

Temperature- and Pressure-Induced Structural Changes in the Perovskite-Type Relaxor Ferroelectric PbSc_{0.5}Ta_{0.5}O₃

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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 T_B , which is well above the temperature of dielectric-permittivity maximum T_m . 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 T_m , is not yet clear. We applied in situ temperature/pressure Raman scattering as well as in-house and synchrotron x-ray diffraction to PbSc_{0.5}Ta_{0.5}O₃ 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 T_B and T_m . The temperature range between T_B and T^* is characterized by a coupling of adjacent off-centred BO₆ octahedra to form initial polar clusters, while the range between T^* and T_m is characterized by a coupling between off-centred B-cations from adjacent polar clusters. Off-centred Pb atoms exist even above T_B and their length of coherence governs the coupling between polar regions comprising B-cation off-center 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 PbSc_{0.5}Ta_{0.5}O₃ also demonstrates the key role of off-centred Pb²⁺ for the ferroic state in this class of materials. PbSc_{0.5}Ta_{0.5}O₃ 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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Abs. No. **93**
Meeting: **DMG 2008**
submitted by: **Mihailova, Boriana**
email: **mi0a007@uni-hamburg.de**
date: **0000-00-00**
Req. presentation: **Vortrag**
Req. session: **S08**