Magnetic ordering of multiferroic $LuMn_2O_5$

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Multiferroic RMn_2O_5 (R = rare earth ions) that exhibits both antiferromagnetic ordering and ferroelectricity, has been the subject of intensive research. Whereas YMn_2O_5 with nonmagnetic Y ions has also been extensively investigated to elucidate the role of Mn ions, the magnetic ordering of $LuMn_2O_5$ has not been studied in detail [1,2]. Our previous neutron diffraction study for $LuMn_2O_5$ showed that (1) magnetic ordering just below T_{N1} ~ 45 K is a two-dimensional incommensurate magnetic (2DICM) one characterized by the magnetic propagation vector $\mathbf{q}_M$ = (0.46, 0, 0.22), (2) as the temperature decreases, $\mathbf{q}_M$ starts to change with temperature at the ferroelectric ordering temperature, T_D = 35 K and a magnetic phase transition to a one-dimensional incommensurate magnetic (1DICM) phase with $\mathbf{q}_M$ = (0.45, 0, 0.25) occurs at T ~ 20 K. However, the commensurate magnetic (CM) phase with $\mathbf{q}_M$ = (0.5, 0, 0.25), which usually appears in RMn_2O_5 as an intermediate magnetic phase [1], was found to be absent in $LuMn_2O_5$. In this study, we performed magnetic structural analysis for single crystal of $LuMn_2O_5$ to understand the origin of the ferroelectric and magnetic features.

Single-crystal neutron diffraction experiments were performed using four-circle off centered diffractometer (FONDER). The wavelength of incident neutrons was 1.2483 Å. The dimensions of $LuMn_2O_5$ single crystal was 1.8 × 1.8 × 3.6 mm^3. Integrated intensities of nuclear and magnetic reflections were collected at T = 5 K by omega scan around each Bragg reflection with a typical scan speed of 1.0 and 0.1 deg/min., respectively. The number of measured nuclear and magnetic reflections were 358 and 279, respectively. Absorption correction was done using DabexN program. Determination of both crystal and magnetic structure was carried out using the FULLPROF program.

Figure 1 shows results of refinement for crystal structure at T = 5 K. Refinement with 22 parameters and reliable 177 nuclear reflections gave R(F) factor = 5.6%.

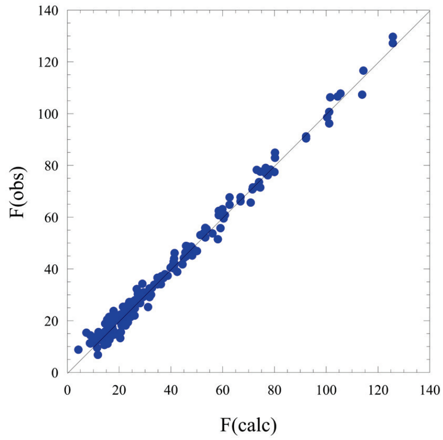

Fig. 1: Results of refinement for crystal structure at T = 5 K.

Refinement of magnetic structure at T=5 K with $\mathbf{q}_M$ = (0.45, 0, 0.25) was performed using 26 refinable magnetic parameters and reliable 98 magnetic reflections, with keeping nuclear-related parameters fixed. Several attempts by changing initial magnetic structure were performed and the best R(F) factor was approximately 13%; the results suggest that magnetic moments of Mn^{3+} ions are sinusoidally modulated, whereas those of Mn^{4+} ions are non-monotonically modulated. A relatively higher R(F) factor as compared with previous magnetic structural analysis for RMn_2O_5 (R=Y, Er, Ho) [1] is attributed to a difficulty of separating neighboring magnetic reflections, which modifies the magnitude of integrated intensities. Further refinement of magnetic structure is in progress.

[1] Y. Noda et al., J. Phys.: Condens. Matter 20 (2008) 434206.
[2] I Kagomiya *et al.*, Ferroelectrics 280 (2002) 131.