

BM02

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Experiment title:

Check of x-ray diffraction as a quantitative probe for non-collinear 4f arrangements

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Names and affiliations of applicants (* indicates experimentalists):

Mehdi Amara*, Laboratoire Louis-Néel, CNRS, BP 166X, 38042 Grenoble

Pierre Morin*,-----

Rose-Marie Galéra*,------

NdMg is a cubic compound (CsCl-type) which displays a multiaxial magnetic structure below $T_R = 35$ K [2]. On the side of the densities of charge, in the plane defined by the moments' directions, this structure corresponds to an antiferroquadrupolar arrangement with a [1/2 1/2 0] wave-vector. This magnetic structure had already been used for checking as feasible the measurement of multipolar diffraction peaks, at reciprocal space nodes $Q = [h \ k \ l] + [1/2 \ 1/2 \ 0]$ [3]. However, these first results were restricted to the observation of two reflections, [5/2 5/2 0] and [3/2 5/2 0], chosen about the expected maximum for the quadrupolar scattering. One crucial point, which was left without answer after our first experiment, regarded the Q dependence of the multipolar intensities, in particular their cancelling at low scattering angles. Indeed, beyond the correct order of magnitude of the peaks intensities, such a behaviour is the unquestionable proof of their multipolar nature.

In order to extend in reciprocal space our investigation of NdMg multiaxial phase, we performed additional measurements in identical conditions, using the 7-circles goniometer D2AM on the BM02 beamline. Thanks to the closed-cycle helium cryostat, the single-crystalline sample was first cooled down to 18.5 K. Then, after optimising the background level, as many multipolar reflections as possible within the beamtime allocated were measured, particularly along the diagonal of the basal plane of NdMg's

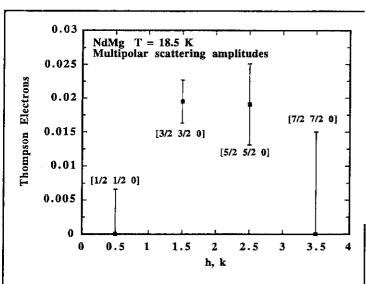


Figure 1 Measured multipolar scattering amplitudes at T = 18.5 K

Reflection	Measured	Computed
[1/2 1/2 0]	0.001 ± 0.006	0.0059
[3/2 3/2 0]	0.0195 ± 0.003	0.0198
[5/2 5/2 0]	0.019 ± 0.006	0.0225
[7/2 7/2 0]	0.001± 0.015	0.0127
[5/2 1/2 0]	0.016 ± 0.005	0.0088
[5/2 3/2 0]	0.013 ± 0.0015	0.0212
[7/2 3/2 0]	0.007 ± 0.003	0.018

Table 1 Measured and computed multipolar scattering amplitudes at T = 18.5 K

multiaxial structure. The location of the measured reflections are listed in Table

1. At least one day of counting time was devoted to each reflection in order to counterbalance the weakness of the signal (with a signal-over-noise ratio less than 10 %). Adjacent crystallographic reflections were systematically measured for the needs of calibration.

The main goal of the experiment, checking the cancelling of the scattering amplitude for low scattering angles, has been reached, as shown on Figure 2. The [1/2 1/2 0] reflection is much weaker than the [3/2 3/2 0] or [5/2 5/2 0]; actually no peak could be identified at the [1/2 1/2 0] position, so that only the maximum intensity consistent with the counting statistics could be defined, resulting in the error bar of Figure 2. The case of the [7/2 7/2 0] is similar, although less counting time was spent for this reflection thus resulting in a larger statistical error. This point is less crucial since the decrease of the scattering amplitude at large scattering angles is common to multipolar and spherical scatterings.

Regarding the quantitative aspect of the analysis, the measured scattering amplitudes are in good agreement with the calculation (Table 1). For the first time, the computed values include all multipolar terms, up to the dodecapolar ones (MFA treatment of NdMg's spin hamiltonian [1], starting from CEF parameters extrapolated in the R-Mg series). Obviously, the relatively large experimental errors are rather tolerant to the model, but a significant result is that beyond the quadrupolar scattering amplitude, one has to take into account the octupolar and dodecapolar contributions. Indeed, due to the large exchange fields exerted on the rare-earth ions, these terms are no longer negligible well below the order temperature.

^[1] Amara M and Morin P, Description of the magnetic phase diagrams in NdZn, 1996 Physica B 222 61-72.

^[2] Deldem M, Amara M, Galéra R M, Morin P, Schmitt D and Ouladdiaf B, Multiaxial magnetic ordering in NdMg, 1998 Journal of Physics: Condensed Matter 10 165.

^[3] Amara M, Galéra R M, Morin P and Bérar J F, Observation of quadrupolar x-ray diffraction peaks in NdMg, 1998 Journal of Physics: Condensed Matter 10 L743.