Investigation of disordered systems using Total scattering: introduction to the method and experimental techniques

Michela Brunelli[a*]

a. Dutch-Belgian Beamline DUBBLE at the ESRF − 71, av. des Martyrs CS 40220 38043 Grenoble Cedex 9

* brunelli@esrf.fr

Structural disorder and/or nano-scale structures are found in many technologically relevant modern materials, such as batteries, catalysts, and guest storage systems. Understanding this disorder is often key to understanding the functional materials properties. While traditional Bragg crystallography is only sensitive to the long-range ordered structure, diffuse scattering features between the Bragg peaks contain information on the local atomic structure. Hence, a combined analysis of Bragg and diffuse contributions to the powder diffraction data provides a versatile approach to probe and characterize these structures.

In powder diffraction, Pair-Distribution Function (PDF) analysis of Total Scattering data is the method for going beyond classical crystallographic analysis by providing quantitative information about local as well as meso-structure, because is sensitive to local static and dynamic disorder. It based on the Fourier transformation of diffraction data into real-space [1, 2].

In this talk, the main characteristics of Total Scattering and its domain of application will be presented. Particular emphasis will be devoted to the experimental implementation of the technique, both for X-ray and neutron powder diffraction.

[1] T. Egami, and S.J.L. Billinge, Underneath the Bragg peaks: Structural Analysis of Complex Materials (Pergamon Materials Series, V. 7: Oxford, 2003)
[2] H.E. Fischer, A.C. Barnes, and P.S. Salmon, Neutron and x-ray diffraction studies of liquids and glasses, Rep. Prog. Phys. **69,** 233–299 (2006)