Correlation between crystal defects and the diffuse scattering in relaxor ferroelectric $(Na_{0.5}Bi_{0.5})TiO_3$

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Relaxor ferroelectrics have attracted considerable attention since the discovery of giant piezoelectricity in relaxor-based single crystals. $(Na_{0.5}Bi_{0.5})TiO_3$ (NBT) forms perovskite structure with two different ions Na^+ and Bi^{3+} at the A-site of ABO_3. A key-concept to understand the relaxor behavior is polar nanoregion (PNR), a local nanometer-sized region with ferroelectric polarization and atomic shift. Such an atomic shift in PNR was observed for a typical relaxor such as PMN and PZN as characteristic diffuse scattering. In NBT, we have revealed anisotropic diffuse scattering which extends along ⟨110⟩-directions. Recently, Noguchi *et al.* succeeded in suppressing Bi-defects in NBT single crystal by high O_2-pressure, and found larger polarizations than those in the crystal grown in air.[1] The purpose of the present work is to compare the diffuse scattering in crystals grown in different O_2 pressure to clarify the correlation between the diffuse scattering and ferroelectric properties. Neutron scattering experiments were performed on the triple-axis spectrometers HQR installed at the JRR-3 Guidehall of JAEA.

Figure 1 shows profiles of $(h, 1, 0)$ scan measured at room temperature. At $T \sim 300$ K, large diffuse scattering appears around (110) and extends along ⟨110⟩-directions. In order to compare diffuse scattering quantitatively, scattering intensities are normalized by sample mass. Profiles consist of sharp peak of (110) Bragg reflection and broad peak of diffuse scattering. Apparently, the diffuse scattering for O_2-10 atm crystal is smaller than that for O_2-0.2 atm crystal. From previous measurement, we found that this anisotropic diffuse scattering shows large temperature dependence and appears strongly along transverse direction, which suggests close correlation between the diffuse scattering and ferroelectric fluctuations. Since number of Bi-defects is expected to be smaller in O_2-10 atm crystal than O_2-0.2 atm crystal, the current results indicate that the diffuse scattering, in other words, PNR are pinned ferroelectric fluctuations at crystal defects.

References

[1] Y. Noguchi *et al.*, Jpn. J. Appl. Phys. 47(9B), 7623 (2008).

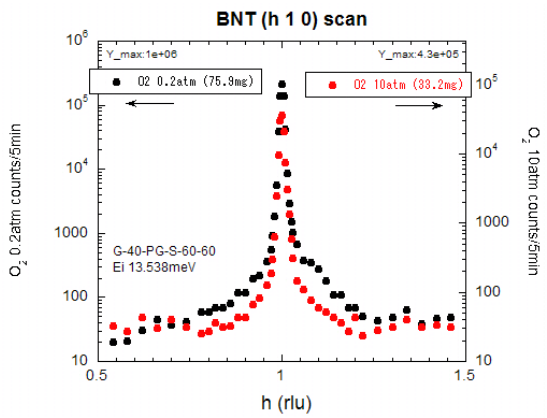

Fig. 1. Profiles of $(h, 1, 0)$ scan for NBT single crystals grown in air (black circles: O_2 0.2 atm) and high O_2 pressure (red circles: O_2 10 atm).