Structure Determination of Ordered Perovskite-type Oxides, Ca2MTeO6 (M = Mn, Co) by Neutron Diffraction

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The B site of the perovskites can accommodate two kinds of metal ions. The general formula of such a system is given as A2B ' B "O6, while the B ' and B " ions are either in an ordered or a disordered arrangement. Many researches including two kinds of magnetism ions, such as Sr2FeMoO6, have been carried out. However, there were few researches on high-oxidation cation of Te6+ in the B site. Ordered perovskite-type oxides, Ca2MTeO6 (M = Mn, Co), belonged to space group P21/n and were insulators at room temperature. However, their electronic conductivities tended large gradually with a rise of temperature. Ca2MnTeO6 and Ca2CoTeO6 showed antiferromagnetism, and their Neel temperatures were 10 K and 7 K, respectively. The effective magnetic moment of manganese ion was 5.8 _B while its valence was bivalence in Ca2MnTeO6.

Neutron diffraction measurements were performed above (50 K) and below (3 K) TN to determine the changes in the crystal and magnetic structures of Ca2MTeO6 (M = Mn, Co). Powder neutron diffraction patterns were recorded using the high efficiency and resolution powder diffractometer, HERMES, of Institute for Materials Research, Tohoku University, installed at the JRR-3M Reactor in JAEA (Tokai). The wavelength of a neutron incident is 1.82646(6) . The crystal and magnetic structures were analyzed using the Rietveld analysis program, RIETN2000.

The neutron diffraction patterns of two samples at 50 K were well fitted with a space group P21/n (No. 14) by Rietveld analysis. The lattice parameter of Ca2MnTeO6 and Ca2CoTeO6 were determined to be a = 5.4917(3) , b = 5.6678(3) , c = 7.8371(5) , β =90.251(4), and a = 5.4448(2) , b = 5.5899(2) , c = 7.7196(3) , β = 90.269(3), respectively. The lattice parameters became smaller with decrease of an ion radius in order of M = Mn, Co. At 3 K, some additional Bragg peaks were observed indicating the magnetic ordering for two samples. Fig. 1 shows the case of Ca2CoTeO6. These magnetic peaks could be indexed on the same crystallographic unit cell, the neutron diffraction patterns of Ca2CoTeO6 at 3 K were refined with a space group P-1 (No. 2). As a result, a direction of magnetic moment seems to turn to the direction deviated from c-axis. However, the refinement for Ca2MnTeO6 did not succeed.

References

[1] Y.J. Shan, Yoko Kanai, Keitaro Tezuka and Hideo Imoto, Advances in Science and Technology 45 2572 ? 2575 (2006).

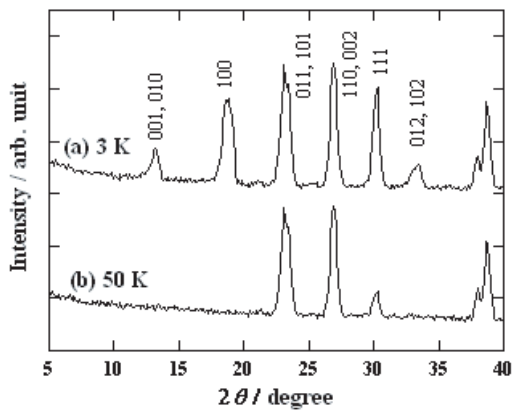

Fig. 1. Powder neutron diffraction patterns of Ca2CoTeO6 at (a) 3 K and (b) 50 K. Indices for magnetic reflections are based on crystallographic unit cell.