ESRF	**Experiment title:** Magnetic Phase Transition of $YMnO_3$ studied by X-ray Magnetic Resonant Diffraction at the Mn K edge.	**Experiment number**: 28-01-636
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Report:

Our interest in the $YMnO_3$ crystal has been mainly driven by their structural and magnetic peculiarities. Several attempts have already been made to determine the magnetic behavior of hexagonal $YMnO_3$ ($P6_3cm$, Z = 6, a = 6.1553(3) Å, c = 11.4026(3) Å at room temperature) [1-4]. The common conclusions that can be drawn are that the magnetic ordering of the Mn sublattice is dominated by antiferromagnetic Mn-O-Mn superexchange, the so-called 120° trigonal structure, where the magnetic moments lie within the basal *ab* plane, which provides a good model to study the crystal as a quasi 2D frustrated spin system. Below $T_N \approx 70$ K, the Mn spins break the basal plane triangular frustration, reorient, and the magnetic moment, observed at 1.7 K, is 2.9 μ_B [1].

Even though the $YMnO_3$ has attracted much attention in the last few decades some important questions still remain unsolved. The aim of our experiment was mainly:

1. To describe a mechanism of the antiferromagnetic phase transition.
2. To characterise the real magnetic structure of the crystal – since on the basis of powder neutron diffraction the $P6_3cm$ magnetic group was proposed [1] which is in disagreement with second-harmonic generation experiments where the $P\underline{6}_3c\underline{m}$ was suggested [3]. Sometimes, neutron powder determination of the magnetic structure is incomplete either due to powder averaging [1] or due to lack of higher Q momentum resolution otherwise available with x-ray synchrotron radiation. On the other hand - although second-harmonic spectroscopy (SHS) is a powerful method - as a macroscopic method it cannot provide a deep insight into the molecular structure and structural changes during the phase transition. Therefore, just as SHS, **magnetic resonant x-ray scattering** depends on the light polarization and the magnetic moment directions of the atoms but in the diffraction experiment we also benefit from the microscopic information.

Based on the neutron diffraction data [1] we set off to examine the (h 0 l) reflections with odd l which appear below T_N and are forbidden for the $P6_3cm$ space group. The crystal sample used in the experiment were cut and polished perpendicular to the hexagonal c-axis in order to give convenient acces to the (h 0 l)

zone. At the same time we were aware that we would be searching for a very weak effect as reported for the XMCD measurements of magnetoresistive manganites at the Mn *K* edge [5].

Unfortunately, due to the big size of the crystal plate (4 x 6 x 2 mm) and the crystal quality, our measurements were strongly affected by a multiple diffraction effect – producing extremely strong reflections at the expected magnetic reflection positions. Since for more than four days we were unable to solve the problem we decided to take advantage of our backup crystals – the $R\mathrm{In}_3$ family.

For a start, a TbIn_3 single crystal was tested for which a magnetic structure has been estimated by neutron diffraction. Similarly as reported [6] we have observed (0.5 0.5 0) type reflections below T_N = 32 K for collinear antiferromagnetic structure, with spins pointing along a fourfold axis. On the basis of the temperature dependence of the (0.5 0.5 0) reflection another phase transition at T_1 = 25 K was confirmed.

GdIn_3, like most RX_3 compounds, crystallizes in the AuCu_3–type cubic structure (*Pm*-3*m*; *Z* = 1; *a* = 4.61 Å). However, apart from its antiferromagnetic ordering, the magnetic structure is still *unknown*. In an attempt to circumvent the extremely high neutron absorption cross-section of Gd, non-diffraction techniques have been used to address the problem. Measurements using ^{119}Sn Mössbauer spectroscopy across the range of the pseudo-binary $\mathrm{Gd}(\mathrm{Sn}_{1-x}\mathrm{In}_x)_3$ alloys indicate that the ground state magnetic structure is a type-II antiferromagnet with the magnetic moments aligned close to [111] for the very rich In compounds (x –> 1.0) at 4.2 K [7]. Surprisingly, during our tests on BM28 a few magnetic reflections of (1/2 1/2 0) type in the temperature range 45 - 10 K were observed with intensities over 10000 cps, which did allow a polarization analysis of the diffracted beam (Fig.1). The only very preliminary results suggest that the GdIn_3 crystal posesses (with great probability) a collinear antiferromagnetic structure, with the spins pointing along a fourfold axis - similarly as for the first magnetic phase of TbIn_3. The temperature dependence of two magnetic reflections confirmed T_N = 47 K. Unfortunately, the limited measurement time left did not allow us to collect enough points at the reduced temperature range [$(T\text{-}T_N)/T_N \leq 0.2$]. Therefore, we can only roughly estimate a critical component: $\beta \approx 0.4$, which seems to be very close to a three-dimensional Heisenberg spin system (Fig. 2). A more detailed study of the system will be published.

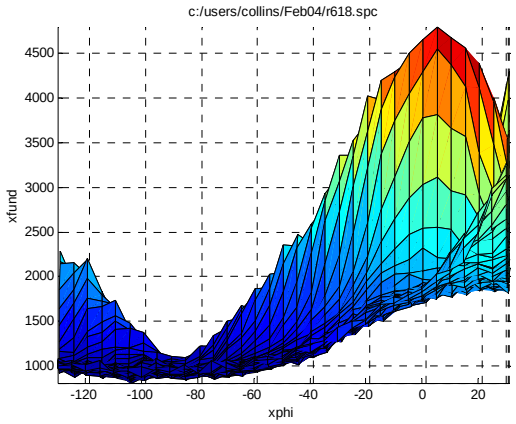

FIG.1: Azimuthal scan of the (0.5 2.5 0) magnetic reflection.

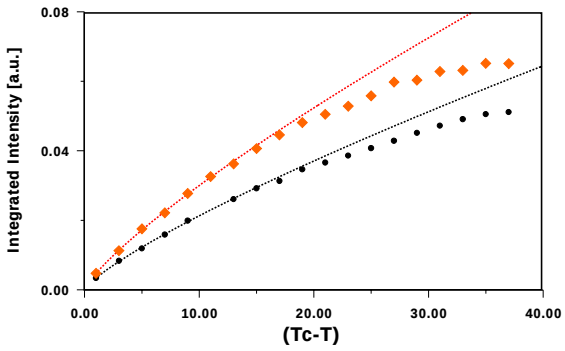

FIG. 2: Temperature dependence of the magnetic intensity of the (0.5 1.5 0) [♦] and (1.5 1.5 0) [●] Bragg reflections. The dashed lines are fits to the power law.

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