Strategy in the age of 360° sweeps

A. Förster, M. Müller, C. Schulze-Briese

DECTRIS Ltd., Täfernweg 1,5405 Baden-Dättwil, CH

andreas.foerster@dectris.com

The rotation method is the most common approach of collecting macromolecular diffraction data. In the days of image plates and charge-coupled device detectors (CCDs), substantial readout time and noise made sophisticated data collection strategies necessary. The correct starting angle of data collection would help minimize the number of images. A rotation increment of up to 1°/image served to raise weak reflections above the detector noise. Datasets took hours to collect.

This is not a sensible way of collecting data anymore. Hybrid Photon Counting detectors, which are installed on essentially all MX beamlines around the world and on many laboratory diffractometers, are free of dark current and readout noise and limited only by Poisson counting statistics. Using rotation increments of around 0.1°/image (fine slicing) decreases the measured background and increases the signal to noise of the experiment. With fast detectors, full 360° datasets can be collected in seconds to a few minutes.

Does the new standard of 360° of data collected at 0.1°/image excuse crystallographers from thinking and optimizing their experiments? Not at all. We show how the full-rotation approach to data collection can accommodate such scenarios as extremely radiation-sensitive samples and experimental phasing. Solving structures by single-wavelength anomalous dispersion from atoms native to the sample becomes possible even with data collected at room temperature. A successful experimental strategy comprises adjustments to beam energy, photon flux, detector distance, starting angle, number of full rotations, orientation of the crystal, and many more.

The recording of data at the highest possible quality makes all subsequent steps of data processing, phasing and model building easier. It will result in a more precise atomic model to answer the biological questions that prompted the structural work. Despite the apparent simplicity of the full-rotation method, data collection, the last experimental step of MX, is as critical as ever. There is no excuse for walking away with less than best data.

Keywords: MX data; Strategy; Low intensity; High multiplicity; Anomalous data