

Poster Presentation

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Aperiodic atomic ordering in PMN recovered from the anomalous x-ray scattering

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Various imaging techniques with atomic resolutions have been developed to study 3D arrangement of atoms in sub-nanometer and nanometer scale. The method presented is based on the measurement of the anomalous portion of 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 diffuse scattering provides information on both the amplitude and the phase of the scattered wave. The sample was $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ (PMN), which belongs to relaxor ferroelectrics. Although the short and intermediate range chemical ordering is responsible for its relaxor behaviour, the real arrangement of cations remains unclear so far. The intensities of x-ray scattering in a large 3D volume of the reciprocal space were measured using an intense x-ray radiation generated by the synchrotron facility. Anomalous x-ray scattering has been obtained as a difference of intensity maps collected at two energies. The energy E1 just below the Nb K absorption edge was chosen in order to get a strong anomalous component in the scattering from Nb atoms. The data acquired at the energy E2 far from the absorption edge were used as the reference. The measured 3D pattern of anomalous scattering, including both discrete diffraction peaks and continuous x-ray diffuse scattering, allows us to reconstruct numerically an average environment around Nb atoms. The reconstructed real-space images clearly show a systematic local ordering of Mg^{2+} and Nb^{5+} cations. This ordering is more significant close to the central reference Nb atom but it is still apparent at the distance of about 3 nm giving thus an idea on the average size of ordered regions. More distant sites are occupied randomly with probabilities of occurrence of Mg^{2+} and Nb^{5+} cations given by their relative fraction in the sample. It is possible to determine conditioned probabilities of site occupancies by the given type of atom provided that the central site is occupied by Nb and to get information on the structure model of the ordered regions in the crystal.

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