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**New Ground State of Relaxor Ferroelectric  $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$**

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**Introduction:** Relaxor ferroelectric materials with extremely high piezoelectric responses are of great interest to both the scientific and industrial communities [1]. Among those the lead perovskite system  $(1-x)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - $x\text{PbTiO}_3$  (PZN-xPT) has been studied extensively, due to its extraordinary piezoelectric properties near the morphotropic phase boundary (MPB) [2,3]. High energy x-ray diffraction studies on  $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$  (PZN) single crystals show that the system does not have a rhombohedral symmetry at room temperature as previously believed [3]. The new phase (X) revealed by our measurements gives Bragg peaks similar to that of a nearly cubic lattice with a slight tetragonal distortion. The Bragg profile remains sharp with no evidence of size broadening due to the polar micro-crystals (MC). On the other hand, studies on an electric-field poled PZN single crystal clearly indicate a rhombohedral phase at room temperature.

**Methods and Materials:** Both electric-field poled and unpoled PZN single crystals were investigated using x-ray diffraction. The crystals are 3x3x1 mm in size and the surfaces of the platelets are (111) crystal planes.

**Results:** 67 keV x-ray diffraction results from the poled PZN single crystal are shown in the top panel of Fig.1. Mesh scans in reciprocal space around the pseudocubic {111} reflections were performed, by doing a series of  $\theta$ -scans at a set of  $2\theta$  values around the pseudocubic {111} reflections. As expected for a rhombohedral structure, the reflections occur at different  $2\theta$ s. Based on the positions the peaks, the rhombohedral lattice parameters can be obtained:  $a=4.0608 \text{ \AA}$ , and  $\alpha=89.935^\circ$ . Weak (111) peak is likely due to a small part of the skin which is not fully poled.

Results from the unpoled PZN single crystal are, however, entirely different. In the lower panel of Fig.1, we show four mesh scans at the pseudocubic (111),(-111),(-1-11), and (-11-1) reflections for the unpoled PZN single crystal, using high energy (67 keV) x-rays. Analysis of the data show that all four {111} reflections have similar d-spacings within 0.05%. The four {111} mesh scans provide the key evidence that the structure of the unpoled PZN single crystal is not rhombohedral as previously believed. To further identify this phase, we performed similar mesh scans at the pseudocubic (100), (010), and (001) reflections. Our results show that the c-axis is about 0.1% longer than the a-and b-axes. However, we did not observe any peak splitting at the {100} reflections corresponding to the tetragonal distortion. This suggests that the system have a nearly cubic symmetry with a slightly tetragonal (T) type distortion, but the true symmetry can only be determined by detailed measurements and analysis of Bragg peak intensities.

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Figure 1: Mesh scans taken around pseudocubic  $\{111\}$  positions of the poled (top frame) and unpoled (bottom frame) PZN single crystals. The x-ray energy is 67 keV. The intensity is plotted in log scale as shown by the scale bar on the right side. Units of axes are multiples of the pseudocubic reciprocal lattice vector  $(111)$   $|\tau_{111}| = \sqrt{3}2\pi a_0$ .

