Temperature Dependence of Field-responsive Mechanisms in Lead Zirconate Titanate Investigated Using Laboratory X-ray Diffraction

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A custom laboratory diffractometer stage capable of simultaneous temperature and electric field measurements was fabricated and validated for studying the field responsive mechanisms of ferroelectric materials (*i.e.* ferroelectric/ferroelastic domain wall motion, piezoelectric lattice strain, and polymorphic phase transitions). The stage was demonstrated by measuring $PbZr_{1-x}Ti_xO_3$ (PZT) based materials, a commercially available PZT and 1% Nb-doped $PbZr_{1-x}Ti_xO_3$ ($0.44 \leq x \leq 0.50$) ceramics, over a temperature range of 25C to 250C. The degree of non-180 domain alignment (η_{002}) of PZT as a function of temperature and composition was quantified. η_{002} of the commercially available PZT ceramic was found to increase exponentially with temperature. The increase in degree of domain alignment, $\Delta\eta_{002}$, with temperature can be expressed well by the Arrhenius relationship. The activation energy for thermally activated domain wall depinning process in PZT was found to be 0.47 eV. Additionally, a field-induced-phase transition in 1% Nb-doped $PbZr_{0.56}Ti_{0.44}O_3$ (PZT56/44) was observed at 250°C. Substantial change in the ratio of rhombohedral-tetragonal phase fractions was observed in the PZT 56/44 after the electrical cycling. The tetragonal phase fraction was increased from 23.5% to 65.3% after electrical cycling. The induced tetragonal phase, at 250°C of PZT 56/44, underwent a large amount of domain switching (η_{002} = 0.45 at 1.75kV/mm). These *in situ* structural details as a function of electric field, and over a wide temperature range, can provide the fundamental information necessary to understand these materials in their technological application.