BL04B2: Disordered structure probed by high-energy x-ray diffraction technique

In this practice, we measure diffraction pattern of amorphous silica (SiO_2) using the two-axis diffractometer dedicated for disordered materials (see Fig. 1 [1]). The energy of incident x-rays is 61.5 keV obtained by a Si 220 monochromator. The scattered x-rays from the sample are collected by a Ge detector using a conventional θ - 2θ step scan method. We analyze the diffraction pattern and obtain Faber-Ziman total structure factor $S(Q)$ [2] by the following equation,

$$S(Q) = \frac{I(Q) - \left\langle |f(Q)|^2 \right\rangle}{\left| \langle f(Q) \rangle \right|^2} + 1$$

$$= \sum_{ij} c_i c_j \frac{\mathrm{Re}\left[f_i(Q) f_j^*(Q) \right]}{\left| \langle f(Q) \rangle \right|^2} S_{ij}(Q) = \sum_{ij} w_{ij}(Q) S_{ij}(Q), \qquad (1)$$

where $S(Q)$ can be obtained by a normalization of the corrected x-ray scattering intensity $I(Q)$. The pair distribution function $g(r)$ is obtained by a Fourier transformation of $S(Q)$,

$$g(r) = 1 + \frac{1}{2\pi^2 \rho r} \int_0^{Q_{\max}} Q\left[S(Q) - 1 \right] sin(Qr) \mathrm{d}Q$$

$$= 1 + \sum_{ij} \frac{1}{\pi r} \int_{-\infty}^{\infty} \int_0^{Q_{\max}} r' [g_{ij}(r') - 1] \cdot w_{ij}(Q) \cos[Q(r - r')] \mathrm{d}r' \mathrm{d}Q, \qquad (2)$$

where Q is the absolute value of wave number ($Q = |\,Q\,| = (4\,\pi/\lambda)\,\sin\theta$, 2θ: scattering angle, λ: wavelength of incident x-rays) and < > means the average per one atom, and c_i and $f_i(Q)$ represents atomic fraction of i and atomic form factor of i, respectively. $w_{ij}(Q)$, $S_{ij}(Q)$, and $g_{ij}(r)$ is weighting factor of i-j correlation for x-rays, partial structure factor for i-j correlation, and partial pair distribution function for i-j correlation, respectively. ρ is an atomic number density. We can assign atomic correlation peaks and derive the coordination number with integrating peak area in the real-space function.

One may realize after the experiment that diffraction data yield only one-dimensional structural information. To reveal the complicated structure in disordered materials, it is necessary to construct 3-dimensional atomic configuration on the basis of diffraction data. The RMC method [3,4] has been shown to be a useful tool to construct a three-dimensional structural model of disordered materials using mainly experimental diffraction data. In the RMC simulation technique the atoms of an initial configuration are moved so as to minimize the deviation from the experimental diffraction data, using a standard Metropolis Monte Carlo

algorithm [5]. In this practice, we try to model 3-dimensional atomic configuration of amorphous silica, which is in consistent with the diffraction data. We hope everybody can find out “order within disorder [6]” in the amorphous materials, since the structure of disordered materials can be understood to exhibit an unique atomic order.

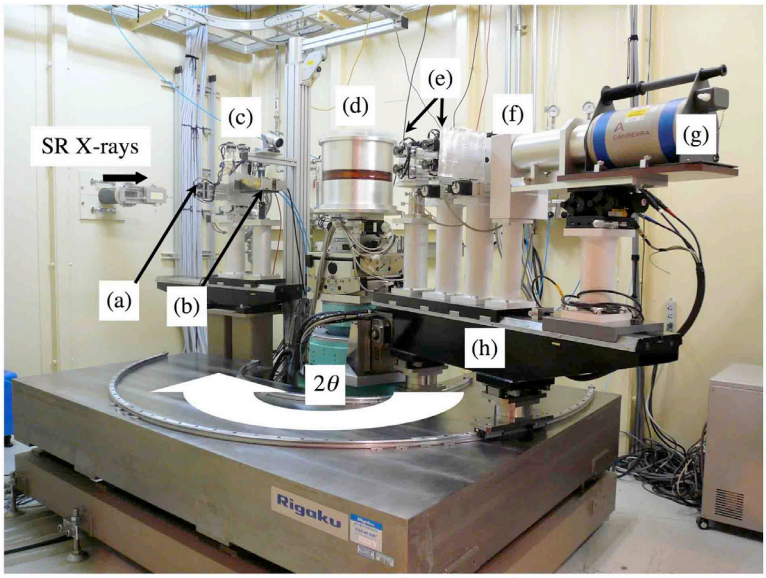

Fig. 1 Photograph of two-axis diffractometer for disordered materials.
(a) incident slit, (b) ionization chamber, (c) CCD camera, (d) vacuum chamber, (e) receiving slits, (f) fully automatic attenuators (g) Ge detector, (h) 2θ arm. Beam stop is hidden behind the receiving slits.

References

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