Time-Resolved Reciprocal Space Mapping of Ferroelectric Perovskites Under an Alternative Electric field

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 $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) is interesting as a potential lead-free piezoelectric and intriguing as the model system for the crystallography of perovskites. The average / local structures of NBT are frequently debated, while their relationship to the physical properties is unclear. The previous reports [1] of the monoclinic (Cc) average symmetry of NBT structure motivate for the in-depth studies of the processes, which are triggered to the polarization rotation and its implication for the physical properties. It is therefore particularly interesting to investigate the response of NBT to such external influences as electric field, change of a temperature or high-pressure, where polarization rotation may be observed and described.

The aim of this work is to probe the lattice response of NBT single crystal to an external electric field. We implemented stroboscopic time-resolved X-ray diffraction (descripted in [2]) to acquire high-resolution reciprocal space maps as a function of time and triangular- shaped 100 Hz cyclic electric field. We focused at the reciprocal space region around {004} reflection and carefully mapped it in-situ using state-of-the-art X-ray optics and synchrotron radiation source (P08 beamline at PETRA III and KMC-3 XPP at BESSY II). We observed that reciprocal space maps are separated into two peak components, where the separation magnitude follows electric field (see the figure). The similar radial separation of {001} was used as the evidence of non-rhombohedral (monoclinic) average symmetry in NBT [1]. We analysed this separation by fitting the observed two-dimensional intensity maps with a pair of two-dimensional Pseudo-Voigt functions to track the individual peaks independently. The results are discussed in the framework of the proposed monoclinic symmetry and allowed polarization rotation.

References

{1} S. Gorman, P.A. Thomas, J. Appl. Cryst., 43, 1409-1414 (2010) {2} H. Choe, J. Bieker, N. Zhang, A. M. Glazer, P. A. Thomas, and S. Gorfman, IUCrJ, 5, 417- 427 (2018)



Figure 1. Top: Time-resolved reciprocal space maps around {004} Bragg peak of Na0.5Bi0.5TiO3 single crystal under applied electric fields. Bottom: Dielectric P-E hysteresis loop.