Poster Presentation

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Improving total scattering data in statistics through detector intensity calibration

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High-resolution atomic pair distribution functions (PDF) require total scattering data with better statistics in a wide range of Q. The wide Q-range data can be obtained by a large area detector along with high-energy X-rays, whereas various systematic errors in X-ray detectors are known to predominate over statistical errors particularly for higher counting intensity. The study focused on a robust technique for reducing systematic errors in a position-sensitive detector, which allows us to obtain total scattering data with statistics in proportion to counting photons.

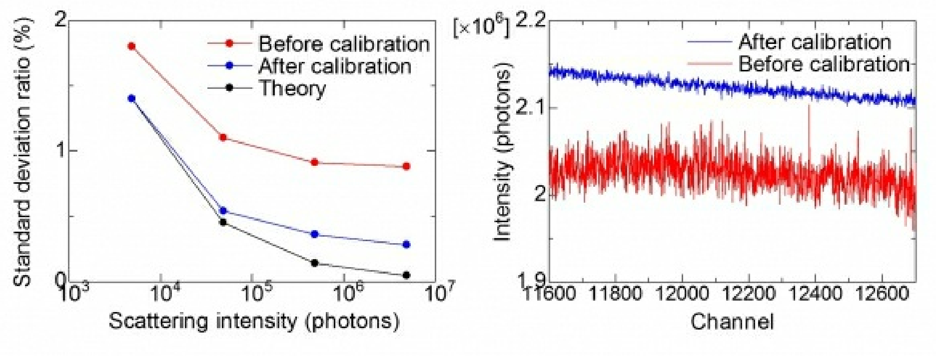
The technique has been examined using a photon-counting microstrip detector (MYTHEN, DECTRIS Ltd.) that has been installed in the Debye-Scherrer camera at the Materials Science beamline BL44B2[1] of SPring-8. The basic idea is that photons counted in one microstrip channel should be the same with those in another channel within statistical errors when each channel receives same X-ray photons. Assuming that the systematic error in one channel are not associated with that in another, each systematic error can be cancelled out by normalizing each intensity with the average of their intensities. To corroborate the assumption, a MYTHEN module, which is composed of 1280 channels, was translated 10 times by 128 channels while glass scattering was measured. The intensity for every channel within a module was calibrated using the 128 mean intensities, each of which was the average of 10 data measured at the same scattering angle. In the end, the procedure was modified to keep systematic errors within statistical errors even at higher intensity[2].

The left figure shows the standard deviation ratios (SDR) to scattering intensity as a function of intensity for 128 channels in a module. Black and red dots are theoretical values calculated according to the Poisson distribution and original ones before applying the calibration method, respectively. The values after calibrating intensity are indicated by blue dots. Surprisingly, the SDR before the calibration for 4.9×10^6 photons is 0.88%, which only corresponds to the statistics of 1.7×10^4 photons. The SDR curve after the calibration is close to that of the theory. In 4.8×10^3 photons, the SDR was reduced from 1.8% to 1.4%, which is comparable to the theory. On the other hand, the calibration at 4.9×10^6 photons lowers the SDR from 0.88% to 0.28%, which is 6 times as large as the theory. The right figure shows the impact of the calibration method on the high-intensity data of 2×10^6 photons. Large fluctuations in intensity before the calibration originates from various systematic errors in the module. Finally, the modified procedure succeeded in reducing these errors nearly within statistical errors as indicated by blue lines.

We demonstrated that the detector intensity calibration for reducing systematic errors plays an important role in obtaining total scattering data with better statistics in a wide range of Q. The results suggest that the precision and accuracy in intensity of Bragg peaks as well as diffuse scattering will improved considerably. We will share some of high-quality PDFs measured by the MYTHEN 12K detector system that incorporates the calibration process.

[1] Kato, K. & Tanaka, H. (2016). Advances in Physics: X 1, 55-80.

[2] Kato, K. Submitted to J. Appl. Cryst.



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