Contribution ID: **13** Type: **Contribution type**

High-precision X-ray total scattering measurements using a high-accuracy detector system

Thursday, 10 June 2021 09:40 (20 minutes)

The total scattering method, which is based on the measurement of both Bragg and diffuse scattering on an equal basis, is still challenging even by means of synchrotron X-rays. This is because such a measurement demands a wide coverage in scattering vector Q, high Q resolution, and wide dynamic range for X-ray detectors. There is a trade-off relationship between the coverage and resolution in Q, whereas the dynamic range is defined by the difference in X-ray response between detector channels (X-ray response non-uniformity: XRNU). XRNU is one of the systematic errors for individual channels, while it appears to be a random error for different channels. So far, the flat-field approach, which needs a uniform reference intensity, has been adopted to correct scattering data for XRNU. However, the conventional approach has failed for the case where the level of the XRNU noise was lower than a few percent because it is difficult to obtain a perfectly uniform intensity. An alternative approach, which is based on the statistical estimation of the reference intensity, has been developed to overcome the limitation.[1] We reported that the level of the XRNU noise of a microstrip detector was successfully reduced from 1% to 0.1%.[1] On the other hand, the approach has a problem with the correcting time. The acquisition of reference data took at least half a day. The long correcting time made it virtually impossible to correct scattering data for XRNU according to the detector and experimental settings. Accordingly, a significant reduction in the correcting time was required. Recently we have improved the statistical approach to reduce the correcting time from half a day to half an hour.[2] I will give a talk about high-precision X-ray total scattering measurements using a high-accuracy detector system, which facilitate electron density studies[3,4] and dual-space structure analysis[5].

References:

[1] K. Kato, Y. Tanaka, M. Yamauchi, K. Ohara, and T. Hatsui, J. Synchrotron Rad. 26, 762 (2019).
[2] K. Kato and K. Shigeta, J. Synchrotron Rad. 27, 1172 (2020).
[3] B. Svane, K. Tolborg, K. Kato and B. B. Iversen, Acta Cryst. A77, 85 (2021).
[4] A. A. Pinkerton, Acta Cryst. A77, 83 (2021).
[5] J. Beyer, K. Kato and B. B. Iversen, IUCrJ 8, 387 (2021).

Primary author: KATO, Kenichi (RIKEN SPring-8 Center)

Presenter: KATO, Kenichi (RIKEN SPring-8 Center)

Session Classification: Session