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).

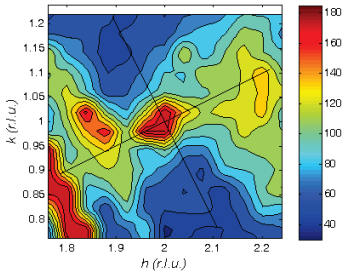

Fig 1. Map of diffuse scattering in (210) Brillouin zone.

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

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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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Software for interpreting diffuse neutron and X-ray scattering data. Michal Chodkiewicz[a], Hans-Beat Bürgi[a], Thomas Weber[b]. [a]*Institute of Organic Chemistry, University of Zürich, Switzerland.* [b]*Laboratory of Crystallography, ETH Zürich, Switzerland.*
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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.