

POWDER DIFFRACTION AS A CALIBRATION AND VERIFICATION TOOL FOR SYNCHROTRON X-RAY BEAM LINES AND APPARATUS

F. J. Rotella, R. W. Alkire and N. E. C. Duke
Structural Biology Center, Biosciences Division, Argonne National Laboratory,
Argonne, IL 60439 USA

Although the primary uses of powder diffraction are in materials phase identification and structure solution and refinement, powder diffraction can also be used as a diagnostic tool in the calibration and operating verification of synchrotron x-ray beam lines and equipment. Three examples of the use of powder diffraction as a diagnostic tool at the bending-magnet and insertion-device beam lines (19BM and 19ID) of the Structural Biology Center at Argonne's Advanced Photon Source will be presented.

The calibration of multi-module CCD area detectors can be verified using powder diffraction from polycrystalline slurries of the protein hen egg-white lysozyme, a *de facto* standard used at protein crystallography synchrotron beam lines. The registry of individual powder "rings" to the pixel within and between CCD modules in lysozyme powder diffraction images indicates that the area detector has been well calibrated.

The precise position of the area detector on a synchrotron beam line – sample-to-detector distance and detector swing angle (2θ) – can be calibrated using powder diffraction. LaB_6 (NIST SRM 660) is the calibration sample of choice at beam lines 19BM and 19ID. After calibration, the refined values for sample-to-detector distance and detector swing angle from lysozyme single-crystal diffraction data are typically within 0.5 mm and 0.25° , respectively, of their nominal values.

Sources of parasitic scattering from beam line components (e.g., beam collimators) observed in area detector x-ray images can be identified from knowledge of the materials comprising the components and the x-ray wavelength and sample-to-detector distance used to measure the diffraction image. Once identified, the components may be redesigned to eliminate the undesired scattering from x-ray images.

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