New aspects in the (x-P-T) phase diagram of $Pb(Zr_{1-x}Ti_x)O_3$ materials

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It is becoming quite apparent that fine details of the crystal structure have a strong influence on the properties of ferroelectric lead-based perovskite solid solutions. In particular, both temperature and pressure can induce significant lattice distortions and structural modifications, thus affecting the overall electronic, dielectric, ferroelectric and piezoelectric performances of PZT materials.
In order to complete the structural investigation of the PZT solid solution and bring new insights on the (x,P,T) phase diagram near the morphotropic phase boundary (MPB) and in the Ti-rich region, X-ray and neutron diffraction as well as Raman spectroscopy measurements were performed in the 0-20 GPa pressure range and 10-350 K temperature range. The local structural information extracted from these complementary techniques have confirmed the extended stability of the monoclinic phase at high pressure and low temperature, and revealed the existence of a new high-pressure induced triclinic structure. The present work establishes the basis for an up-to-date (x,P,T) phase diagram, revealing that both low temperature and high pressure can tune the MPB in the (x-T) and (x-P) planes to include compositions that do not normally lie in the MPB region. In the current technological and commercial competition towards higher performances, the comprehensive study of the variation of the crystal structures and accompanying atomic displacements as a function of pressure and composition appears as an attractive way for the design of reliable PZT-based devices with optimized properties.