Crystal structure of $BiFeO_3$-$PbTiO_3$ Mutiferroic composite in the vicinity of MPB region

H. Kimura[1], S. Hagiya[1], Y. Noda[1], and S. Lee[2]
[1]*IMRAM, Tohoku University*
[2]*HANARO, KAERI, Korea*

Composite between two ferroelectric materials has attracted much attention because of the enhancement of dielectric as well as piezoelectric properties in the region of Morphotropic Phase Boundary (MPB). Among many composite materials, $BiFeO_3$-$PbTiO_3$ system has been intensively studied because the possible enhancement of multiferroic properties due to the antiferromagnetism of $BiFeO_3$ and ferroelectricity of $PbTiO_3$. Although structural studies have also performed already and reported so far, there are still some controversies about the magnetic and dielectric phase diagrams as well as about the existence of MPB region.

In the present study, we performed X-ray and neutron powder diffraction (XPD and NPD) studies of (1-x)$BiFeO_3$-$x$$PbTiO_3$ composite ($0 \leq x \leq 0.5$) to investigate the detailed crystal and magnetic structure as a function of x and to verify the existence of MPB region. Powder specimens were prepared by solid state reaction under $T = 900°C$ with 48 hours. XPD experiments were carried out at our laboratory and NPD experiments were performed at High Resolution Powder Diffractometer HRPD installed in HANARO reactor of KAERI. Crystal structure analyses were carried out by using both the XPD and NPD data simultaneously.

Figure 1 shows NPD profiles for several x of (1-x)$BiFeO_3$-$x$$PbTiO_3$. As shown in Fig. 1 (a), magnetic Bragg peak disappears around $x = 0.5$. On the other hand in Fig. 1 (b), superlattice peak indicating the $R3c$ space group disappears above x =0.33, suggesting that the structural phase transition from Hexagonal to tetragonal occurs. At $x = 0.33$, antiferromagnetic order and tetragonal structure coexist. Note that pure $PbTiO_3$ has a same tetragonal symmetry but non-magnetic, indicating that around $x = 0.33$, new structural and magnetic phase appear. However, no lower symmetry phases such as orthorhombic and monoclinic have been observed in the present study, suggesting that there is no MPB region in this system. Previous report suggests that at $x = 0$, the space group was identified as monoclinic Cc. However in our study, crystal structure of $x = 0$ can be solved with hexagonal $R3c$ which is higher symmetry than Cc. XPD and NPD experiments with higher resolution are required to settle these contradictions.

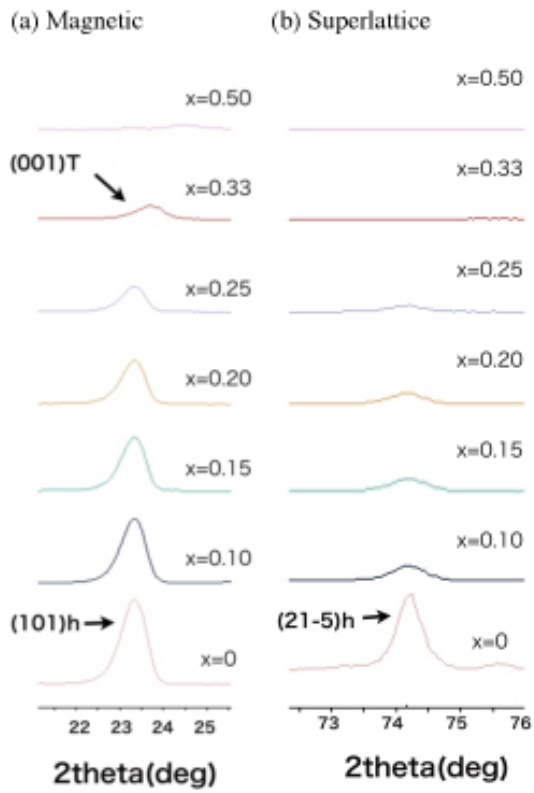

Fig. 1. NPD profiles as function of x for (a) magnetic reflection and (b) superlattice reflection