

Magnetic Structure of Transition Metal Oxides with LiNbO₃-Type Structure

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We have recently succeeded in fabricating a novel LiNbO₃-type ferrite with small Sc³⁺ occupying the A-sites, ScFeO₃, via the solid-state reaction at high pressure and high temperature. Magnetization measurements using a SQUID magnetometer revealed that the resultant materials exhibit a ferromagnetic ordering even at room temperature due to the strong magnetic interaction between Fe³⁺ ions via oxide ions. We have also attempted to determine the crystal structure of these compounds by synchrotron XRD and optical second harmonic generation (SHG) measurements. The SHG measurements indicated that these compounds crystallize in a polar structure of the space group *R3c* (No.161) at room temperature, which is the same as that in multiferroic perovskite BiFeO₃. In LiNbO₃-type ScFeO₃, the ordered arrangement of Sc³⁺ and Fe³⁺ ions in the rhombohedral lattice leads to the polar structure, which is different from the nonpolar corundum-type structure (*R3̄c*, No.167) where Sc³⁺ and Fe³⁺ ions are randomly distributed in the lattice. However, the structural refinement for the synchrotron XRD pattern was equally good by using either polar *R3c* or nonpolar *R3̄c* structural models, due to the similar atomic scattering factor between Sc and Fe elements.

To address this issue, we have measured the neutron powder diffraction (NPD) of pressure-induced ScFeO₃. We performed Rietveld refinement of NPD data at 300 and 5 K; the result at 5K is shown in Fig. 1. For both profiles, the magnetic diffractions were observed at the low angles and therefore the magnetic structure was considered in the refinement. When the occupancy factors, *g*, of Sc, Fe, and O were allowed to vary, they remained approximately unity (*g*(Sc) = 0.98(6), *g*(Fe) = 0.94(6), and *g*(O) =

1.10(7)), confirming the fully Sc/Fe ordering as well as the absence of oxygen deficiency.

The observed magnetic reflections are characterized with a propagation vector *k* = 0 so that the magnetic unit cell is identical to the chemical one. By considering different spin directions, the best fit was obtained when the spins are aligned within the *ab* plane (*R*_{wp} = 1.48%). The magnetic moment was found to be $\mu = 3.53(14)\mu_B/\text{Fe}$ at 300 K and $\mu = 3.71(10)\mu_B/\text{Fe}$ at 5 K, indicative of the long-range magnetic ordering of Fe³⁺ ions in the high-spin 3d⁵ configuration (*S* = 5/2). The weak ferromagnetic component evaluated from the magnetization curve at 5 K is 0.035 μ_B/Fe , corresponding to the canting angle of 0.2°. Determination of such a small canting angle is beyond the capability of NPD refinement: a trial refinement involving the canting angle gave a ferromagnetic component of 0.7 μ_B (equivalent to a 5.6° canting of 3.71 μ_B moment) within the *ab* plane, but without improving the *R* factors.

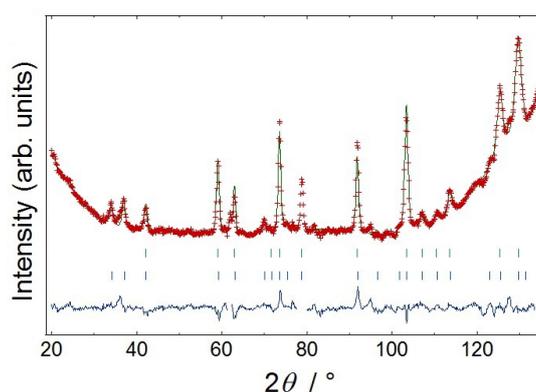


Fig. 1. NPD pattern of LiNbO₃-type ScFeO₃ at 5K