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Electric field induced monoclinic distortion and polarization rotation in $Na_{0.5}Bi_{0.5}TiO_3$

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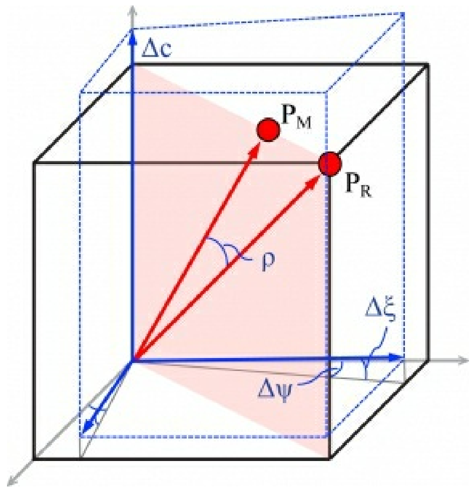
Na0.5Bi0.5TiO3 (NBT) perovskite-based ferroelectric has been in focus of attentive research during the last decade. NBT is interesting for materials scientists as a base for lead-free piezoelectrics: many NBT-dominated solid solutions exhibit morphotropic phase boundaries and strongly enhanced physical properties. Because of its rich phase transitions pattern [1], NBT is also an attractive model system for crystallography and physics of functionally distorted perovskites. The structure-property relationships in NBT are debated; the fine structure and symmetry of room temperature NBT are frequently reassessed. Many recent studies (e.g. [2]) suggest that the average periodic structure of NBT has monoclinic (Cc), rather than rhombohedral (R3c) symmetry. This symmetry lowering means that the vector of spontaneous polarization can be rotated, rather than extended / reverted only and that this rotation may trigger strong electro-mechanical response even in pure NBT crystals. Despite the strong technological interest to any properties enhancement mechanisms in perovskites, neither polarization rotation nor the mechanism of monoclinic lattice distortion are adequately investigated and understood.

Here we report in-situ single crystal X-ray diffraction for the direct probe of the electric-field-induced monoclinic distortion of the average NBT crystal lattice. We conceive this study as the first test of the monoclinic ferroelectric phase in "action". We implement the stroboscopic multi-channel data-acquisition system (as described in [3]) and use the high-resolution four-circle X-ray diffractometer (P08) at the PETRA III storage ring. We collect reciprocal space map around representative ({002}) Bragg reflection under cyclic (100 Hz) sub-coercive (< 14 kV / cm) electric field. We observe that the reflection splitting (due to the monoclinic lattice distortion and the presence of monoclinic domains) opens and closes as a function of electric field magnitude and direction. We found that the time and field-dependence of the sub-peaks positions in the reciprocal space maps can indeed be accounted by the continuous variation of the monoclinic lattice parameters (and therefore polarization rotation) as shown in the Figure. We found that one of the purely intrinsic (e.g. lattice distortion) piezoelectric coefficient reaches the value of 110 pC / N. This proves the importance of the monoclinic symmetry and polarization rotation for the enhancement of electromechanical response in NBT.

[1] Jones G.O., Thomas, P.A. (2002). Acta Cryst B58, 168-178.
[1] Gorfman S., Thomas, P.A. (2010). J. Appl. Cryst. 43, 1410 - 1414.
[2] Gorfman S. (2014). Cryst Rev 20(3), 210 - 232.



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