Magnetic structural analysis of isosceles-triangular lattice antiferromagnet $Mn(Nb_{1-x}Ta_x)_2O_6$

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Columbite compounds MnB_2O_6 (B=Nb, Ta) is one of model materials of Heisenberg antiferromagnets, where Mn magnetic ions form an isosceles triangular lattice in the *a*-*b* plane. Earlier neutron diffraction measurements [1,2] revealed that $Mn(Nb_{1-x}Ta_x)_2O_6$ exhibits a non-collinear magnetic structure, where a cant angle of Mn spins changes with *x*. However, there are many inconsistencies between reported magnetic structures, possibly due to deviations of compositions from the chemical formula and the difficulty of separating nuclear and magnetic reflections in powder diffraction data.

Single-crystal neutron diffraction experiments for $MnNb_2O_6$ (x=0) were performed using four-circle off centered diffractometer (FONDER). A single crystal of $MnNb_2O_6$ with dimensions of approximately $2\times2\times2$ mm^3, grown by floating zone melting method, was used. The wavelength of incident neutrons was 1.2476 Å. The single crystal was inserted into 3K refrigerator to achieve a low temperature below the Neel temperature of 4.3 K. Integrated intensities at 234 Bragg points were collected at T=3.0 and 8.0 K by omega scan with a typical scan speed of 0.1 deg/min. Determination of both crystal and magnetic structure was carried out using the FULLPROF program.

To check magnetic Bragg reflections, we first performed reciprocal lattice scans along the *a** direction at T = 3.0 and 8.0 K. We found that both nuclear and magnetic reflections generally appear at (h,k,l) reciprocal lattice points with h,k,l = integer, being consistent with previous works [1,2]. Figure 1 shows results of refinement for crystal structure at T = 8 K above T_N. Refinement with 133 nuclear reflections gave R(F) factor = 4.2% and refined nuclear parameters were consistent with those of previous works [2].

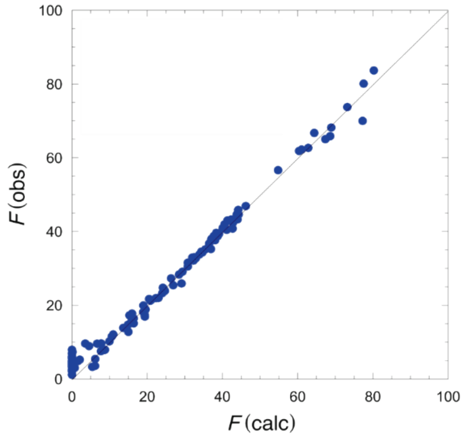

Fig. 1: Results of refinement for crystal structure at T = 8 K.

For the determination of magnetic structure below T_N, integrated intensities of magnetic reflections were obtained by subtracting data at T = 8 K from those at T = 3.0 K. Preliminary magnetic structural analysis showed that observed magnetic structure factors were explained within a magnetic structural model proposed by Nielsen [2]; however, a deviation between observed and calculated magnetic structure factors was evident for some reflections. Such deviation can be attributed to competing contribution of G-type and A-type magnetic structures. Further magnetic structural analysis of $MnNb_2O_6$ and single-crystal growth of $Mn(Nb_{1-x}Ta_x)_2O_6$ with x = 0.5 and 1 is now in progress.

[1] W. Scharf et al., Solid State Comm. vol.18 (1976) 249; V.S. Klein et al., Acta Cryst. vol.A32 (1976) 587.
[2] O.V. Nielsen et al., J. Phys. C: Solid State Phys. vol.9 (1976) 2401.