Poster

Correcting the axial divergence from high-resolution powder diffraction data

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High-angular resolution powder diffraction, with well-defined and resolved diffraction peaks, is used generally to obtain high-quality data for complex structure refinements. The ID22 beamline at ESRF has very high angular resolution, arising from the combination of the highly collimated beam from the new EBS ring, wavelength selection via a cryogenically-cooled Si 111 monochromator, and use of a 13-crystal Si 111 multi-analyser stage between the sample and the detector. Since 2021, ID22 is equipped with a Dectris Eiger2 X 2M-W CdTe pixel detector receiving the X-rays transmitted by the thirteen crystals [1]. A great advantage of this arrangement is the axial resolution provided by the 2D detector. By exploiting this axial resolution, the effect of axial divergence, which causes the low- angle asymmetry in the peak shape of powder diffraction patterns, can be removed. Indeed, due to the curvature of the Debye-Scherrer cones, axially-diverging photons satisfy the Bragg condition at the analyser crystal at lower angles of the detector arm than those scat- tered closer to the diffraction plane and so appear to be diffracted at lower 2θ angles. By recording the axial position at which a photon arrives at the detector, its true 2θ angle from the sample can be calculated [2]. The overall effect is that peaks at low angle are more symmetric and narrower when such corrections are applied (Fig. 1a), also improving the angular resolution. A second advantage of this arrangement is that the axial acceptance of the detector can be increased as 2θ increases, thus improving the statistical quality of the high angle data (Fig. 1b). ID22 has implemented this approach systematically, as an automatic procedure, into its collection of high- resolution powder diffraction data.

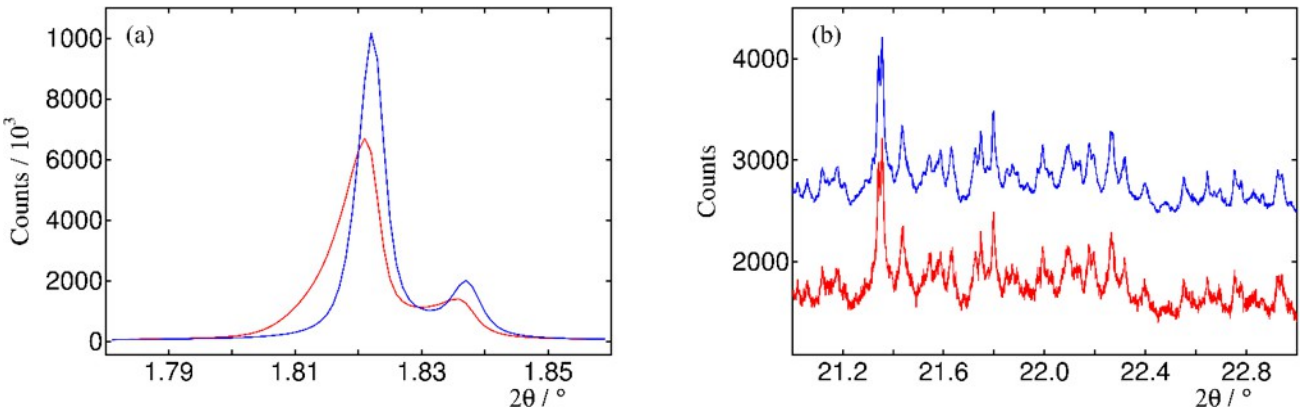

Figure 1. Low-angle (a) and high-angle (b) parts of a high-resolution powder diffraction pattern of zeolite ZSM-5 at 35 keV showing (red) standard processing with a fixed 4-mm large axial aperture and (blue) advanced processing exploiting the axial resolution of the 2D detector.

[1] Fitch, A., Dejoie, C., Covacci, E., Confalonieri, G., Grendal, O., Claustre, L., Guillou, P., Kieffer, J., de Nolf, W., Petitdemange, S., Ruat, M. & Watier, Y. (2023). *J. Synchrotron. Rad.* **30**, 1003.

[2] Fitch, A. & Dejoie, C. (2021). *J. Appl. Cryst*. **54**, 1088.