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Report:

The heavy fermion superconductor UPt$_3$ is attracting much interest because it has been established as an unconventional superconductor as seen by the existence of three distinct superconducting phases in the magnetic field-temperature plane. In zero-field the two superconducting phase transitions occur at $\approx$ 0.475 K and $\approx$ 0.520 K. It is usually thought that this complex phase diagram arises from the lifting of the degeneracy of a multicomponent superconducting order parameter.

One candidate for such a symmetry-breaking field is the short range antiferromagnetic order characterized by a Néel temperature of $T_N \approx$ 6 K and an extremely small ordered magnetic moment (0.02 (1) μ_B/U-atom) oriented along the a^* axis.

Recently, we have investigated the magnetic response of UPt$_3$ on a microscopic scale by muon Knight shift studies [1]. The conclusion of that work was that UPt$_3$ is characterized by a two component magnetic response. The muon results immediately raise the question of whether the observed magnetic behavior is due to an unknown weak lattice modulation.

Following the publication of the muon paper, a work reporting electron and high energy x-ray diffraction experiments has been published. It shows that UPt$_3$ has a trigonal crystal structure rather than the hexagonal close-packed structure usually assumed [2]. The fact that the symmetry of the crystal structure is lower than usually assumed suggests that the symmetry-breaking field needed to explain the superconducting phase diagram could be of crystalline origin rather than magnetic.

If UPt$_3$ had an hexagonal close-packed crystal structure, (h, h, l) reflections should be systematically absent for odd values of l. However, Walko *et al.* [2] have recorded Laue patterns with 75 keV x-rays in which $(0, 0, 7)$ and $(0, 0, 5)$ are clearly observed.

Last June we investigated the crystal structure of UPt$_3$ at room temperature at ID15A. We chose a relatively high energy x-ray beam of 130 keV for two reasons: 1) to work with a sufficiently small absorption coefficient as Walko *et al.* and 2) to minimize the influence of the harmonics of the x-ray beam.

We started the measurements with the three axes diffractometer using a germanium detector. We first established that the ratio of the intensity of a reflection due to the second harmonic (260 keV) relative to a reflection from the first harmonic was about 2×10^{-4}. Combining this intrinsic low flux to the possibility of energy analysis allowed by the germanium detector, it turned out that the contamination of the beam with higher order harmonics was not a problem. Then, we recorded a number of rocking curves for different reflections. Forbidden reflections of the type $(0, 0, l)$ with odd values of l were clearly observed. In particular, the $(0, 0, 7)$, $(0, 0, 5)$, $(0, 0, \bar{7})$ and $(0, 0, \bar{5})$ reflections were detected. However, we found that the intensities were strongly dependent on the orientation of the sample about the scattering vector. An example is presented in Fig. 1. This is a clear indication that multiple scattering is at play.

We then decided to record Laue patterns. The data were collected using the oscillation method with a MAR two-dimensional camera. The efficiency of such a detector is known to decrease extremely rapidly with energy. However, the problem of the multiple scattering is still present. To deal with it, we chose to record Laue patterns for values of the azimuthal angle taken between $-5°$ and $5°$ about the mean value, in steps of $0.5°$. For a given reflection, we decided to select the smallest intensities among the 21 Laue patterns. As clearly seen from Fig. 1, many measurements are expected to give an intensity at a plateau value.

Because of the limited dynamical range for detection with the MAR camera (16 bits), many patterns have to be recorded for a given set-up. In fact, we found that 10 pictures were sufficient. $(00l)$ reflections with $l = \pm 3$ and ± 1 were observed; see Fig. 2 for an example. Reflections with $l = \pm 5$ and ± 7 were not detected.

In order to increase the number of reflections for a reliable determination of the crystal structure, we have collected patterns for different experimental geometries. The analysis is under way. However, since forbidden (in the hexagonal space group) reflections were detected, we already know that, in agreement with the conclusion of Walko *et al.*, UPt_3 does not crystallize in the previously accepted hexagonal structure.

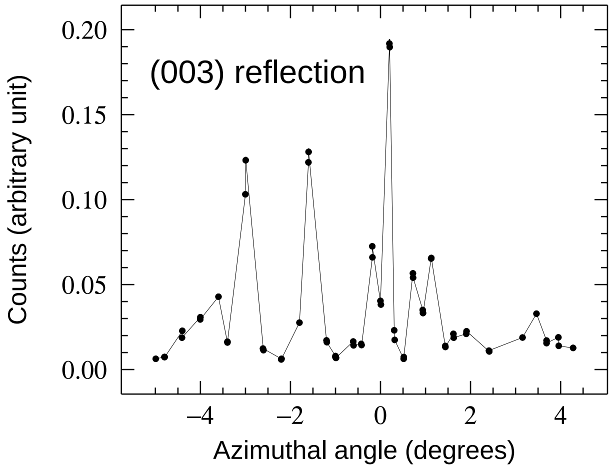

Fig. 1: angular scan around the scattering vector for the (003) reflection. The observed peaks as a function of the azimuthal angle are the signature of multiple scattering effects.

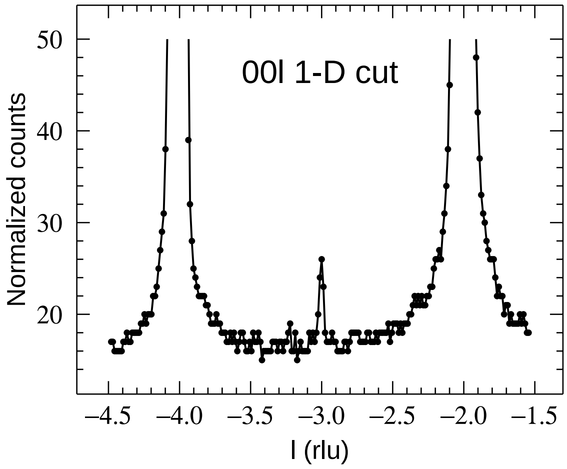

Fig. 2: 1D cut of a Laue pattern along the [00l] direction showing the $(00\bar{4})$, $(00\bar{3})$, $(00\bar{2})$ reflections. The intensity ratio $I(00\bar{2})/I(00\bar{3})$ = 3.1 $\times 10^3$ with an uncertainty of $\sim 15\%$. To cope with multiple scattering effects we have only selected the Laue patterns in the azimuthal scans with the smallest intensity at $(00\bar{3})$ position. The half width at half maximum are similar for the three reflections.

References

[1] A. Yaouanc *et al.*, Phys. Rev. Lett. **84**, 2702 (2000).
[2] D.A. Walko *et al.*, Phys. Rev. B **63**, 054522 (2001).