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Local Study on the Composition and Temperature Induced Structural Change of PZT

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The crystal structure and its relationship with the high piezoelectric performance of PbZr1-xTixO3 (PZT) have been studied for years, especially near the morphotropic phase boundary (MPB). Now the bridging monoclinic Cm phase in the MPB separating the not-group-subgroup-related R3c and P4mm has been widely accepted. However, in recent high-resolution powder diffraction experiments and Rietveld refinement analyses, the presence of the monoclinic Cm phase was found across the whole composition from the MPB to the rhombohedral region. Around the MPB, the structure seems to become more complicated, with a mixture of three phases[1]. It was also found that the local structure of PZT can be different from its average structure by examining the anisotropic displacement ellipsoids of both Pb and O: 1) the Pb atoms in the rhombohedral phase are displaced away from the threefold symmetry axes to create locally monoclinic symmetry that averages out to form an overall rhombohedral symmetry[2]; 2) at high temperature, the local effect of the low-temperature oxygen octahedra tilts remained even in the cubic phase[3]. In order to better study the local structures of PZT, we have carried out a series of high-resolution neutron diffraction experiments on both powder samples using Pair Distribution Function (PDF) analysis and single crystal samples using Diffuse Scattering (DS) analysis. The difference between the average and local structures is confirmed. The local distribution of the Pb displacements directions are plotted out for different compositions in PZT (x = 0.20, 0.30 and 0.40), which reveals on approaching MPB, the Pb atoms are tend to displace on one monoclinic mirror plane forming a macroscopic monoclinic phase. This is the first time that the local monoclinic short range order in Zr-rich PZT has been observed.

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