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, accuracy, Q (scattering vector) resolution, and Q range [1]. Such extraordinary data have allowed valence electron density studies in a wide range of materials, even powders [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. Towards total scattering "spectroscopy"

Total scattering is based on simultaneous measurements of coherent scattering such as Bragg and diffuse scattering, which means that incoherent scattering such as Compton scattering must be disregarded in the measurement process. In most cases, however, Compton scattering has been measured with coherent scattering and then subtracted from the mixed data in the analytical process. Therefore, the reduced data often suffer from considerable degradation in the signal-to-noise ratio and systematic errors, especially at high Q.

We have attempted total scattering "spectroscopy" to discriminate coherent scattering from incoherent scattering in the measurement process. Forward scattering, where Compton scattering is insignificant, can be measured with OHGI (Fig. 1). On the other hand, backscattering, where Compton scattering is one order of magnitude higher than coherent scattering in light materials, is measured by moving a silicon drift detector (SDD) (Fig. 1). The SDD has an energy resolution of about 300 eV FWHM at 30 keV. Judging from the Compton shift, it is found that the energy resolution meets the requirement for total scattering spectroscopy at backscattering.

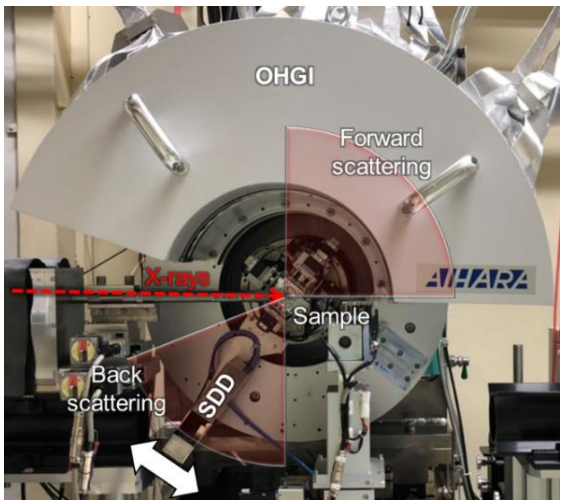

Fig. 1. Setup for total scattering spectroscopy.

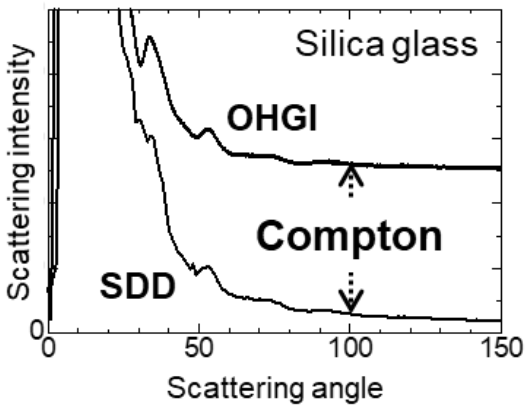

Fig. 2. Contribution of Compton scattering.

Figure 2 shows the mixed data collected with OHGI and the spectroscopic data obtained with the

SDD in silica glass. The development of total scattering spectroscopy is still in progress, but these results clearly indicate that total scattering spectroscopy is a unique and promising approach to achieving high-Q values of more than 30 Å^{-1}, leading to a real-space resolution higher than 0.1 Å.

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