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.

[1] Krivoglaz M.A., *X-Ray and Neutron Diffraction in Nonideal Crystals,* Springer Berlin/Heidelberg 1995.

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

correlations known as polar nanoregions. Above T_d, in the paraelectric phase, a weak but definite longitudinal diffuse scattering is observed [2]. Its intensity is nearly temperature independent and it was initially suggested that this DS originates from weakly correlated ionic displacements due to short-range chemical ordering of Mg^{2+} and Nb^{5+} ions in B sublattice. At the same time it is naturally to suggest another mechanism assuming the scattering by elastic lattice deformations that are unavoidable in mixed crystals (Huang scattering).

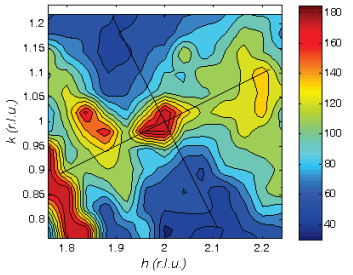

Fig 1. Map of diffuse scattering in (210) Brillouin zone.

We have measured 2-dimensional maps of diffuse scattering in model relaxor $PbMg_{1/3}Nb_{2/3}O_3$ in several Brillouin zones at T=650K where the butterfly-shaped diffuse component is absent. In low-symmetry zones (310) and (210) the DS has pronounced anisotropy and cannot be considered as purely longitudinal. For all experimentally studied zones we performed model calculations using formalism of Huang scattering [3]. It is shown that the observed anisotropy can be reproduced by model calculations of DS on elastic lattice deformations produced by simple cubic symmetry defects. Weak diffuse scattering intensity near zone centers indicates strong lattice deformations screening in real space due to high concentration of defects. It is shown that the weak satellite maxima near Bragg reflections observed in this and previous neutron scattering [2] studies can be described as effect of finite experimental resolution and do not evidence for superstructures or mesoscopic ordering.

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Keywords: Neutron diffuse scattering, Disordered ferroelectric oxides, Anisotropic elasticity

FA3-MS22-P07

Twins in $SrFe_{0.95}Mo_{0.05}O_{2.58}$: Debye Simulation of XRD Patterns. Svetlana Cherepanova[a], Ulyana Ancharova[b], Olga Savinskaya[b], Alexander Nemudry[b]. [a]*Boreskov Institute of Catalysis, Novosibirsk, Russia.* [b]Institute of Solid State Chemistry and Mechanochemistry, *Novosibirsk, Russia.*
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Mixed conducting compound $SrFe_{0.95}Mo_{0.05}O_{2.58}$ used as membrane material for oxygen separation in catalytic reactor possesses specific XRD pattern. It consists of intensive main peaks, which are correspond to cubic perovskite structure with $a_{per} = 3.930(1)$ Å, and weak superstructure ones (<2%). Some of these peaks are broader then main ones. Others have narrow top and wide bottom or asymmetric shape. $SrFeO_{2.5}$ is well known to have an orthorhombic brownmillerite structure, which can be derived from the cubic perovskite one by ordering of oxygen vacancies. Their cell parameters are connected as: $a_{bm} \approx a_{per}\sqrt{2}$, $b_{bm} \approx 4a_{per}$ and $c_{bm} \approx a_{per}\sqrt{2}$. Refinement gives $a_{bm} = 5.662(1)$ Å, $b_{bm} = 15.570(1)$ Å and $c_{bm} = 5.522(1)$ Å for cell parameters of $SrFeO_{2.5}$. Increase in Mo content (x) in solid solutions $SrFe_{1-x}Mo_xO_{2.5+1.5x}$ leads to gradual convergence of reduced cell parameters (see table).

x	$a_{bm}/\sqrt{2}$, Å	$b_{bm}/4$, Å	$c_{bm}/\sqrt{2}$, Å
0	4.004(1)	3.893(1)	3.905(1)
0.01	3.994(1)	3.895(1)	3.903(1)
0.03	3.974(1)	3.907(1)	3.904(1)
0.05	3.93(1)	3.93(1)	3.93(1)

Thus at x=0.05 all reflections can be indexed in orthorhombic cell with parameters $a_{bm} = c_{bm} = a_{per}\sqrt{2}$, $b = 4a_{per}$, where a_{per} is determined from main peaks. Such behavior of cell parameters and shape of XRD peaks can be explained by the formation of microstructure consisting of nanosized 90° twins. That results in matching of three equivalent and mutually perpendicular orthorhombic cells. To confirm this we simulated XRD patterns with use of Debye equation, which gives spherically averaged intensity scattered on model particle. There are no any restrictions on atomic arrangement of the particle. Any type of disorder can be taken into account when massive of atomic coordinates is created. Our model particles were constructed consisting of brownmillerite-type blocks of different sizes. From one block to other *b*-axis is rotated by 90°. Simulation of XRD pattern shows that such microdomain texture is suitable for $SrFe_{0.95}Mo_{0.05}O_{2.58}$ sample. We managed to fit the unusual shape of weak XRD peaks that was impossible by means of other methods of full profile analysis. Existence of mutually perpendicular domains is also confirmed by HREM.

Keywords: X-ray diffraction of defect structures, twins, diffuse scattering

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Single crystal structure determination from Bragg diffraction has become a largely routine operation. The information obtained is limited, however: It is the content of the crystallographic unit cell averaged over time and space. If a crystal structure shows disorder, some of the scattered intensity is lost from the Bragg peaks and distributed throughout reciprocal space as diffuse scattering. The interpretation of such scattering is far from routine.
We are developing software for analysing diffuse scattering from disordered single crystals whose average structure is (at least approximately) known. Disordered crystals are simulated and analysed. The model parameters used for crystal simulation are optimized with respect to experimental data.