

## **X-RAY and NEUTRON DIFFRACTION ANALYSIS OF Nb-DOPED AND UNDOPED PZT 95/5**

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Pb(Zr<sub>0.95</sub>Ti<sub>0.05</sub>)O<sub>3</sub>, often referred to as "PZT 95/5", resides near the ferroelectric-antiferroelectric phase boundary in the PbZrO<sub>3</sub>-PbTiO<sub>3</sub> phase diagram. It has been observed that undoped PZT 95/5 transforms from a ferroelectric compound (R3c) to an antiferroelectric phase upon cooling to approximately -100C. On the other hand, a small fraction of Nb-doping stabilizes the R3c phase to temperatures well below the -100C range. This transition suppression and the consequential structural aspects for each composition are the motivation of our investigation of these two compositions. Time-of-Flight neutron diffraction analyses of both PZT 95/5 and Nb-doped composition have been accomplished utilizing the High-Pressure-Preferred-Orientation (HIPPO) powder neutron diffractometer at LANSCE. Pressed and sintered pellets of each composition were cooled and reheated *in-situ* to measure the structural changes across the transitional temperature regions. Structural refinements at each temperature region were completed using the GSAS Rietveld Refinement software.

In the process of our investigation, we have observed a new ordering of PZT 95/5 in the temperature range -50C to 200C. We have modeled undoped PZT 95/5 at room temperature as a super-cell with twice the a-axis length of the typical reported R3m phase. This new cell was diagnosed based on small peaks observed in the neutron diffraction spectra. We have also observed these weak reflections via high-temperature XRD. Our observations indicate that PZT 95/5 is in the new super-lattice R3m structure at room temperature, and transitions to the R3c cell upon cooling to -50C. Nb-doped PZT 95/5 displays the R3c structure at room temperature and transforms to the R3m super-cell upon heating above 50C. The R3m phase remains stable for both doped and undoped PZT 95/5 until the paraelectric transition to cubic Pm3m symmetry at approximately 200C.

\*Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

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