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Supporting information for article:

Energy Optimization of a Regular Macromolecular Crystallography Beamline for Ultra-High Resolution Crystallography

Gerd Rosenbaum, Stephan L. Ginell and Julian C.-H. Chen

S1. Differences between even and odd harmonic beam profiles

There are two distinct differences between the even and odd harmonics. The even harmonics have a peculiar angular profile of the flux density: it is zero on-axis, increases with angle and then falls off, i.e. it has the shape of a donut. The finite size of the electron beam smoothes the profile and fills in the donut hole: for the APS, at 30 keV, the angular peak in the horizontal direction is only ~40% higher than the center (horizontal source size 0.60 mm FWHM) and ~75% higher in vertical direction (source size 0.02 mm FWHM). For the 40 keV and 50 keV contaminations, the angular peaks are at larger angles. If the beamline has an adjustable aperture this feature could be used to substantially decrease the 40 keV and 50 keV flux without sacrificing much of the 30 keV flux. At the focal plane, the angular profile converges into the image of the source. However, for the necessarily sizable crystals (~0.2 mm^3) needed for ultrahigh resolution data acquisition, the beam is not focused at the sample in order to use a large volume of the crystal. The non-uniform beam profile is mostly smoothed out by rotation of the crystal during data collection.

A second difference between the even and odd harmonics is the degree of polarization. Whereas for the odd harmonics it is safe to assume 100% polarization in the horizontal plane for processing the data it is slightly less for the even harmonics and may need to be considered. For beamline 19-ID with undulator A tuned for 4th harmonic at 30 keV it is 97% averaged over the angular divergence limited by the primary aperture (81 µrad x 40 µrad, h x v).