Magnetic structure in AFeO3 with Fe4+

Yamamoto T., Takeiri F., Kageyama H.
Kyoto University

There have been known a small class of perovskite oxides that contain iron in an unusually high valence state of Fe4+ like SrFeO3 and CaFeO3. Their electronic properties are peculiar. Normal Fe2+- and Fe3+-oxides such as Fe2+O and LaFe3+O3 are antiferromagnetic insulators governed by the Kanamori-Goodenough rule, while these Fe4+-oxides exhibit a shift toward metallicity and ferromagnetism. SrFe4+O3 is a cubic metal in the proper screw spin structure with propagation vector along [111] [1]. CaFe4+O3 shows a metal-to-insulator transition by charge-disproportionation to Fe3+ and Fe5+ at 290 K [2]. It is notable here that Fe3+L (t2g3eg2L, S=2), i.e., a charge transfer from O to Fe, is the realistic picture in these oxides [3]. The compounds with Fe4+ are thus quite attractive in terms of both experimental and theoretical views, but the knowledge of the Fe4+ physics is still far from satisfactory due to few model materials.

Until recently, perovskite BaFeO3 was only reported as thin film and the discussion about oxygen defects involves ambiguities and inconsistencies. However, three years ago, we reported BaFeO3 without any oxygen defect. BaFeO3 shows a proper screw spin structure along [100] having a different propagation vector from that of SrFeO3 [4]. In addition, we have found that this material exhibits a complete saturation magnetization (3.5 μ B) by the application of a tiny magnetic field (˜0.3 T). Thus, this material represents the first example to show ferromagnetism at ambient pressure. Subsequently, we have synthesized a powder sample of (Sr1-xBax)FeO3 ($0 < x < 1$) without any oxygen defect, and demonstrated magnetic phase diagram. We revealed a propagation vector [111] of (Sr1-xBax)FeO3 ($0 < x < 0.8$) (Figure 1b) [6]. Here, we want to emphasize is that the magnetic phase diagram in AFeO3 (A = Sr1-xBax) is very well consistent with that predicted by a theory demonstrated by Mostvoy (Figure 1a) [5]. However, there still exist unrevealed magnetic phase, A-AFM, in between A-HM (magnetic structure of BaFeO3) and G-HM (magnetic structure of SrFeO3).

In order to explore this phase and reveal the phase boundary, we carried out neutron diffraction measurements of (Sr1-xBax)FeO3 ($0.8 < x < 1$). We expected that satellite peak can be found if it is screw magnetism. We now analyze the experimental data.

We also performed a neutron diffraction for a perovskite oxynitride with the B site of Manganese. In (Sr1-xBax)FeO3, the screw magnetic structure appear without tilting of FeO6 octahedra, while a screw magnetic structure appears in the manganese perovskite oxynitride because of frustration of magnetic interactions due to a large tilting of MnO6 octahedra. In this machine time, we measured solid solution of the manganese oxynitride and antiferromagnetic oxide perovskite. The result indicates that the magnetic peak pattern changes from the screw magnetism changes to G-type antiferromgnetism (Figure 1c). This indicate that the screw magnetism is unexpectedly robust against atomic substitution. We now analyze details.

The powder neutron diffraction experiment was performed by using BT1 at NIST, US, which was transferred from HERMES with the approval of Institute for Solid State Physics, The University of Tokyo (proposal no. 14650), Japan Atomic Energy Agency, Tokai, Japan.

[1] T. Takeda et al., J. Phys. Soc. Jpn., 1972, 33, 967.
[2] S. Kawasaki et al., J. Phys. Soc. Jpn.,

1998, 67, 1529.
[3] A. E. Bocquet et al., Phys. Rev. B, 1992, 45, 1561.
[4] N. Hayashi, T. Yamamoto, H. Kageyama et al. Angew. Chem. Int. Ed., 50, 12547?12550 (2011).
[5] M. Mostovoy et al., Phys. Rev. lett, 2005, 94, 137205.
[6] N. Hayashi, T. Yamamoto, H. Kageyama et al. J. Phys. Soc. Jpn., 82, 113702 (2013).

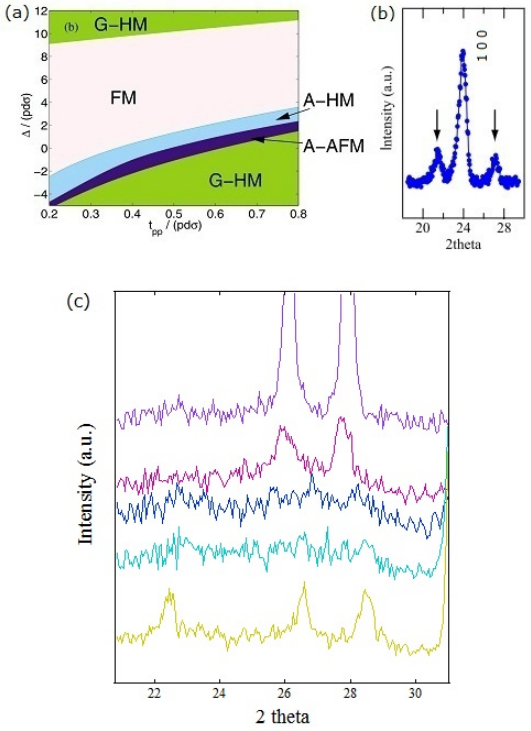

Fig. 1. Figure 1. (a) Referred from [5]. (b) Magnetic satellite peak around 100 in (Ba0.6Sr0.4)FeO3. The arrows correspond to magnetic peaks. (c) Low temperature diffraction patterns of manganese perovskite oxyniteride.