Transformation Stress Induced Metastable Tetragonal Twins in PZN-(7-8)%PT Single Crystals

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High-resolution synchrotron X-ray diffraction (HR-XRD) was used to investigate a two-phase coexistence of the rhombohedral (R) and a metastable tetragonal at room temperatyure 25 °C in unpoled $Pb(Zn_{1/3}Nb_{2/3})O_3$–(7-8)%$PbTiO_3$ (PZN-(7-8)%PT) single crystals of compositions close to the morphotropic phase boundary (MPB). Reciprocal space mappings (RSM) of H0L-plane and HK-plane scans were obtained from x-ray beam of 10 keV. All the diffraction patterns were obtained from (001) fractured surfaces of the single crystal. With two pairs of slits between the sample and the detetctor, the typical scattering vector resolution in the vertical scattering plane was set to ~ $1x10^{-3}$ nm^{-1}. PZN-7%PT (Fig. 1a) and PZN-8%PT (Fig. 1b) reveal a single broad R peak at L =2.000. In contrast, diffraction peaks lying in other Bragg's positions besides the L = 2.000 were detected detected in the RSMs shown in Figs. 1(c) and 1(d), which were taken from different samples prepared from the same wafers. Judging from their Bragg's position, the peaks at L = 2.010-2.016 are likely to arise from phases other than the *R* phase (L = 2.000). Since their Bragg's position coincides with that of the $(100)_T$ phase, one plausible room temperature structure of PZN-(7-8)%PT single crystal is thus a (R+T) phase mixture. T denotes the tetragonal phase. Alternatively, one may also assign the diffraction patterns to that arising from one of the monoclinic (M) phases.

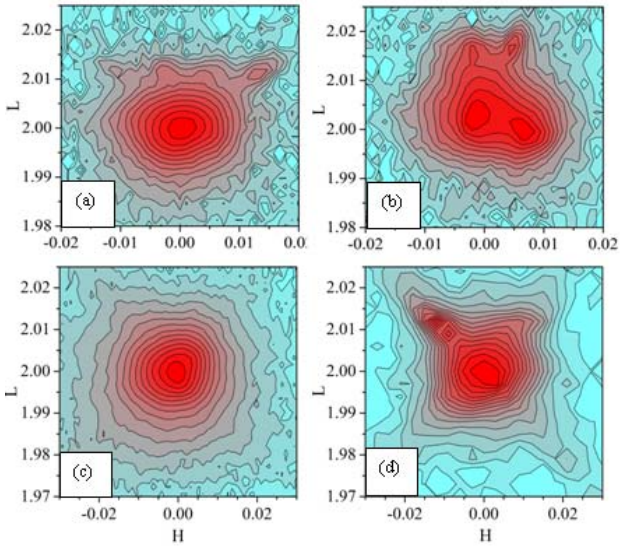

Fig. 1: Room temperatire RSMs of H0L-plane scan of unpoled (a) and (b) PZN-7%PT, and (c) and (d) PZN-8%PT.

By means of HK-plane scan, the high resolution of the x-ray beam in BL17B1 confirms a four-fold symmteric $(100)_T$ domains ($\Delta\omega \neq 0^o$) with 45° (110) twin boundaries at L = 2.010 (Fig. 2a), while at L = 1.980 (Fig. 2c) a four symmetry ($\Delta\omega \neq 0^o$) and one central ($\Delta\omega = 0^o$) peaks corresponding to both twinned and non-tilted $(001)_T$ domains were detected. The diffuseness of the $(001)_T$ diffractions in the figure may be attributed to the small amount (variant) of $(001)_T$ domains present in the sample. Meanwhile the HK-plane scan at L = 2.000 (Fig. 2b) reveals a single R diffraction peak.

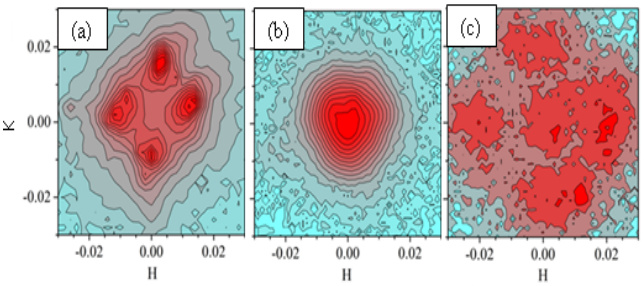

Fig. 2: Room temperature RSMs of HK-plane scan of unpoled PZN-8%PT at (a) L = 2.010, (b) L = 2.000, and (c) L = 1.980.

Our investigations indicate that the room temperature T phase in PZN-(7-8)%PT single crystals is a metastable phase stabilized by the transformation-cum-cooling stress in the crystal. This is manifested by the "missing" $(001)_T$ diffraction peaks from (00L) planes on the fractured surface, a result attributed to the stress relaxation effect in the surface layer of the fractured crystal causing the meastable $(00l)_T$ domain in the surface layer to transform to the equilibrium rhombohedral phase. The above difficulty has been resolved by making HK-plan scans on the same samples.