

High-pressure Raman spectroscopy of Ba-doped $\text{PbSc}_{0.5}\text{Ta}_{0.5}\text{O}_3$ and $\text{PbSc}_{0.5}\text{Nb}_{0.5}\text{O}_3$ relaxor ferroelectrics

Welsch, Anna-Maria¹ Mihailova, Boriana¹ Gospodinov, Marin² Güttler, Bernd³ Bismayer, Ulrich¹

¹Universität Hamburg Grindelallee 48, 20146 Hamburg, Germany ²Institute of Solid State Physics, Tsarigradsko Chausse 72, 1784 Sofia, Bulgaria ³PTB Braunschweig, Bundesallee 100, Braunschweig, Germany

Relaxors are ferroelectric materials showing remarkably high dielectric permittivity, diffuse phase transition over a temperature range and significant frequency dispersion of the dielectric permittivity as a function of temperature. The number of applications relaxor ferroelectric materials have in new technologies, has been significantly increased in recent years and expanding further. Practical needs forced many different approaches in the research on relaxors in order to better understand their unique nature. This type of materials was found mainly among the perovskite-type lead-containing oxides with the general formula $(\text{Pb}, \text{A}')(\text{B}', \text{B}'')\text{O}_3$. The structure of these compounds is very flexible and allows introducing cations of different valence and ionic radius in both A- and B-sites. The existence of various cations at the same crystallographic site has a considerable impact on relaxor properties, since the charge imbalance creates local electric fields which hinder the development of long range ferroelectric order. Off-centre shifts of both types of cations exist in relaxors at ambient pressure and temperatures above the temperature of the dielectric permittivity maximum. Hence, polar nanoregions are typical of relaxors in a wide temperature range although the average structure remains non-polar, cubic.

High-pressure studies allow better understanding of the structural complexities in relaxors, because mechanical loading can slow down the dynamic structural fluctuations existing above and in the vicinity of T_m . Pressure studies on relaxor structure are relatively rare and up to now mostly relaxors of the general formula $\text{PbB}'_{1/3}\text{B}''_{2/3}\text{O}_3$ have been focused upon.

$\text{PbSc}_{0.5}\text{Ta}_{0.5}\text{O}_3$ (PST) and $\text{PbSc}_{0.5}\text{Nb}_{0.5}\text{O}_3$ (PSN) are relaxors of type $\text{PbB}'_{1/2}\text{B}''_{1/2}\text{O}_3$, which undergo a phase transition to a normal ferroelectric state. We studied the local structure and the effect of A-site doping by applying high pressure Raman scattering on single crystals of stoichiometric PST and PSN as well as the Ba-doped varieties, $\text{Pb}_{0.78}\text{Ba}_{0.22}\text{Sc}_{0.5}\text{Ta}_{0.5}\text{O}_3$ (PBST) and $\text{Pb}_{0.92}\text{Ba}_{0.07}\text{Sc}_{0.51}\text{Nb}_{0.49}\text{O}_3$ (PBSN). Raman spectroscopy is very sensitive on short time/length scale and enables the observation of local structural transformations. We conducted Raman spectroscopic experiments at room temperature from ambient pressure up to 10 GPa. Of special interest was the evolution of the spectral peaks originating from (i) the Pb-localised Raman-active F_{2g} mode near 55 cm^{-1} ; (ii) the B-site cation-localised IR-active F_{1u} mode that generate anomalous Raman scattering near 240 cm^{-1} due to the off-centring of the B-cations, (iii) the Raman-active A_{1g} mode near 830 cm^{-1} related to the BO_6 octahedral stretching (all assigned according to the $Fm-3m$ symmetry). Complementary x-ray diffraction studies were conducted to compare the pressure-induced changes in the local and the average structure. The presence of Ba at A-sites alters the way PST and PSN structures adjust to the elevating pressure and the critical points at which the corresponding pressure-induced phase transitions take place.

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submitted by: **Welsch, Anna-Maria**
email: **anna.maria.welsch@uni-**
hamburg.de
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