follows that the width of the diffraction maximum in reciprocal space is proportional to the square root of the dislocation density, however the shape of the maximum strongly depends on the correlation of dislocation positions. The results were compared with dislocation curves obtained from the standard algorithm [1] using an upper cut-off radius. It has been demonstrated that for some of the correlation types (dislocation bunching and anti-bunching), similar results of the standard algorithm can be found for a suitably chosen cut-off radius, however the shape of the diffraction maximum for dislocations in subgrain boundaries cannot be approximated by the standard method.

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Keywords: diffuse x-ray scattering, dislocations, Monte-Carlo simulation

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Phase Transitions in the lead-free mixed perovskite piezoelectrics. Maxim Korablev-Dyson[a], Sergey Vakhrushev[b], Dmitry Chernyshov[c]. [a]*Saint-Petersburg State Polytechnical University, Russia.* [b]*Ioffe Physico-Technical Institute, Russia.* [c]*SNBL/ESRF,France.*
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Most of the high-performance piezoelectric materials, which are widely used in sensors, actuators and other electronic devices, are based on the lead containing perovskites (e.g. PZT – lead zirconate-titanate). High electromechanical properties of these compounds are usually attributed to the existence of so-called morphotropic phase boundary (MPB), i.e. nearly vertical phase boundary at the composition-temperature phase diagram. In the vicinity of this MPB the phase state is easily changed by small external action. Recently the efforts of the specialists all over the world got attracted to the development of the environmental friendly lead-free piezoelectrics with the electromechanical coupling close to that in PZT and related compounds. The Li doped mixed potassium-sodium niobates $Lix(K_{0.5}Na_{0.5})_{1-x}NbO_3$ (KNN:Li) are now considered as the most prospective systems for practical applications [1]. These materials demonstrate the MPB but the origin of this "easy" phase boundary remains unclear.
One of the reasons of the absence of the data on the lattice dynamics of KNN and doped KNN is difficulty of crystal growing. Recently our German collaborators have succeeded to grow high quality single crystals of KNN and Li-doped KNN. First results of the study of these single crystals were published in Ref.[2].We have performed the 3-d study of the diffuse scattering in the $Li_{0.02}(K_{0.5}Na_{0.5})_{0.98}NbO_3$. We have followed the temperature evolution of the 3-d scattering pattern on cubic-tetragonal-orthorhombic phase transformation. Due to the high luminosity of the instrument we have succeeded to do the measurements with the single domain (both in T and O phases) crystal. In cubic phases 3 "shining plane" in the diffuse scattering are seen corresponding to 3 ionic chain displacements in real space. On C-T phase transition one corresponding plane disappears. On T-O phase transition (MPB region) two remaining "shining plane" in the diffuse scattering disappear and C-T plane reappears (it is evident from evaluation of additionally performed IXS-measurements). It means that in the close vicinity of the transition point the crystal is effectively cubic again and its symmetry can be easily altered by weak external action. IXS data demonstrated that the phenomenon is dynamic in nature.

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Keywords: piezoelectrics, X-ray diffuse scattering, X-ray inelastic scattering

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Local order and diffuse scattering in ferroelectric oxides. M. Paściak, D. Goossens, R. Whitfield, R. Withers, T. R. Welberry. *Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia.*
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Ferroelectric materials are nowadays broadly employed as capacitors and transducers of different types, e.g. actuators. It is well known that important properties of a given material are the derivative of the degree of its structural order. It has been also known for decades, that local structure of ferroelectrics, can be studied via measurement of structured diffuse scattering [1]. The interpretation of the experiments has been disputed over the years, but there has been a recent revival of intrest due to the broad range of evidence of diffuse scattering for ferroelectric relaxors [2].
In this work we show recent experimental data for a number of ferroelectric materials acquired with different scattering methods: x-rays, neutrons and electrons. Some common features of the diffuse scattering patterns have been extracted and explained with the help of various atomistic simulation techniques [3]. These include Monte Carlo simulations, molecular dynamics and *ab-initio* techniques. The results are discussed in the context of (local) structure – property relationships with a special emphasis on mechanisms leading to the occurrence of a dielectric constant anomaly.

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Keywords: diffuse scattering, ferroelectrics, atomistic simulations

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Diffuse neutron scattering in high-temperature phase of relaxor $PbMg_{1/3}Nb_{2/3}O_3$. Roman Burkovsky[a], Sergey Vakhrushev[b], Kazuma Hirota[c], Masato Matsuura[c]. [a]*St-Petersburg State Polytechnical University, Russia* [b]*Ioffe Physical-Technical Institute, Russia.* [c]*Osaka University, Japan.*
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Relaxor ferroelectrics [1] are perovskite-like mixed crystals with random occupations of equivalent lattice positions by nonisovalent ions. These compounds have unusual and very promising dielectric and piezoelectric characteristics and present a challenge in interpreting of their properties from the point of view of microscopic structure and lattice dynamics. Below the characteristic Burns temperature T_d relaxors show strong butterfly-shaped temperature dependent diffuse scattering (DS) associated with formation of local polar