BL44B2
RIKEN Materials Science I

1. Data-driven total scattering measurements

BL44B2 is recognized to give exceptional total scattering data in various aspects such as precision and accuracy in scattering intensity, Q (scattering vector) resolution, and Q range [1]. Such extraordinary data have allowed valence electron density studies in a wide range of powdered materials [2] and short- and long-range-order analyses on an equal basis [3]. The success in these studies is due entirely to a continuous effort towards the development of hardware (OHGI) [4] and software (ReLiEf) [5] by a data-driven approach.

2. Pushing the limits of total scattering by Compton-free measurements

Compton scattering is one of the most significant noise sources for total scattering measurements, especially at higher Q, where the intensity of incoherent (Compton) scattering is much higher than that of coherent (total) scattering. For example, the incoherent intensity of SiO_2 is one order of magnitude higher than the coherent intensity in the Q range over 20 $Å^{-1}$. The resolution and noise of the resulting pair distribution function would be determined by how Compton scattering is processed. Using an empirical formula, Compton scattering is commonly subtracted from measured scattering data in the process of obtaining the structure factor $S(Q)$. The subtraction process, however, is extremely complicated, because the Compton correction is correlated with other corrections, which leads to a large systematic error in $S(Q)$. Even though the Compton correction may succeed, the signal-to-noise ratio of total scattering data does not improve. We are aiming at separating incoherent and coherent scattering in the measurement process to push the limits of total scattering.

Energy-dispersive semiconductor detectors, such as silicon drift detectors (SDDs) and CdTe detectors (CTDs), were adopted to separate incoherent and coherent scatterings in a wide range of scattering angles. At 30 keV, the energy resolution of an SDD is twice as high as that of a CTD, whereas the quantum efficiency of a CTD is three times as high as that of an SDD. Therefore, multiple SDDs were installed in the powder diffractometer of BL44B2 to cover forward scattering, discriminating incoherent scattering adjacent to coherent scattering. On the other hand, multiple CTDs were installed in the diffractometer to cover backscattering, which improved the statistics of coherent scattering. In the conventional approach with SDDs, an energy window is set to separate the two types of scattering. The problem for the energy-window approach is that both scatterings considerably overlap, especially at forward-scattering angles. To overcome this problem, we introduced a curve fitting procedure for each spectrum measured at each scattering angle. Consequently, we obtained Compton-free total scattering data from forward to backscattering.

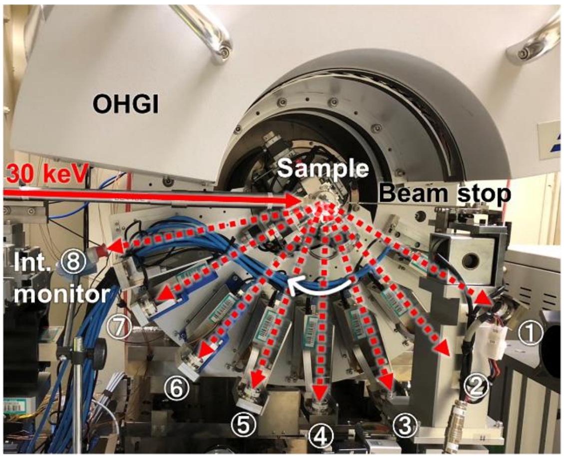

Fig. 1. Multiple energy-dispersive detectors for separating Compton and coherent scatterings.

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