Symmetry determination of piezoelectric
(1-x)Pb(Mg_{1/3}Nb_{2/3})O_3-xPbTiO_3 single crystal near morphotropic phase boundary

KYOHYUN KIM, DAVID PAYNE, JIAN-MIN ZUO, University of Illinois, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING COLLABORATION — The symmetry of (1-x)Pb(Mg_{1/3}Nb_{2/3})O_3-xPbTiO_3 single crystal (PMN-xPT) is investigated at the morphotropic phase boundary with x=31%. The XRD result indicates that the average symmetry of annealed PMN-31%PT single crystal is in close agreement with the monoclinic M_C (Pm) phase, but with strain. The local symmetry of PMN-31PT are then investigated at three different directions of [001]_C, [010]_C, [011]_C and [111]_C by using convergent electron diffraction (CBED) technique with a probe size of 2 nm. The dynamical theory is used to simulate the CBED patterns for the reported phases of PMN-xPT. The CBED results show that significant deviations of the experimental CBED patterns from the simulations. The deviations in the CBED results are considered as a result from a local distortion induced by the different B cations of Mg^{2+}, Nb^{5+} and Ti^{4+}. The local symmetry of PMN-31%PT is not defined by any reported phases and the symmetry of PMN-31%PT seen in X-ray diffraction is the average of local structures.

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