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Pressure-induced FE to AFE Phase Transition of PZT95/5-2Nb: A Neutron Diffraction and Dielectric Study.

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Zr-rich, Nb-doped lead zirconate titanate powder and ceramic samples with composition near $Pb_{0.99}(Zr_{0.95}Ti_{0.05})_{0.98}Nb_{0.02}O_3$ (known as PZT95/5-2Nb) have been studied in the range of hydrostatic pressure 0 - 6.2 kbar and temperature 10 - 295K by time-of-flight neutron diffraction and dielectric measurements. At 295K the diffraction study shows that the sample undergoes a sharp phase transition from the rhombohedral ferroelectric R3c phase ($F_{R(LT)}$) to the antiferroelectric orthorhombic Pbam phase (A_O) at 2.1 kbar; at 200K this transition occurs at 1.1 kbar. The transformation is incomplete: after the initial sharp drop of the $F_{R(LT)}$ content, 20% of the sample remains in this low pressure phase. Above the transition, the fraction of the $F_{R(LT)}$ phase, which exists as a minority phase in the high pressure A_O phase, continues to decrease, but even at our highest pressure of 6.2 kbar, ~8% of the sample remains in the $F_{R(LT)}$ phase. The 10% volume contraction at the $F_{R(LT)}$ –to- A_O transition unexpectedly results in the retained minority $F_{R(LT)}$ being anisotropically "clamped", with its a axis slightly expanded and c axis contracted at the phase transition. On pressure release, 26% of the $F_{R(LT)}$ phase remains at ambient pressure in the "clamped" state because of the majority A_O phase. The most pronounced structural changes of the $F_{R(LT)}$ result from temperature changes rather than pressure and these involve the B metal site oxygen octahedra distortions.

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