	Experiment title: Search for structural anomalies in the itinerant antiferromagnet UGa_3	Experiment number: HE1170
Beam-line: BM16	**Date of experiment**: from: October 3rd 2001 to: October 5th 2001	**Date of report**: 1st/03/2002
Shifts: 9	**Local contact(s)**: Dr. Fauth Francois	*Received at ESRF:*

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Report:

Experimental data and band structure calculations suggest that UGa_3 can be classified as an itinerant antiferromagnet. It orders at T_N = 67 k with type II structure (+-+- stacking of ferromagnetic (111) planes). Additional anomalies were observed below T_N at $T_1 \approx 40$ K and $T_2 \approx 8$ K. The 40 K singularity associated with a big change of extinction of the (0 0 2) nuclear reflection was shown to be due to a reorientation of the U-moments possibly linked to a small crystallographic distortion. Moreover, recent Ga NMR/NQR results cannot be reconciled with the occurrence of a simple cubic type II antiferromagnetic structure. The origin of the 8 K anomaly is even more speculative, it was tentatively ascribed to a peculiar itinerant nature of the ordered state of UGa_3.

The aim of the experiment was to search for any small crystallographic distortions for the different magnetic phase. The diffraction patterns were recorded between 250 K and 20 K on two samples sealed under argon in small capillaries (0.4 mm). The two samples powdered from the same polycrystalline rod differed only by the size and mosaicity of

the crystallites (different crushing time). The results were the same for both samples except that broaden peaks were observed for the sample with smaller grain sizes. At high temperature (250 K), the refinement as shown Fig. 1 is excellent (χ^2 = 1.26), it correspond as expected, to a cubic phase (AuCu3 type, space group $Pm\bar{3}m$) with a cell parameter a = 4.25152(1) Å. However good agreement between experimental and theoretical intensities was only obtained assuming a rather large Ga deficiency in the investigated samples (U/Ga = 1/2.82). By decreasing the temperature new diffraction peaks appears below about 240 K. Fig. 2 shows the diffraction pattern recorded at 30 K. It can be indexed considering two set of peaks. One set corresponds to the cubic phase observed at high temperature (a = 4.24045(1) Å). The other was assigned to a trigonal phase (a = 2.98317(5) Å, γ = 70.70º) which alternatively can be indexed in an hexagonal representation with parameters a = 3.45193(5) Å, c = 6.6593(2) Å. It is interesting to note that the a parameter of the trigonal phase is close to the U-Ga or Ga-Ga nearest neighbor distance ($4.24045/\sqrt{2} = 2.99845$) found in the cubic phase. Here again best fits to the data indicate that the cubic phase is Ga deficient. It is thus suggested that the new set of peaks observed at low temperature could be due to a gallium phase although it did not correspond to any known phases of the (P, T) diagram. It would be interesting to check if the puzzling result we found is really linked to the Ga deficiency of the investigated samples. To shed further lights on this problem, we plan to perform similar experiments on samples obtained by crushing single crystals to verify the stoechiometry of these samples.

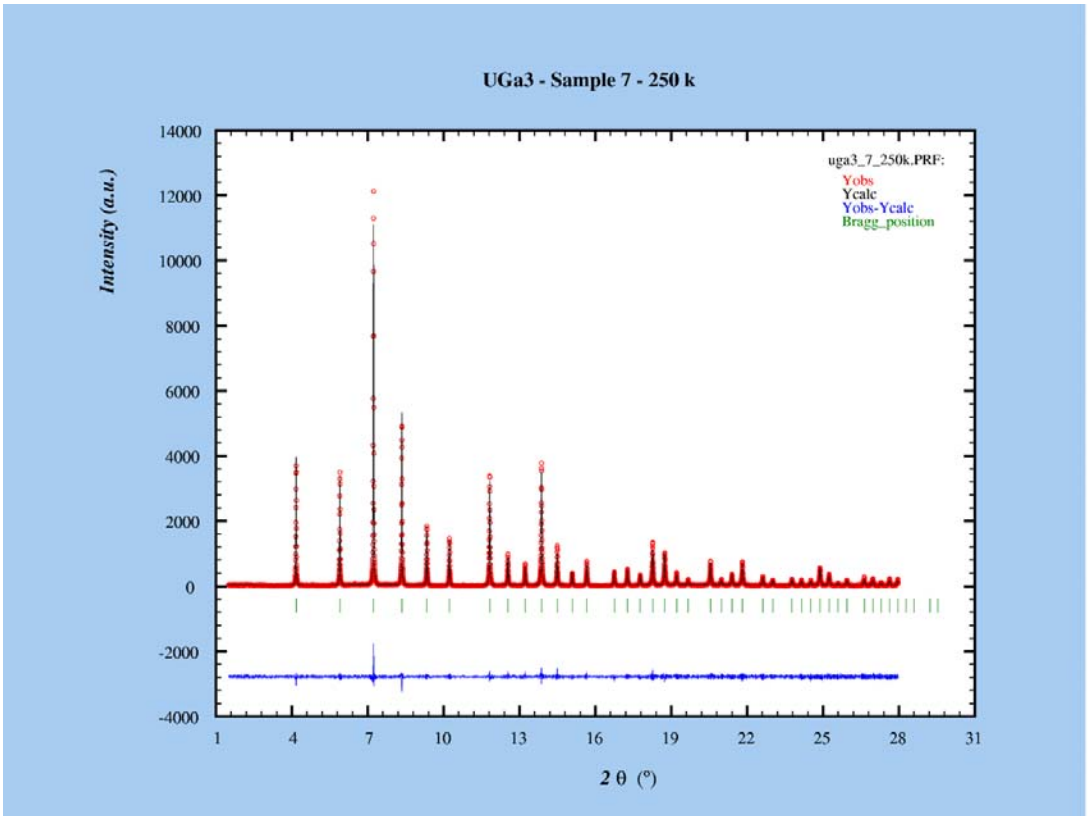

Figure 1: Diffraction pattern at 250 K. The marks correspond to the diffraction pattern of the cubic $Pm\bar{3}m$ structure.

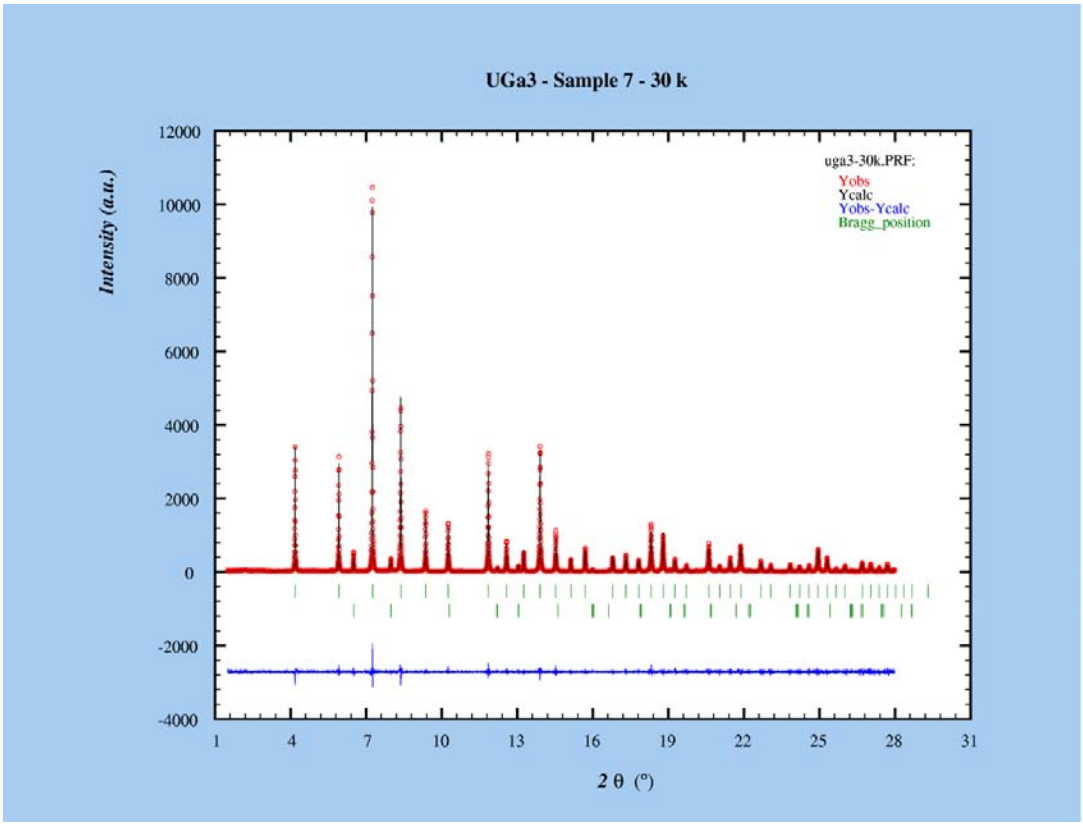

Figure 2: Diffraction pattern at 30 K. The upper marks correspond to the diffraction pattern of the cubic $Pm\bar{3}m$ structure, the lowest marks correspond to the diffraction pattern of the trigonal $R\bar{3}$ structure.