

MS44 Total scattering: pdf analysis and diffuse scattering in X-Ray, neutron and electron diffraction

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MS44-O1 Confined liquid structure and chemical kinetics from total neutron scattering

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Catalysis is, to put it mildly, extremely important. Around 80% of industrial chemical processes rely on a catalyst at some point, and 90% of all man-made materials use a catalyst in at least one step of the reaction. That said, there are still no experimental techniques that allow the structure and kinetics of (heterogeneous) catalytic processes to be resolved in situ. Here I will show the use of total neutron scattering in the determination of relevant information for the hydrogenation of benzene over Pt/MCM-41. I will begin with the structure of the reactant and product liquid, show how the chemical kinetics of the underlying processes can be obtained, and touch on the experimental determination of confined liquid structure.

Keywords: total scattering, catalysis, liquid structure, kinetics

MS44-O2 Correlated disorder in relaxor ferroelectrics

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The aim of this contribution is report our insights in the correlated occupational and displacement disorder in perovskite ferroelectric crystals of relaxor type.

We begin by exposing our recent investigation of the short-range correlations in the distribution of cations in perovskite B-sites of lead magnesium niobate single crystal, the enigmatic model ferroelectric relaxor material. This analysis is based on the resonant x-ray diffuse scattering data taken in a sizeable volume of the reciprocal space, including both discrete diffraction peaks and continuous x-ray diffuse scattering, and on subsequent direct numeric reconstruction of the average atomic occupation around a given Nb⁵⁺ cation up to the distance of several nanometers. Example of the experimental data is shown in Fig. 1.

We then discuss these results in the context of other experimental and theoretical studies of the B-site distribution in lead magnesium niobate single crystal, as well as its relation to the A-site displacement disorder and the implications for the peculiar dielectric properties of lead magnesium niobate single crystal and similar materials.

This work was supported by the Czech Science Foundation (project 15-09142S).

References

[1] M. Kopecky, J. Kub, J. Fabry, and J. Hlinka, Phys. Rev. B, **93**, 054202 (2016).

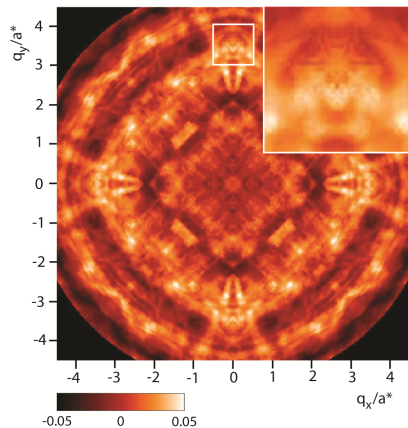


Figure 1. The intensity map of the anomalous part of the x-ray diffuse scattering from the PMN single crystal in the $(0\ 0\ 0.25a^*)$ plane of the reciprocal space. The inset shows enlarged part of the scattering intensity from the marked regions.

Keywords: diffuse scattering, resonant x-ray scattering, short-range correlations, disorder, relaxor, lead magnoniobate