BL44B2
RIKEN Materials Science I

1. Introduction

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 of these studies is due entirely to a continuous effort toward the development of hardware (OHGI) [4] and software (ReLiEf) [5] by a data-driven approach.

2. Recent activities

D2*G* [6]: A data-driven approach to *G*(*r*)

Another challenge for the total scattering PDF user is to derive the PDF from total scattering data through the structure factor $S(Q)$. We have developed an unbiased approach to the reduced atomic pair distribution function $G(r)$ in terms of the random errors in $S(Q)$ (Fig. 1). The χ factor in reciprocal space is proposed to measure the systematic errors in $S(Q)$.

Experimental total scattering data, which are inevitably incomplete even though synchrotron X-rays are used as a probe, cannot uniquely determine the PDF. To date, nevertheless, no particular care has been devoted to the incompleteness of data. In the present study, an approach to such an inverse problem has been developed to determine the most unbiased PDF within the random errors in $S(Q)$. In addition, the χ factor defined by the random errors was found to measure the systematic errors in $S(Q)$. In contrast to conventional approaches, the resulting PDFs for both crystalline (Si) and amorphous (SiO_2) samples were virtually free from spurious ripples at no cost of real-space resolution. The reliability of the PDF was confirmed with the atomic displacement parameter of Si obtained by PDF analysis. These results are based on not only the estimated random errors but also prior knowledge of the average number density and the pair "density" function, which should be considered as part of the information contained in the data. Thus, our approach could be referred to as a data-driven approach to $G(r)$, D2G, via the pair "density" function.

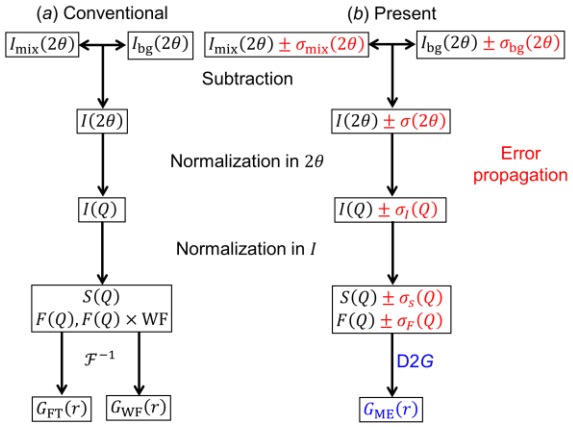

Fig. 1. Data reduction procedures for determining the reduced pair distribution function $G(r)$ from the total scattering intensity data, $I(2\theta)$, through the (*a*) conventional and (*b*) present approaches.

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