Temperature- and Pressure-Induced Structural Changes in the Perovskite-Type Relaxor Ferroelectric PbSc0.5Ta0.5O3

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Relaxors are ferroelectrics with a broad, frequency-dependent maximum of the dielectric permittivity over a temperature range and a number of technological applications. The majority of relaxors are Pb-based perovskite-type oxides of the general formula (Pb,A)(B,B)O3. Relaxor behavior is related to the rather complex nano-scale structure of these materials. Polar nanoclusters occur at a characteristic temperature TB, which is well above the temperature of dielectric-permittivity maximum TM. At low temperatures the ferroic distortion of the unit cell is very weak and often unresolved by diffraction methods. The mechanism of nucleation and growth of polar nanoclusters, as well as the reason for the suppression of long-range ferroelectric ordering below TM, is not yet clear. We applied in situ temperature/pressure Raman scattering as well as in-house and synchrotron x-ray diffraction to PbSc0.5Ta0.5O3 in order to gain new insights into the structural features of Pb-based perovskite-type relaxor ferroelectrics. The temperature evolution of phonon anomalies and the pseudo-cubic unit cell parameter reveals the existence of a characteristic temperature T* between TB and TM. The temperature range between TB and T* is characterized by a coupling of adjacent off-centred BO6 octahedra to form initial polar clusters, while the range between T* and TM is characterized by a coupling between off-centred B-cations from adjacent polar clusters. Off-centred Pb atoms exist even above TB and their length of coherence governs the coupling between polar regions comprising B-cation off-centre shifts and, consequently, directs the formation of the ferroelectric state to a proper, long-range ordered or non-ergodic, relaxor state. The pressure evolution of the structure of PbSc0.5Ta0.5O3 also demonstrates the key role of off-centred Pb2+ for the ferroic state in this class of materials. PbSc0.5Ta0.5O3 undergoes a pressure-induced phase transition involving elastic softening. The critical pressure is associated with a decoupling of the displacements of the B-site and Pb cations in the existing polar nanoregions, leading to the suppression of B-cation off-center shifts and enhancement of the ferroic distortion in the Pb-O system.
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