

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).

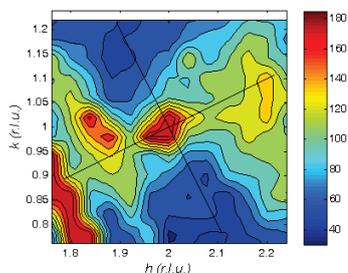


Fig 1. Map of diffuse scattering in (210) Brillouin zone.

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.

[1] L. E. Cross, *Ferroelectrics*, 76: p. 241-267., 1987. [2] H. Hiraka, S.H. Lee, P.M. Gehring, G.Y. Xu, and G. Shirane, *Physical Review B*, 70., 2004. [3] M. Krivoglaz, *X-Ray and Neutron Scattering in Nonideal Crystals*. 1996, Springer, Berlin.

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*Boriskov Institute of Catalysis, Novosibirsk, Russia.*

^b*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia.*

E-mail: svch@catalysis.ru

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 correspond to cubic perovskite structure with $a_{per} = 3.930(1)$ Å, and weak superstructure ones (<2%). Some of these peaks are broader than 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

Acknowledgements. This research was supported by grants of RFBR project № 08-03-00964-a and the Integration project №82 of SB RAS

FA3-MS22-P08

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.*

E-mail: michalc@oci.uzh.ch

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.

They include energy terms (for Monte-Carlo and other energy based simulations), joint probabilities (in crystal growth models) and parameters accounting for local distortions from the average structure. Models are constrained to show the symmetry of the average structure and of the observed diffuse scattering. Usage of a-priori chemical or structural knowledge is extensively supported. Various tools for analysis of the simulated crystals are provided.

As this type of calculations is known to be computationally demanding, especially if a global optimization of the parameters is performed, the software is targeted for use with supercomputers.

Keywords: diffuse scattering, software design, supercomputing

FA3-MS22-P09

The phase transition in the $(\text{NbSe}_4)_{10/3}\text{I}$ charge-density-wave system. J.Kusz^a, M.Zubko^a, A.Prodan^b, H.J.P. van Midden^b, J.C.Bennett^c, H.Böhm^d. ^a*Institute of Physics, University of Silesia, Katowice, Poland.* ^b*Jožef Stefan Institute, Ljubljana, Slovenia.* ^c*Department of Physics, Acadia University, Wolfville, Canada.* ^d*Institut für Geowissenschaften, University of Mainz, Germany*
E-mail: kusz@us.edu.pl

$(\text{NbSe}_4)_{10/3}\text{I}$ belongs to the $(\text{MX}_4)_n\text{Y}$ family of linear chain compounds. At room temperature it is a semimetal which changes at lower temperatures into a semiconductor [1]. The compound shows nonlinear transport properties with a charge density wave transition at 285K. A transmission electron microscopic study confirmed that the transition is of the Peierls type [2]. Single crystals of $(\text{NbSe}_4)_{10/3}\text{I}$ were grown from the elements by means of a transport reaction in a two-zone furnace. The Xcalibur four-circle diffractometer (Oxford Diffraction) was used for data collections in the temperature range 80-300 K. A reversible transformation from a tetragonal into a monoclinic lattice with a domain structure was observed on cooling through the Peierls transition.

Single crystal X-ray analysis performed at room temperature confirms that the structure of $(\text{NbSe}_4)_{10/3}\text{I}$ belongs to the space group $P4/mcc$ with cell parameters $a = 0.9464$ nm and $c = 3.1906$ nm. Its one-dimensional nature is characterized by NbSe_4 chains, aligned along the c axis. The niobium atoms are coordinated by Se antiprisms, stacked along the c axis in a screw-like arrangement. In accord with literature [3] the iodine atoms were found in two types of channels. In the first, running along the $[00z]$ direction, four iodine atoms are closely bonded to four selenium atoms, while in the channels along the $[\frac{1}{2}\frac{1}{2}z]$ direction only two iodine atoms are weakly bonded to eight selenium atoms in a square antiprismatic arrangement.

A weak diffuse scattering is detected perpendicular to the c^* direction in the entire temperature range examined. It is an indication of a short range order, which is present in both high and low temperature phases. Simulations of the disorder were performed with the DIFFUSE program package [4, 5], giving an insight into the real structure of $(\text{NbSe}_4)_{10/3}\text{I}$.

[1] Z.Z.Wang, P.Monceau, M.Renard, P.Gressier, L.Guemas, A.Meerschaut, *Solid State Commun.* 47(1983), 439. [2] C.Roucau, R.Ayrolesw, P.Gressier, A.Meerschaut, *J.Phys.* C17(1984), 2993. [3] A.Meerschaut, P.Gressier, L.Guemas, J.Rouxel, *J.Solid State Chem.* 51(1984), 307. [4] Th.Proffen, R.B.Neder, *J.Appl. Cryst.* 30(1997),

171. [5] R.B.Neder, Th.Proffen, *Difuse Scattering and Defect Structure Simulation*, Oxford University Press, 2008.

Keywords: charge density waves, diffuse X-ray scattering, one-dimensional conductors

FA3-MS22-P10

Undulation fluctuations in the smectic A phase of goethite nanorods. A.V. Petukhov^a, E. van den Pol^a, D.V. Byelov^a, D.M.E. Thies-Weesie^a, G.J. Vroege^a.

^a*van 't Hoff laboratory for physical and colloid chemistry, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands.*

E-mail: a.v.petukhov@uu.nl

Anisometric (i.e., very non-spherical) colloidal particles are able to form liquid crystals, just like rod-like or disc-like molecules do. Here the application of microradian x-ray diffraction to characterize the structure of the smectic phase formed in the suspensions of goethite $[\alpha\text{-FeOOH}]$ particles (average size $280 \times 70 \times 30$ nm) will be described [1,2]. In particular, an unusual shape of the smectic reflections was observed with strong diffuse 'streaks' in the direction along the smectic layers [3]. This unusual peak shape is rationalized in terms of *sliding* fluctuations, in which the particle director stays fixed while the layers undulate by sliding the particles along each other. This undulation mode is different from the usually considered *splay* layer undulations, in which the nematic director follows the fluctuations of the layer normal. While the *splay* undulations destroy the long-range positional (Landau-Peierls instability), we show that the *sliding* fluctuations do not. Diffuse x-ray scattering tails around the smectic Bragg reflections allow one to distinguish which type of the fluctuations is dominant.

[1] B.J. Lemaire, P. Davidson, J. Ferre, et al., *Phys. Rev. Lett.*, 2002, 88, 125507; B.J. Lemaire, P. Davidson, P. Panine, et al., *Phys. Rev. Lett.*, 2004, 93, 267801. [2] G.J. Vroege, D.M.E. Thies-Weesie, A.V. Petukhov, B.J. Lemaire and P. Davidson, *Advanced Materials*, 2006, 18, 2565; D.M.E. Thies-Weesie, J.P. de Hoog, M.H. Hernandez Mendiola, *Chem. Mater.*, 2007, 19, 5538; E. van den Pol, A.V. Petukhov, D.M.E. Thies-Weesie et al., *Phys. Rev. Lett.*, 2009, 103, 258301; E. van den Pol, A.V. Petukhov, D.M.E. Thies-Weesie, G.J. Vroege, *Langmuir*, 2010, 26, 1579. [3] E. van den Pol, PhD thesis (Utrecht University, 2010); Chapter 4; A.V. Petukhov et al., to be published.

Keywords: colloids, crystal disorder, small-angle x-ray scattering

FA3-MS22-P11

PDFView - A Program for Processing 3D Pair Distribution Function Data. Thomas Weber.

Laboratory of Crystallography, Department of Materials, ETH Zurich, Switzerland.

E-mail: thomas.weber@mat.ethz.ch

The three-dimensional pair distribution function method (3D-PDF) provides a direct access to information about disorder in crystals based on diffuse scattering data. It could be shown that this method allows qualitative and quantitative modeling of disorder in periodic crystals [1] as well as in quasicrystals [2, 3]. Though straightforward from a conceptual point of view, 3D-PDF investigations are currently time consuming and cumbersome tasks, because standard tools for data processing and refinement are not yet available. In this