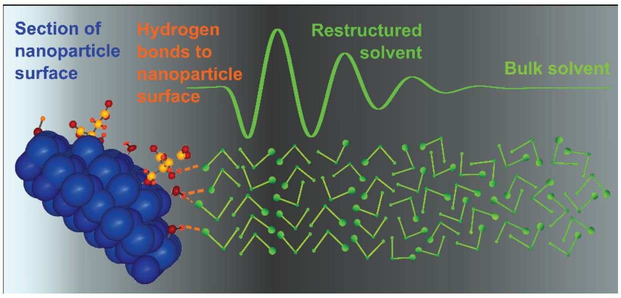

Figure 1. Solvent restructuring of ethanol at a ZnO nanoparticle interface (hydrogen atoms omitted for clarity) and resulting density oscillation observable by PDF. [5]

Keywords: nanoscopic solvation shell; nanoparticle; organic solvents;

MS24. Short range order and diffuse scattering

Chairs: Alexei Bosak, Thomas Weber

MS24-O1 Short-range order in cubic $RbNbWO_6$ and phase transition to tetragonal phase. Interpretation of X-ray diffuse scattering using group theory approach

Dorota Komornicka[1], Marek Wołcyrz[1], Adam Pietraszko[1], Wiesława Sikora[2], Andrzej Majchrowski[3]

1. Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50-950 Wrocław 2, Poland
2. Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Al. Mickiewicza 30, 30-059 Kraków, Poland
3. Institute of Applied Physics, Military University of Technology, 2 Kaliskiego St., 00-908 Warszawa, Poland

email: d.komornicka@int.pan.wroc.pl

A complex scheme of atomic displacements (modes; cf. Perez-Mato et al. [1]) that break the *Fd*-3*m* symmetry of the high-temperature (T_c > 395 K) cubic phase of $RbNbWO_6$ and ultimately lead to a phase transition to the tetragonal phase was determined using the group theory approach (program MODY [2]). The resulting set of modes was used to construct a model of the disordered crystal that provides diffuse scattering (calculated with DISCUS program from DIFFUSE package [3]) that is consistent with the experimental results. Particularly characteristic extinctions are well reproduced (cf. Withers et al. [4]).

The resulting solution reveals a disordered structure of cubic $RbNbWO_6$, which is a system of intersecting {111}-type planes in which Nb/W atoms (statistically occupying centers of oxygen octahedra) are shifted along three symmetry-equivalent $\langle 110 \rangle$ directions parallel to these planes. Oxygen atoms also move in a characteristic manner, but their shifts are considerably smaller and do not substantially affect the diffuse scattering pattern. The movements of Rb atoms are large but uncorrelated.

The obtained picture of the local structure of cubic $RbNbWO_6$ makes it necessary to change the interpretation of existing physical measurements, particularly dielectric measurement. Furthermore, the determined structure of the low-temperature tetragonal phase that exists below 395 K was found to be non-polar (*I*-42*d* space group).

Group theory analysis provides a coherent picture of the phase transition from the disordered cubic phase to the ordered tetragonal phase. At T_c, in a multimodal crystal of the high-temperature phase, mode symmetry breaking occurs, and each of the four displacive modes is decomposed: only 1/4 of the atoms of every mode of k =

(x, x, x) retain their ⟨110⟩-type in-plane displacements; the displacements of the remaining atoms undergo reorientation to fulfill the conditions imposed by the k = (0, 0, 0) mode. The former group of displacements defines the direction of the appearing tetragonal axis.

[1] J. M. Perez-Mato, D. Orobengoa and M. I. Aroyo, 2010 *Acta Crystallogr. Sect. A* 66, 558. [2] W. Sikora, F. Białas and L. Pytlik, 2004 *J. Appl. Crystallogr.* 37, 1015. [3] T. Proffen and R. B. Neder, 1997 *J. Appl. Crystallogr.* 30, 171. [4] R. L. Withers, M. I. Aroyo, J. M. Perez-Mato and D. Orobengoa, 2010 *Acta Crystallogr. Sect. B* 66, 315.

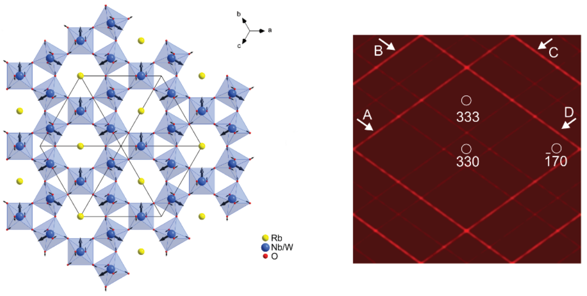

Figure 1. Scheme of atomic displacements in one of {111} $RbNbWO_6$ planes (left side) which reproduce the experimental diffuse scattering pattern. On the calculated section of the reciprocal space (right side) extinct diffuse streaks are marked with letters A – D and their directions are indicated by arrows.

Keywords: short-range order, X-ray diffuse scattering, phase transition, group theory

MS24-O2 Diffuse scattering experiments with relaxor ferroelectics: probing complexity of primitive cubic perovslite

Dmitry Chernyshov[1]

1. Swiss-Norwegian Beam Lines at the European Synchrotron Radiation Facility, Grenoble, France

email: dmitry.chernyshov@esrf.fr

Lead-based relaxors are puzzling ferroelectrics with centrosymmetric perovskite-like average structure and frequency dependent maximum of dielectric permittivity. The core of polar response in relaxors is local deviations from centrosymmetric structure due to a structural disorder; diffuse scattering is therefore expected to provide valuable information on the disorder. Here we focus on the experimentation and discuss diffuse scattering data for PMN relaxor collected as a function of temperature, pressure, and electric field. Different experimental problems and ways we present diffuse scattering are discussed. The anisotropy and shape of diffuse scattering can be successfully parameterized with a combination of two contributions. First term mimics thermal diffuse scattering, the corresponding microscopic glass-like realization corresponds to a fluctuation regime. The second term is located very near Bragg nodes and develops with cooling; it presumably represents frozen atomic displacements pinned by the static compositional disorder. The latter effect indicates an emergence of numerous long-lived states that is a hallmark of a dipole glass. The pressure does suppress polar correlations in a specific glass-like relaxor state, and above 40 kbar new non-polar phase becomes stable, while electric field leads to relatively small changes in the shape and intensity of diffuse scattering.

Keywords: diffuse scattering, relaxor, disorder, synchrotron radiation