ESRF	**Experiment title:** Examination of magnetic surfaces by x-ray resonant scattering	Experiment number: *HE-495*
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Report:

The challenge of surface magnetism on UO_2 is that the crystal surfaces must be prepared ex-situ and the experiments are not done in UHV, because they require temperatures below 30 K, and that the magnetic structure is a complicated so-called 3**q** arrangement. We concentrated on the (100) surface [an earlier run had examined also the (111)], which appears to be the best surface despite it being polar in nature. Extensive *magnetic* truncation rods were characterised at the lowest temperature and are shown below.

In an experiment at the NSLS X22C beamline we obtained detailed specular intensity (not shown) at 8 keV to characterise the *atomic* planes near the surface. (This cannot be done at the same time on ID20 because of the grazing incidence geometry necessary for the magnetic surface experiments.) The top layer has a large interlayer spacing, a low density, and is probably a hydrocarbon molecule at low coverage. The next layer is oxygen and the third layer is uranium with a density only a few percent lower than the bulk. Interplanar relaxation effects are relatively small, and can be reliably modeled. With just a single low-density layer of "dirt", this is a considerable improvement on our earlier work, and is the result of extensive preparation in Karlsruhe. Obviously, these model parameters need to be included when fitting the magnetism.

The magnetic structure of UO_2, despite having the simple propagation vector of $\mathbf{q}$ = <001>, is rather complicated as it has been proposed [1] that the three independent **q** vectors, $\mathbf{q}_1$ = [001], $\mathbf{q}_2$ = [010], and $\mathbf{q}_3$ = [100], exist simultaneously within the crystal. This is called the 3**q** structure. It is not possible to distinguish this from the simple 1**q** structure by intensity measurements at magnetic Bragg peaks, and usually some symmetry breaking perturbation, such as a magnetic field or uniaxial stress, has to be applied to distinguish these structures [2]. However, the magnetic truncation rods represent a continuous distribution of intensity across the Brillouin zone (see figure) and there are interference effects that arise when fitting the 3**q** structure which allow us to verify that it is correct. Thus, in the 3**q** arrangement there is a definite phase relationship between $\mathbf{q}_1$ and $\mathbf{q}_2$ which does not exist if they come from different physical regions of the crystal. Furthermore, with a single q arrangement the moments can lie in two possible directions. The result will be a superposition of the two, shown separately simulated below. The fit is reasonable – recall that it must also include the nature of the atomic planes at the surface – and gives us confidence that we now understand the magnetic surface of the (100) UO2 antiferromagnetic at low temperature. A separate publication is being prepared on this interesting "side effect" to our surface experiments.

The experiment then went on to examine some of the rods as a function of temperature. More details of this are given in the proposal.

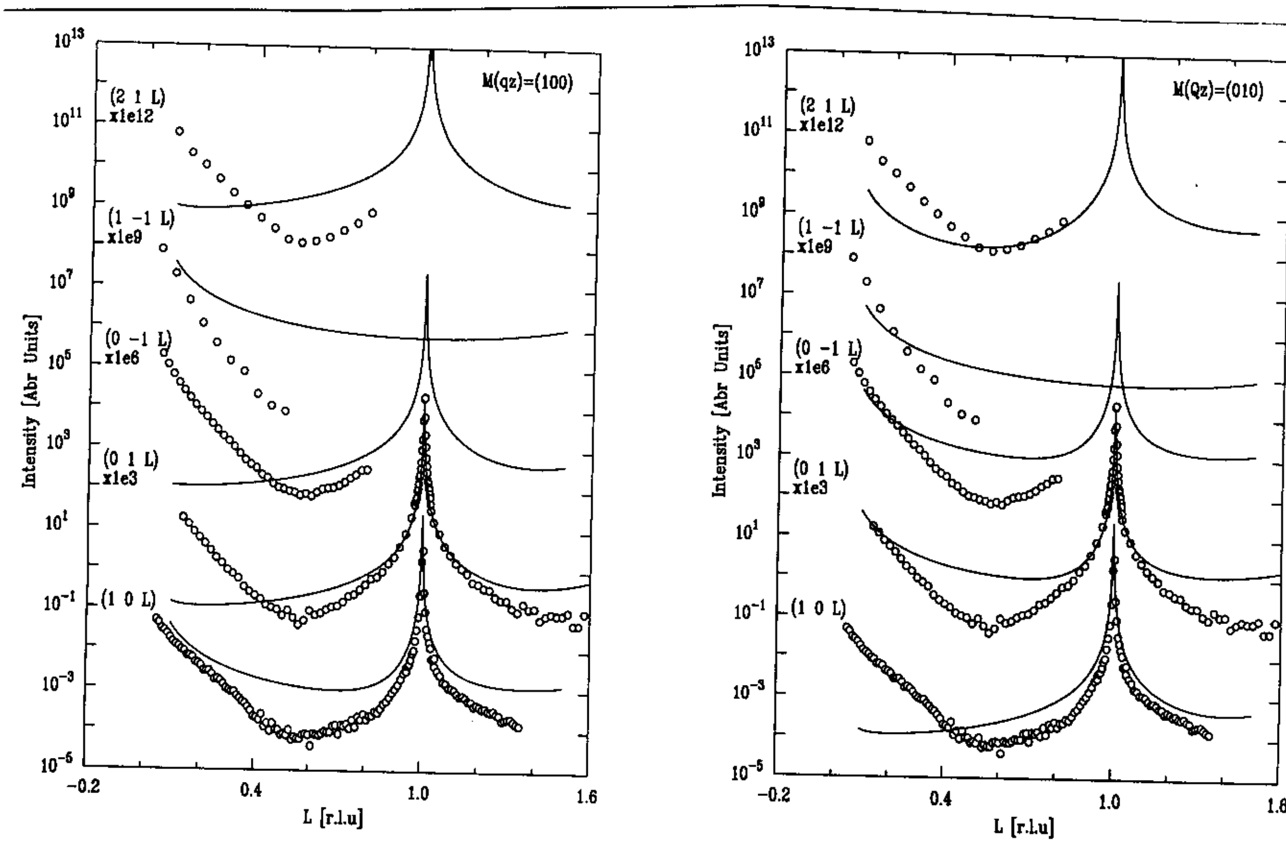

Figure 1

Intensity as a function of position for five magnetic truncation rods in UO_2 at T = 12 K. Data taken with polarisation analysis. The solid line is a best fit to the data for each moment direction and is shown separately. One has to add these incoherently to reproduce the data.

Refs:

[1] See R. Caciuffo et al., Phys. Rev. B 59 13892 (1999) and references therein.

[2] J. Rossat-Mignod in Methods in Exp. Physics (Academic Press) 1987, Vol. 23C, pp. 69-158