Morphotropic Phase Boundary and Magnetism in $BiFeO_3$-$SrTiO_3$

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Relaxor ferroelectrics are a class of materials characterized by a large dielectric constant over a wide temperature range, with the constant exhibiting gradual temperature dependence and significant frequency dependence. To explain these properties, the existence of "polar nanoregions" (PNRs), which is randomly oriented and very local polar region, is widely acknowledged. In this study, we focused on relaxor ferroelectrics having magnetic ions. Although few studies exist on such materials, relaxor-like behavior has been observed in systems such as (1-*x*)$BiFeO_3$-*x*$BaTiO_3$ and $LuFeMO_4$ (M=Co, Mg). We investigated the relationship between magnetism and relaxor dielectric properties by conducting macroscopic measurements and neutron experiments on (1-x)BiFeO3-xBaTiO3 and LuFeCoO4 single crystals [1,2].

In previous neutron diffraction experiments on (1-*x*)$BiFeO_3$-*x*$SrTiO_3$ single crystals, the anisotropic nuclear diffuse scattering induced by PNRs and the board magnetic reflections have been detected. It is expected that magnetic order is suppressed by PNRs, leading to the formation of nano-sized magnetic domains. In 2/3$BiFeO_3$-1/3$BaTiO_3$, superparamagnetism originated from these PNR-induced nanomagnetic domains was also observed, This novel relationship between magnetic and dielectric properties was also observed in $LuFeCoO_4$.

In this study, we focused on the morphotropic phase boundary (MPB) of the (1-x)$BiFeO_3$-x$SrTiO_3$ (BFO-xSTO) system to explore new candidate materials for relaxor ferroelectrics having the magnetic ions. From X-ray diffraction studies, the presence of an MPB in the BFO-xSTO system is expected at x = 0.3. This study aims to elucidate the relationships among the MPB, dielectric properties, and magnetic properties of BFO-xSTO by conducting a detailed analysis of its crystal and magnetic structures near the MPB.

We conducted powder neutron diffraction experiments on BFO-xSTO (x = 0.1, 0.3, 0.4, and 0.6) and a reference sample of 2/3$BiFeO_3$-1/3$BaTiO_3$ at the HERMES spectrometer. In the neutron diffraction profiles of BFO-0.4STO measured at 3 K and 300 K, the temperature-dependent magnetic reflections were clearly observed. These reflections are attributed to antiferromagnetic ordering. Notably, magnetic reflections persist even at 300 K, indicating the presence of magnetic order at this temperature. Furthermore, weak ferromagnetism observed in magnetization measurements suggests that the (1-*x*)$BiFeO_3$-*x*$SrTiO_3$ has the canted antiferromagnetic structure.

As the present measurements prioritized surveying a wide compositional range, they were limited to room-temperature data. In order to clarify the relationships among the MPB, dielectric properties, and magnetic properties, a detailed investigation of temperature dependence of the crystal and magnetic structures is necessary for future work.

[1] M. Soda, *et al.*, J. Phys. Soc. Jpn. **80**, 043705 (2011).
[2] M. Soda and T. Masuda, J. Phys. Soc. Jpn. **85**, 034713 (2016).