Small-Angle X-ray Scattering (SAXS)

Naoto Yagi
Hiroshi Sekiguchi
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1. Learning what is SAXS ...and WAXS

Non-crystalline diffraction ... what is diffraction? what is scattering?
Hierarchy in non-crystalline materials
Pitfalls in SAXS

2.Visiting three beamlines: BL40XU, BL40B2, BL45XU

These three SAXS beamlines in SPring-8 have different x-ray sources and optics. To have an actual look at these beamlines is a valuable experience.
BL40XU:
http://www.spring8.or.jp/wkg/BL40XU/instrument/lang-en/INS-0000000353/instrument_summary_view
BL40B2:
http://www.spring8.or.jp/wkg/BL40B2/instrument/lang-en/INS-0000001280/instrument_summary_view
BL45XU:
http://www.spring8.or.jp/wkg/BL45XU/instrument/lang-en/INS-0000000334/instrument_summary_view
BL03XU

3. Understanding optics for SAXS

Using the above three beamlines as examples, designs of SAXS beamlines are explained.
BL40XU: helical undulator --- double focusing mirrors
BL40B2: bending magnet --- double crystal monochromator --- bent cylindrical mirror
BL45XU: tandem vertical undulators --- double crystal diamond monochromator --- double focusing mirrors
BL03XU: undulator --- double crystal Si monochromator --- double focusing mirrors
Other beamlines: BL20XU and beamlines in other facilities.

4. Understanding detectors for SAXS

Several different types of detectors are used at the above three beamlines. Apart from basic detectors such as ion chambers, they are all area detectors.
RAXIS: image plate detector
X-ray image intensifier + CCD camera: high sensitivity and fast readout
CMOS flatpanel: solid-state area imager
PILATUS: photon-counting pixel detector

5. Protein solution scattering measurements at BL40B2

Data acquisition using samples such as calmodulin.

6. Practicing data analysis

Introduction to widely used SAXS data processing software (fit2D, PRIMUS, etc.)

Important formulae:

Definition of “q”

$$q = 4\pi \frac{\sin(2\theta/2)}{\lambda}$$

Guinier Plot ... R_g is radius of gyration

$$I(q) \propto \exp(-\frac{q^2 R_g^2}{3})$$

Pair distribution function ... Fourier transform of autocorrelation function

$$P(r) = \frac{r}{2\pi^2}\int_0^\infty I(q) q \sin(qr) dq$$

Scattering from a sphere (radius=R)

$$I(q) = I_e V^2 \rho_0^2 \left[\frac{3[\sin(qR) - (qR)\cos(qR)]}{(qR)^3}\right]^2$$

Scattering intensity

$$I(q) = I_e \left|F(q)\right|^2 = I_e \int_v \rho(r_k) e^{-iq\cdot r_k} dr_k \int_v \rho(r_k) e^{iq\cdot r_k} dr_k$$