MS28-P6 **Atomic ordering in PbMgTaO recovered from the anomalous x-ray scattering.** Zbyněk Šourek, Miloš Kopecký, Jiří Kub, Jan Fábry, and Jiří Hlinka, *Institute of Physics of the Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21 Prague 8, Czech Republic*
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Three-dimensional arrangement of atoms in sub-nanometer and nanometer scale is very important from the point of view of physical and chemical properties of materials. For this reason diverse imaging techniques with atomic resolutions have been developed. The method presented here is based on the measurement of anomalous x-ray scattering in large volume of the reciprocal space. It can be shown that, by analogy to x-ray holography with atomic resolution, the anomalous portion of diffuse scattering provides information on both the amplitude and the phase of the scattered wave. Consequently, the anomalous x-ray scattering can be employed to the 3D reconstruction of atomic arrangements extending up to the distances of several nanometers. The sample was a lead magnesium tantalate (PMT), which belongs to a class of ferroelectric materials known as relaxor ferroelectrics. PMT has a cubic perovskite ABO_3 structure with fluctuations of cations Mg^{2+} and Ta^{5+} on the B-sites. It is known that the short- and intermediate-range chemical ordering is responsible for relaxor behaviour of PMT, but the particular arrangement of cations remains unclear so far. The intensities of x-ray scattering in a large 3D volume of the reciprocal space were measured at the ESRF. Anomalous x-ray scattering has been obtained as a difference of intensity maps collected at two energies. The energy E_1 just below the Ta K absorption edge was chosen in order to get a strong anomalous component in the scattering from Ta atoms, whereas the data acquired at the energy E_2 far from the absorption edge were used as the reference data. The measured 3D pattern of anomalous scattering, including both the diffraction peaks and x-ray diffuse scattering, allows us to reconstruct numerically an average environment around Ta atoms. The real-space image shows a systematic local ordering of Ta and Mg atoms up to the distance of several nanometers. The conditioned probabilities of the site occupancies by the given type of atom provided that the central site is occupied by Ta were determined yielding information on the structure model of the ordered regions in the crystal.

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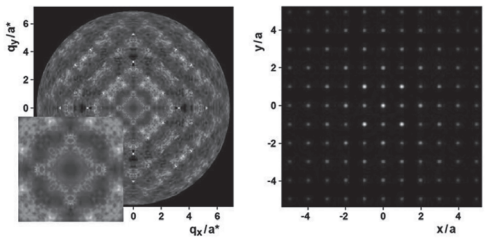

Figure (Left) The anomalous portion of x-ray diffuse scattering from the $PbMg_{1/3}Ta_{2/3}O_3$ single crystal in the plane (0 0 0.7a^*) of the reciprocal space obtained from intensity maps measured at the photon energies of 67.01 keV and 60.00 keV. (Right) The real-space image of the average surroundings of Ta atoms; the atomic plane is parallel to the (001) crystallographic plane at $z = 0$.

Keywords: short-range order; anomalous scattering; ferroelectric relaxors

MS31-P1 **Importance of hydrogen atoms in small molecules.** Horst Borrmann, *Max Planck-Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany*
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Due to the very weak scattering power of hydrogen it is frequently argued that hydrogen atoms cannot be determined reliably in course of X-ray diffraction experiments. A detailed analysis of the results after quite routine experiments on some small organic molecules revealed very interesting but even surprising results. In one case the clear assignment of positions of hydrogen atoms proved quite an unexpected configuration of the molecule. A second case is even more unusual since the analysis of isotropic displacement parameters reveals a very clear trend for hydrogen atoms in the molecule. Obviously modern experimental conditions allow for quite reliable information on hydrogen atoms even with 'routine' experiments. These results also show that low temperatures are not always a 'must' in small molecule crystallography. Lowering the temperature is certainly going to provide additional information and may improve quality of the data, however, experimental conditions are very important and need careful consideration. Obviously, quality criteria put forward in *Richard Harlow's hydrogen challenge* [1] ought to be carefully considered in structure evaluation.

[1] Harlow, R. L. (1996). *J. Res. Natl. Inst. Stand. Technol.* **101,** 327-339.

Keywords: hydrogen atoms; small molecules; low temperature