MS24-P9 Combined 3D-ΔPDF and Monte Carlo analysis of disorder in $NaLaF_4$

Ruggero Frison[1], Thomas Weber[2], Tara Michels-Clark[3], Michal Chodkiewicz[4], Anthony Linden[1], Hans-Beat Bürgi[1,5]

1. Department of Chemistry, University of Zurich, CH-8057 Zurich Switzerland
2. Laboratory of Crystallography, Department of Materials, ETH Zurich, CH-8093 Zurich Switzerland
3. Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
4. Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Zwirki i Wigury 101, 02-089 Warszawa, Poland.
5. Department of Chemistry and Biochemistry, University of Bern, CH-3012 Bern Switzerland

email: ruggero.frison@uzh.ch

Many crystalline materials of scientific and technological interest posses disordered local structure arrangements that give rise to distinct diffuse scattering intensity. With the availability of high quality 3-D diffraction data and high performance computing infrastructures, detailed investigations of diffuse scattering data that were not possible only a few years ago are now within reach. From the 3-D data, the 3D-Difference Pair Distribution Function (3D-ΔPDF) can be calculated and the various types of disorder present in the structure identified and quantified in terms of an abstract model of interatomic vectors [1,2]. These results are extended by building and optimizing large Monte Carlo (MC) model crystals using parallelized algorithms [3,4]. Such MC simulations lead to a specific (and possibly improved) atomistic disorder model. $NaLaF_4$ was chosen for a case study; it is an efficient up-conversion phosphor [5] belonging to the family of rare earth-doped (Er^{3+}, Yb^{3+}) sodium lanthanide tetra fluorides [6]. Its distinctive, planar X-ray diffuse scattering was remeasured with synchrotron radiation at SNBL@ESRF, analyzed with the dual 3D-ΔPDF / MC approach and modeled in terms of occupational and positional disorder of the La, Na and F atoms. The final model along with possible alternative models will be discussed on the basis of our modeling strategy. We conclude that the dual modeling strategy provides an efficient procedure for the quantitative analysis of diffuse scattering data.

We thank Dr. Dmitry Chernyshov and the technical staff of SNBL@ESRF for their help during measurement.

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Keywords: 3D-PDF, Monte Carlo modelling, Diffuse scattering, Computing