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Domain wall dynamics, local diffusion, and phonons in a lead-free relaxor ferroelectric

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Ferroelectric materials are used in many applications, e.g. as ultrasonic transducers. The most commonly used ferroelectrics like Pb_xZr_(1-x)TiO_3 contain lead, which makes them potential hazards for human health and our environment. Consequently, lead-free ferroelectrics are currently being developed with the aim of replacing the lead-containing materials in the medium term. However, the microscopic mechanisms which determine the ferroelectric properties have to be identified before the properties can be optimized for specific applications.

The ferroelectric parameters of solid solutions near the morphotropic phase boundary of (1-x)Bi_(1/2)Na_(1/2)TiO_3-xBaTiO_3 around x = 0.06 were cited as d_33 = 125 pC/N and ε_33^T / ε_0 = 580. These values are comparable to those of commonly used lead-containing ferroelectrics. The diffuse x-ray scattering experiments performed by our group revealed features related to the local octahedral tilting order and stacking faults between different tilt domains. These features react strongly to the application of an external electric field and their temperature dependence is clearly correlated with the dielectric permittivity. Potential phonon anomalies may also help to identify the mechanisms leading to the good ferroelectric properties.

We investigated the temperature dependence of the structural dynamics of a single crystal with x = 0.04 using inelastic and quasielastic neutron scattering. Most phonon branches are not well defined, but hints of possible anomalies are visible. The quasielastic scattering (QENS) was measured at different positions in reciprocal space, focusing on the field-dependent diffuse scattering. We observed a very strong temperature and Q dependence. This indicates that different mechanisms like enhanced domain wall mobility and local cation hopping strongly influence the dielectric properties in different temperature ranges.

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