

What is hidden in the background of Bragg diffraction. Diffuse scattering and PDF analysis not only with neutrons

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Many modern materials exhibit a considerable portion of structural disorder, playing a key role in their functionalities. Routine crystallographic structure solutions based on positions and integrated intensities of Bragg peaks only reveal their average structure. In order to access the details of local atomic arrangements and their short-range correlations one has to study the shape of the Bragg lines and the diffuse scattering below and between them.

In the past decade(s) increasing popularity has gained the pair distribution function (PDF) technique. Originally employed to investigation of amorphous structures and liquids, it has been extended to treat also crystalline systems. Its application consists in calculating the Fourier transform of a complete powder diffraction pattern, including the slowly varying part of the signal underneath the Bragg peaks and taking into account instrumental contributions to the line widths [1,2]. The resulting real-space atomic distance distribution by itself often permits qualitative discussions of changes in nearest neighbor distances as a function of chemical composition or of thermodynamic parameter variations (eg. [3]).

More involved and more quantitative interpretations of the PDF necessarily call for (much) more computing effort following one of the two possible approaches. In the first approach, a model-free technique of reverse Monte-Carlo (RMC) is used to build up a model structure providing a diffraction pattern coinciding with the observed one within statistical limits [4]. In an ideal case progress in computing power may permit to treat data obtained by various experimental probes (X-ray, neutron and electron scattering, EXAFS, NMR etc.) simultaneously to remove ambiguities inherent in each single technique [5]. In the second approach molecular dynamics and/or *ab-initio* computational techniques are employed to build up a dynamical model of the studied system, which is then successively refined to match the observed pattern. At the present state of the art DFT molecular dynamics can deal with disorder in quite complicated structures [6].

References

1. Th. Proffen et al., *Z. Kristallogr.* 218 (2003) 132–143
2. S.J.L. Billinge, M.G. Kanatzidis, *Chem. Commun.* (2004) 749–760
3. I.K. Jeong et al., *Phys. Rev. Lett.* 94 (2005) 147602
4. R.L. McGreevy, *J. Phys.: Condens. Matter* 13 (2001) R877–R913
5. I. Levin et al., *Chem. Mater.* 31 (2019) 2450–2458
6. M. Pasciak et al., *Phys. Rev. B* 99 (2019) 104102