ESRF	**Experiment title:** **Crystallographic symmetry of antiferromagnetic MnO**	**Experiment number**: 1-01-260
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Report:

In MnO, the transition to the antiferromagnetic state at $T_N \cong 120$ K is accompanied by a strong rhombohedral contraction along <111>, thus distorting the high-temperature NaCl type structure. At 10K, the angle of the pseudocubic cell is as large as 90.62°. The magnetic configuration is type-II, characterized by the wavevector [1/2, 1/2, 1/2]. Despite the long tradition of attention to MnO, further points concerning the magnetic structure could be resolved only recently. From high-resolution neutron powder diffraction, it is now established that the magnetic structure is collinear with the moments ordered perpendicular to the unique [111] direction. Therefore, the true crystallographic symmetry of antiferromagnetic MnO must be lower than rhombohedral. We proposed to collect high resolution powder patterns in the temperature range of 10-125 K, as an attempt to detect the presence of an additional small structural distortion. This project is a follow-up to our earlier SNBL work on CoO, in which a reduction from tetragonal to monoclinic symmetry in the antiferromagnetic state could be unambiguously established [Jauch et al, Phys Rev **B64**, 052102, *2001*]. In the case of CoO, it could be shown that the monoclinic deformation angle scaled with the well-known tetragonal distortion of the pseudo-cubic cell.

We initially made a check of the sample quality by measuring the room temperature powder diffraction pattern of commercial MnO powder (Aldrich Chem Co.) at room temperature at a wavelength of 0.6Å. The full pattern, demonstrating the good quality of the diffraction peaks, is shown below in Fig 1. The lattice constant of 4.445 Å in s.g. Fm-3m are in good agreement with the literature values.

We subsequently installed the powder capillary in the He cryostat on BM1B and measured part of the powder pattern at 293K, 10K and 5K. The wavelength was changed to 0.8Å in order to provide good sensitivity to the expected lattice distortions (both the known tetragonal and the possible monoclinic distortions). The resulting diffraction patterns at room temperature and 10K measured between 47º and 48º are shown in Fig 2. The peak at 47.454º is the (420) reflection from the cubic room temperature phase. We can see that the expected tetragonal distortion is easy to observe, resulting in peaks of reflection (4,0,-2) at 47.393º and (4,2,0) at 47.829º. Unfortunately, our angular resolution was limited by the sample quality. Although the peak widths at room temperature were only approximately 0.033º FWHM, this is about a factor of 3x wider than the intrinsic diffractometer resolution. Both of the peaks shown in Fig 2 which appeared at 10K had a peak width which was substantially larger than at room temperature (0.058º FWHM for the peak at 47.393º and 0.070º FWHM for the peak at 47.829º). A similar increase in peak widths was observed, for example, for the (331) reflection at 46.183º, which split into 3 peaks as a result of the tetragonal distortion.

It is therefore not possible for us to draw definite conclusions concerning the postulated monoclinic distortion in the antiferromagnetic phase of MnO. Although the increase in peak widths seen in the tetragonally split peaks point in this direction, the increase in width could also arise from strain in the crystal lattice. It will be necessary to produce starting material which has a peak width close to the intrinsic width of the diffractometer (ca 0.01º of 2θ) before we can proceed further with this project. A suitable annealing procedure may help to reduce the intrinsic peak width of the MnO powder.

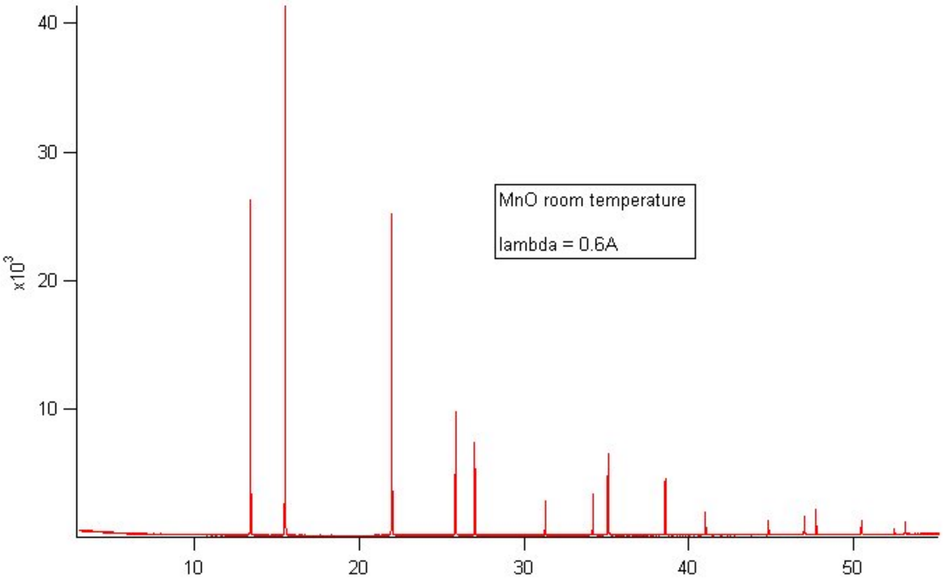

Fig 1 : MnO room temperature powder pattern at 0.6Ă

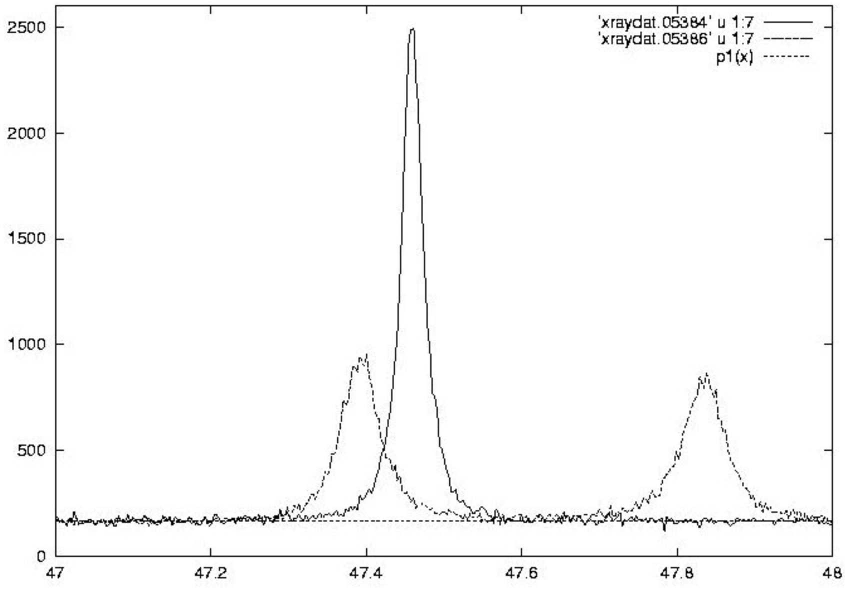

Fig 2 : Comparison of powder diffraction pattern from MnO at room temperature and 10K