used because of the lower viscosity, allowing easier mixing with the powder sample and insertion into the narrow kapton capillary. The remainder of the capillary was then filled with Stycast and, once fully cured, it was inserted into a drilled-out plexiglass rod, which was sealed with a plexiglass plug, glued with further Stycast and finally enveloped within a 4 mm polyimide tube.

The channel-cut Si 111 monochromator of ID22 provided an incident beam wavelength of 0.354155 Å. The sample capillary was mounted on the axis of the diffractometer and span inside a liquid-helium-cooled cryostat allowing reaching a base temperature of 2 K. A NIST 640c Si standard was used to calibrate the Si-111 multianalyser stage. In the first part of the experiment, the diffraction pattern was measured at several temperatures, from 2 to 300 K, with acquisition times up to four hours. No lattice distortion has been observed and the tetragonal structure (Space Group P4/mmm) persists in the superconducting phase. The temperature (T) dependence of the lattice parameters has then be obtained from the Rietveld refinement of diffraction patterns collected on warming from 5 K up to 260 K, with a counting time of 1 hour at each temperature. The main results are summarized below.

- The temperature dependence of the linear thermal expansion coefficients α_a and α_c, shows that upon cooling the expansion is isotropic down to 150 K, and anisotropic for lower temperatures. This results in a *c/a* ratio that decreases with increasing T to become almost constant above ~150 K. An anomaly is observed at T_c for both α_a and α_c. As a consequence, also the volume thermal expansion coefficient α_V has a jump at T_c, a factor ~20 larger than the change predicted by the Ehrenfest relation between the variation of α_V at T_c, the change in the specific heath ($\Delta C_V/T$ = 0.11 J mol^{-1} K^{-2}) and the pressure derivative of T_c ($\partial T_c/\partial P$ ~0.4KGPa^{-1}).







- Marginal evidence is obtained for an anomalous behaviour below T_c of the *a* and *c* lattice parameters. Whilst *a* decreases linearly with decreasing T, *c* has a small expansion at T_c and becomes constants at lower temperatures. As a consequence, the volume expansion deviates from the curve expected for the conventional anharmonic behaviour described by a simple Grüneisen-Einstein model. The observed differences are about two times larger than the error bars obtained by multiplying the statistical errors by a factor five.