“Use of Coherence Methods in X-ray Powder Diffraction”

Ian Robinson
London Centre for Nanotechnology
University College
London

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Abstract

Multibend Achromat Upgrades are being developed at a number of Synchrotron Radiation facilities, including ALBA. By greatly reducing the beam emittance, the coherent fraction of the X-rays produced by the undulators is correspondingly increased. The “diffraction limit” is reached where all X-rays up to a certain energy cutoff are fully coherent. This energy is expected to move into the hard X-ray range, with the consequence that ordinary diffraction experiments, such as powder diffraction at the MSPD beamline, become coherent diffraction experiments. While imperfect optics and beam vibrations might obscure the coherent diffraction effects, there is strictly no formal way to lose the coherence. So it will be important for users of MSPD to know how their data may be affected by the coherence.

Of course there are great opportunities to use Coherence Methods to extract more information from X-ray Powder Diffraction experiments. One common data analysis technique, called the Williamson-Hall method [1], plots the measured powder diffraction line widths against the total momentum transfer. The slope of this line is a widely used quantitative measure of “microstrain”, attributed to local distortions of the crystal lattice within each powder grain. When the illuminating beam is made coherent, each Bragg peak recorded in a powder pattern acquires fine structure in the form of fringes surrounding the peak centre. These fringes can be analysed using the Bragg Coherent Diffractive Imaging (BCDI) method to obtain real space 3D images of the crystal grain complete with the local distortions appearing as the image phase [2]. In this way the microstrain can be imaged, grain by grain, in the powder diffraction sample.

Another commonly used analysis method is to calculate the Pair Distribution Function (PDF) and complete the analysis of the crystal structure in real space [3]. PDF is particularly powerful for nanocrystalline materials with grain sizes below 100nm. This often requires Reverse Monte Carlo simulation of the real space distribution of matter to “fit” the PDF. With coherent BCDI images of typical grains of the material, these simulations could be directly tested.

[1] G.K.Williamson and W.H.Hall, Acta Metall. 1, 22-31 (1953)
[2] Ian Robinson and Ross Harder, Nature Materials 8 291-298 (2009)
[3] Takeshi Egami and Simon J.L. Billinge , “Underneath the Bragg Peaks: Structural Analysis of Complex Materials” (Pergamon press, 2003)