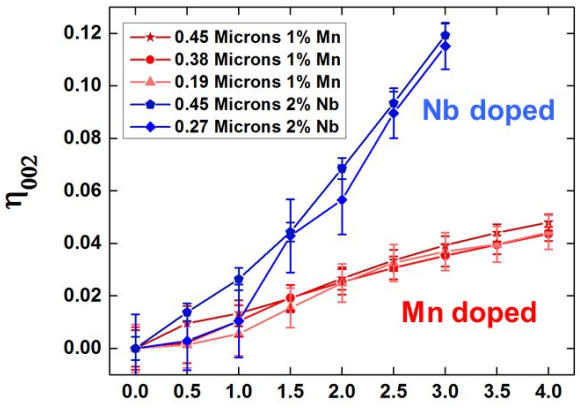
Domain Reorientation and Extrinsic Scaling Effects in Polycrystalline, {001} Textured $PbZr_{0.3}Ti_{0.7}O_3$ Thin Films

L.M. Denis[1], G. Esteves[2], J. Walker[1], H. Zhou[2], M. Wallace[1], C. Fancher[2], J.L. Jones[2], and S. Trolier-McKinstry[1] *
[1]Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA, USA
[2]Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC, USA
*Lyndsey Denis; Email: lmd342@psu.edu

Extrinsic scaling effects in the piezoelectric and dielectric responses were studied in polycrystalline, {001} textured $PbZr_{0.3}Ti_{0.7}O_3$ (PZT 30/70) thin film of varying thicknesses (0.2 to 1 µm thick), dopant type (2% Nb and 1% Mn) and release state (clamped, 25% released, 50% released and 75% released from the substrate). Ferroelectric/ferroelastic domain reorientation was measured using *in situ* synchrotron X-ray diffraction at the Advanced Photon Source. Domain reorientation of 90^0 domain walls was quantified for responses parallel to the applied electric field. As expected, with increasing field (to a maximum of 5 times the coercive field), it was observed that the 00*l* type domains are preferred parallel to the electric field. Little variation in the percent of 90^0 domain reorientation was observed in films of thicknesses below ~0.5 µm, suggesting that there exists a critical thickness below which 90^0 domain reorientation is suppressed. For a film thickness of 0.45 µm, PZT 30/70 thin films doped with 2% Nb exhibited two times more 90^0 domain reorientation than films doped with 1% Mn at 1.5 times the coercive field. The difference in the extent of 90^0 domain reorientation between films doped with 2% Nb vs. 1% Mn increases as the applied electric field increases, seen in the figure below. Additionally, 90^0 domain reorientation in {001} textured PZT 30/70 thin films of various thicknesses was studied by quantifying the contribution of substrate clamping on the extrinsic size effects. The degree of substrate clamping was varied from 0% (fully clamped to the substrate) to 75% released from the substrate, i.e. 75% of the film's electroded area is released from the substrate. This was accomplished by dry etching a ~100 µm diameter trench in the silicon substrate beneath the electroded area using XeF_2 gas. The results in terms of the thickness dependence of extrinsic size effects for both donor and acceptor doped PZT films will be discussed and compared with low field Rayleigh analysis.



The volume fraction of reoriented 002 domains (η_{002}) for different thicknesses and doping type (1% Mn and 2% Nb) of polycrystalline PZT 30/70 thin films under applied electric fields up to 4 times the coercive field (E_c).