

## Local Atomic Structure of Ferroelectric PZT.

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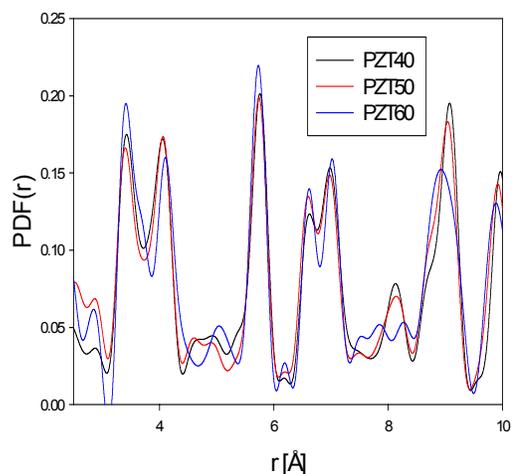
**Introduction:** The perovskite-like solid solutions of  $\text{PbZrO}_3$ - $\text{PbTiO}_3$  (PZT) are applied as solid-state actuators that couple strain to electric response and are of particular interest in under-water applications/warfare like sonars. The PZT Zr rich solid solutions are anti-ferroelectric below 250 C and up to 7% of  $\text{PbTiO}_3$  in orthorhombic  $\text{Pbam}$  structure. Higher content  $\text{PbTiO}_3$  solutions are ferroelectric. PT-PZ phase diagram is characterized by the almost vertical morphotropic phase boundary [1] at 48-52% of PT, which separates Zr rich rhombohedral region ( $R3m$  and  $R3c$  depending on temperature and Ti content) from tetragonal Ti rich region ( $P4mm$ ). At this phase boundary the solid solutions of PZT exhibit exceptionally high, stable over wide range of temperatures piezoelectric response. The extremely high electromechanical coupling observed in this region has been related to the morphotropic boundary, however, microscopic origin has never been proposed. Similarly the driving force of the structural transition is not well understood. Recently high-resolution x-ray diffraction study of the PZT sample at the morphotropic phase boundary at low temperatures revealed previously unknown monoclinic phase  $\text{Cm}$  (1).

**Methods and Materials:** We have studied three PZT compositions near the phase boundary with  $\text{Zr}=0.4, 0.5$  and  $0.6$ . Powder samples were enclosed in the Displex and cooled down to 20-35 K degree. Monochromatic scattering at  $E=23$  keV was done in the reflection geometry. Data was corrected for background, absorption and multiple scattering. Structure factor was normalized at high scattering vector and by Fourier transformation atomic pair distribution function (PDF) was obtained.

**Results:** The PDF of PZT with different composition is shown in the **Figure 1**. It should be noted that in the x-ray diffraction relatively high weight is coming from heavy (high Z) atoms. Therefore the pair distribution function obtained in the x-ray experiment describes mostly Pb and Zr with small contribution from Ti and oxygen atoms. It is seen that beyond 3 Å the PDF are very close to each other. This result suggests that local atomic arrangements of Pb and Zr do not change significantly when crossing from rhombohedral to tetragonal phase through the morphotropic boundary.

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**References:** B. Noheda *et al.*, Appl. Phys. Lett. 74, 2059 (1999)



**Figure 1.** Atomic pair distribution function of  $\text{Pb}(\text{ZrTi})\text{O}_3$