

BL44B2

RIKEN Materials Science I

1. Introduction

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. Recent Activities

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 SiO₂ 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. With 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 Compton correction is correlated with other corrections, which leads to a large systematic error in $S(Q)$. Even though 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 FY2023, a significant problem to be solved was found in CTDs during development. Current and mechanical noises significantly degenerated the energy resolution. To deal with current noise, the material for mounts and screws was changed from metal to resin. On the other hand, a vibration isolator was inserted between the mount and the diffractometer to cope with mechanical noise. However, it was difficult to set the detector in position due to the isolator. Therefore, the mechanical noise source, which is a spinning motor, was modified by optimizing its speed. Ultimately, CTDs are free of current and mechanical noises, and

the original performance is achieved.

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