Version 1.51

Open-source Python software for six-circle diffraction with an inelastic x-ray scattering (IXS) spectrometer

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Abstract

We have made an open-source six-circle diffractometer code using Python 3. This code specifically targets the case of a four-circle Eulerian cradle geometry with an incident beam that has been tilted out of the nominal diffraction plane by, e.g., a Kirkpatrick-Baez (KB) mirror pair, though it is also more general. The 4-circle + KB case is especially relevant for diffractometers or spectrometers where the two-theta arm motion is constrained to be in a horizontal plane, as is common for, e.g., inelastic x-ray scattering (IXS) spectrometers, where the two-theta arms are often heavy and >5 m long. The code numerically inverts the diffraction equations, allowing the user to fix any 3 parameters out of the 5 angular motions (theta, phi, chi, mu and gamma) and 3 auxiliary angles (omega, alpha and beta). Commands tailored to inelastic x-ray scattering (IXS) at SPring-8 with a 2-dimensional analyzer arrays are included.

1. Introduction

X-Ray diffraction is commonly employed to investigate the details of material structure, often to elucidate specific and subtle features of single crystal samples. Various standard diffractometer geometries have evolved for these single crystal experiments with different features as may be indicated by specific experimental details (sample environment, angle ranges, types of detection, etc). At one extreme is the diffraction apparatus used in inelastic x-ray spectrometers, where the two-theta arms are often both very long (3 to 10 m) and extremely heavy (~1000 kg or more) as, instead of carrying a detector, they carry an energy analysis setup, or even an array of analyzers (see e.g. (Baron, 2016)). These spectrometers usually move the analyzer / two-theta arm in the horizontal plane, to avoid the problems associated with gravity and gravitational induced bending when moving in the vertical direction. If the incident beam is then also in the horizontal plane (and the analyzer is in that plane), then the spectrometer setup is just that of a 4-circle diffractometer (e.g. (Busing & Levy, 1967)). However, at modern synchrotron radiation facilities, focusing elements are often placed upstream of a spectrometer to reduce the incident beam size and these can tilt the incident beam out of the horizontal plane. This is not generally compatible with a simple 4-circle geometry, but can be treated in a six-circle geometry, e.g., (Lohmeier & Vlieg, 1993).

The present paper describes the geometry and mathematics behind an open-source python based software for six circle diffraction calculations. These calculations include both the direct determination of the specific momentum transfer in the crystal system, (H,K,L), from the angles of the diffractometer, and also solve the inverse problem of determining the possible angles needed to reach a specific (H,K,L) momentum transfers. The latter is the more difficult problem, and the code solves it in the general case numerically with default precision that is typically ~0.0001 deg, or better, and that can be improved if so desired. The code was developed and operates under Python 3.7.3, numpy 1.16.4, scipy 1.3.0

The code also includes some routines specific to the IXS setups at SPring-8, allowing the calculation of the momentum transfers for arrays of analyzers as are present, at BL43LXU and BL35XU, as well as some auxiliary routines for specifying the incident beam characteristics, and for plotting the momentum transfers of the analyzer arrays.

2. Diffractometer layout and angle definitions.

The essential angles for the diffraction setup under consideration are shown in figure 1 and described in table 1. Three circles, θ, χ and ϕ determine the sample orientation in the laboratory, one circle, μ, gives the tilt of the incident beam out of the 4-circle scattering plane (the plane normal to the θ and 2θ axes) as may induced by the focusing optics, and two circles, 2θ and γ determine the position of the detector or analyzer. In the event that μ and γ are both zero, this geometry reduces to that of a 4-circle diffractometer.

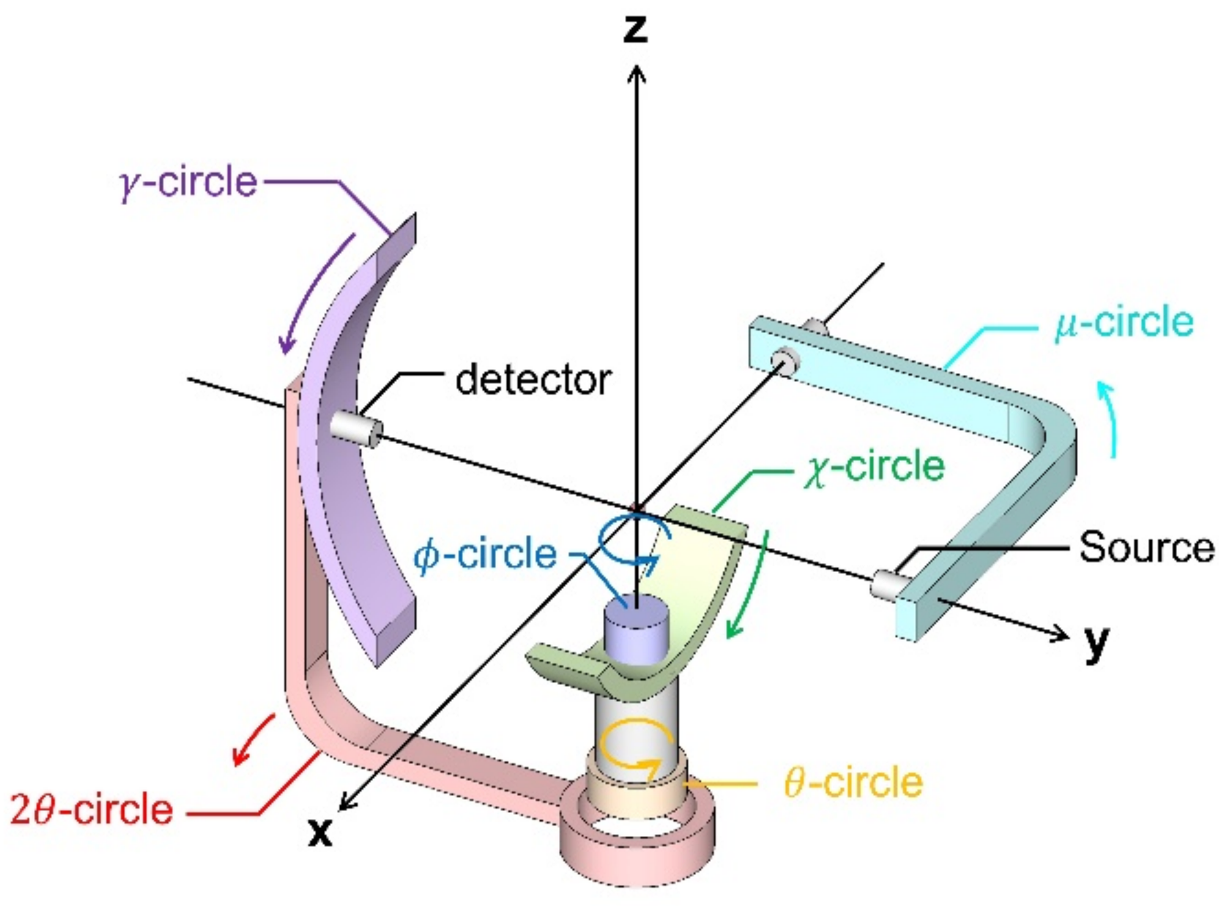

Figure 1. Schematic of the circles relative to the laboratory (xyz) reference frame. Arrows indicate direction of positive motion. See also the text and table 1.

Name	Symbol	Roman	Comment	Zero and Sign
Two-Theta	2θ	tth	Moves the detector (in the 4-circle scattering plane) Axis position/orientation is fixed in the lab Axis coincident with th. In a 4-circle geometry (mu=gam=0), this is the scattering angle.	Origin (tth=0) when the tth arm is in the plane of the incident beam. Right-Handed Motion about the z axis
Theta	θ	th	Changes the sample orientation. Axis position/orientation is fixed in the lab Axis coincident with tth	Origin (th=0) when the chi axis is in the plane of the incident beam
Chi	χ	chi	Changes the sample orientation Motion is on top of the th stage Chi axis is always perpendicular to the th/tth axes	Axis is right handed about the incident beam direction when th=0, mu=0 Chi=0 when phi and th axes coincide
Phi	ϕ	phi	Changes the sample orientation Motion is on top of the chi-stage. Phi axis is always perpendicular to the chi axis	Arbitrary zero. Coincident, and right handed, with th/tth axis when chi = 0
Mu	μ	mu	The incident beam angle relative to the plane of tth and th motion, Axis position/orientation is fixed in the lab frame	Zero if the incident beam is in the plane of th/tth motion. Positive for a downward reflected/travelling beam
Gamma	γ	gam	Moves the detector/analyzer out of the plane of th/tth motion. The axis is perpendicular to the tth/th axis and is on top of the tth arm	Zero when the detector/analyzer is in the plane of the sample and th/tth motion. Positive when above.
Omega	ω	-	Defined as omega = th-tth/2 or $\omega = \theta - 2\theta/2$	-
Azimuth	-	Az	Q-space/(H K L) reference vector – often chosen as the sample normal – for determining α, β and ψ	See text
Psi	ψ	-	Angle of **Q** about the azimuth – see text.	See text
Alpha	α	-	Grazing angle of the incident beam on the surface defined by the plane normal to the azimuthal vector	Positive when the dot-product of the incoming beam and the azimuth <0 Bragg Geometry if α,β have the same sign
Beta	β	-	Grazing angle of the outdoing beam to the surface defined by the plane normal to the azimuthal vector	Positive when the dot-product of the outgoing beam and the azimuth is >0 Laue Geometry if α,β have different signs
Scatt. Angle	SA or 2Θ	-	This is the total scattering angle as is directly related to the momentum transfer : $\lvert\boldsymbol{Q}\rvert = (4\pi/\lambda)\sin(2\Theta/2)$	Defined >=0

Table 1. Description of axes and angles

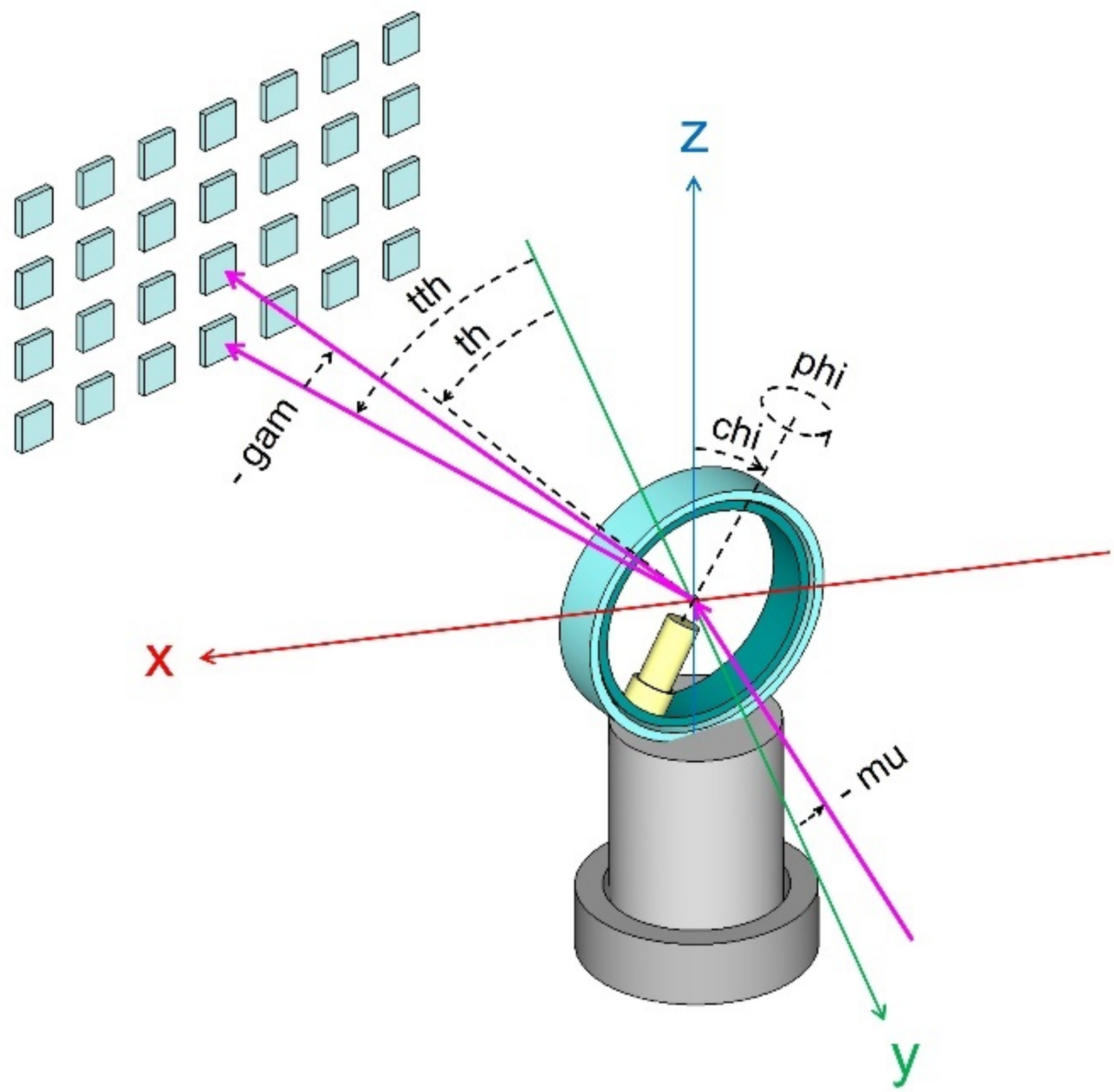

Figure 2. Schematic of the spectrometer at BL43LXU including the (4x7) analyzer array as placed at the end of the two-theta arm.

3. Rotation Matrices & Equations

Laboratory coordinates are defined as follows: the x-y plane is the horizontal plane; the positive z-axis points upward; the positive y-axis is along the line from the sample to the X-ray source (y points upstream). At BL43LXU, the positive x-axis is towards the experimental hall.

2.1 Rotation matrices

Rotation of ϕ-circle is right-handed with respect to z-axis, when $\chi = 0$.

Rotation matrix $\mathbf{\Phi}$ is:

$$\boldsymbol{\Phi} = \begin{bmatrix} cos\,\phi & -sin\,\phi & 0 \\ sin\,\phi & cos\,\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Rotation of χ-circle is left-handed with respect to y-axis, when $\theta + \omega = 0$.

Rotation matrix $\mathbf{X}$ is:

$$\boldsymbol{X} = \begin{bmatrix} cos\,\chi & 0 & -sin\,\chi \\ 0 & 1 & 0 \\ sin\,\chi & 0 & cos\,\chi \end{bmatrix}$$

Rotation of ω-circle is right-handed with respect to z-axis.

Rotation matrix $\mathbf{\Omega}$ is:

$$\boldsymbol{\Omega} = \begin{bmatrix} cos\,\omega & -\,sin\,\omega & 0 \\ sin\,\omega & cos\,\omega & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Rotation of θ-circle is right-handed with respect to z-axis.

Rotation matrix $\mathbf{\Theta}$ is:

$$\boldsymbol{\Theta} = \begin{bmatrix} cos\,\theta & -\,sin\,\theta & 0 \\ sin\,\theta & cos\,\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

For a vector $\boldsymbol{v_b}$ in reciprocal-lattice coordinates, its coordinates in laboratory system $\boldsymbol{v_l}$ is:

$$\boldsymbol{v_c} = \boldsymbol{B}\boldsymbol{v_b}$$

$$\boldsymbol{v_\phi} = \mathbf{U}\boldsymbol{v_c}$$

$$\boldsymbol{v_\chi} = \mathbf{\Phi}\boldsymbol{v_\phi}$$

$$\boldsymbol{v_\omega} = \mathbf{X}\boldsymbol{v_\chi}$$

$$\boldsymbol{v_\theta} = \mathbf{\Omega}\boldsymbol{v_\omega}$$

$$\boldsymbol{v_l} = \mathbf{\Theta}\boldsymbol{v_\theta}$$

Here, v_c is the coordinates in crystal cartesian system, $\boldsymbol{v_\phi}$, $\boldsymbol{v_\chi}$, $\boldsymbol{v_\omega}$, and $\boldsymbol{v_\theta}$ are coordinates in ϕ-stage, χ-stage, ω-stage, θ-stage systems, respectively, U is the orientation matrix, and

$$\boldsymbol{B} = \begin{bmatrix} b_1 & b_2 \cos\beta_3 & b_3 \cos\beta_2 \\ 0 & b_2 \sin\beta_3 & -b_3 \sin\beta_2 \cos\alpha_1 \\ 0 & 0 & 2\pi/a_3 \end{bmatrix},$$

where the a_i's and α_i's and the b_i's and β_i's are the direct and reciprocal lattice parameters, respectively. So far all equations are very similar to Ref [1], except that in Ref [1] it uses right-handed ration for χ and left-handed rotation for ϕ, ω, and θ, whereas this paper uses left-handed rotation for χ and right-handed rotation for ϕ, ω, and θ. The definition of these angles in this paper is consistent with that of SPEC's FOURC code.

For the primary and deflected X-ray beam, rotation of μ-circle is right-handed with respect to x-axis; rotation of 2θ-circle is right-handed with respect to z-axis; rotation of γ-circle is right-handed with respect to x-axis when 2θ=0. Therefore, the wavevector of primary beam in laboratory system is

$$\boldsymbol{p_l} = k \begin{bmatrix} 0 \\ -\cos\mu \\ -\sin\mu \end{bmatrix},$$

while the wavevector of deflected beam in laboratory system is

$$\boldsymbol{d_l} = k \begin{bmatrix} \sin 2\theta \cos\gamma \\ -\cos 2\theta \cos\gamma \\ -\sin\gamma \end{bmatrix},$$

where $k = 2\pi/\lambda$. Therefore, the scattering vector in laboratory system is

$$\boldsymbol{s}_l = k \begin{bmatrix} \sin 2\theta \cos\gamma \\ \cos\mu - \cos 2\theta \cos\gamma \\ \sin\mu - \sin\gamma \end{bmatrix}$$

When θ_d notates half of deflection angle:

$$|\boldsymbol{s_l}| = 2k \sin\theta_d = k\sqrt{2 - 2\sin\mu\sin\gamma - 2\cos\mu\cos\gamma\cos 2\theta}$$

Therefore,

$$\sin\theta_d = \frac{\sqrt{2 - 2\sin\mu\sin\gamma - 2\cos\mu\cos\gamma\cos 2\theta}}{2}$$

$$\cos 2\theta = \frac{1 - \sin\mu\sin\gamma - 2\sin^2\theta_d}{\cos\mu\cos\gamma}$$

$$\theta_d, \theta \in [0, 90°]$$

2.2 Basic equations

2.2.1 Diffraction-plane system

Considering the diffraction equation:

$$\boldsymbol{s_l} = \boldsymbol{v_l}$$

This is the basis of most six-circle calculations in this paper. For the ease of finding $\boldsymbol{s_l}$ and calculating azimuth angles ψ in following parts, a right-handed diffraction-plane system is defined: the x-y plane is the diffraction plane which contains the primary X-ray beam and the deflected X-ray beam; the positive x-axis is along $\boldsymbol{s_l}$; $\hat{\boldsymbol{z}} = \hat{\boldsymbol{x}} \times \frac{\boldsymbol{p_l}}{|\boldsymbol{p_l}|}$.

A normal matrix $\boldsymbol{D}$ is defined to translate a vector in the diffraction-plane system to the laboratory system.

$$\boldsymbol{v_l} = \boldsymbol{D}\boldsymbol{v_d}; \quad \boldsymbol{v_d} = \boldsymbol{D}^{-1}\boldsymbol{v_l}; \quad \boldsymbol{s_l} = \boldsymbol{D}\begin{bmatrix}1\\0\\0\end{bmatrix}$$

The diffraction-plane system and the corresponding matrix $\boldsymbol{D}$ is a “novel” point of this paper. It provides a flexible extension from four-circle calculation to six-circle calculation. When $\mu = 0$ and $\gamma = 0$, $\boldsymbol{D} = \boldsymbol{I}$.

2.2.2 Orientation matrix

Using above equations, one may easily find v_{c0}, $v_{\phi 0}$ and, v_{c1}, $v_{\phi 1}$for the primary reflection and the secondary reflections. The method to find orientation matrix is the same as Ref [1]. Therefore, after knowing all angles of θ, ω, χ, ϕ, μ, and γ, the scattering vector in the reciprocal-lattice system is

$$\boldsymbol{v_b} = \boldsymbol{B}^{-1}\boldsymbol{U}^{-1}\boldsymbol{\Phi}^{-1}\boldsymbol{\mathrm{X}}^{-1}\boldsymbol{\Omega}^{-1}\boldsymbol{\Theta}^{-1}\boldsymbol{D}\begin{bmatrix}1\\0\\0\end{bmatrix}$$

2.2.3 Reference vector and azimuth angle

For one reference vector (frequently normal to sample surface) $\boldsymbol{v_b}$ in the reciprocal-lattice system, its coordinates in the diffraction-plane system is

$$\boldsymbol{v_d} = \boldsymbol{D}^{-1}\boldsymbol{\Theta}\boldsymbol{\Omega}\boldsymbol{\mathrm{X}}\boldsymbol{\Phi}\boldsymbol{U}\boldsymbol{B}\boldsymbol{v_b}$$

In this paper, the azimuth angle ψ is defined as

$$\psi = \mathrm{atan}(v_{dz}, v_{dy}),$$

which means $\psi = 0$ when the reference vector is in the upper-stream side in the diffraction plane, and ψ increases if the reference vector right-handed rotates with respect to x-axis in the diffraction-plane coordinates.

To do six-circle calculation with a fixed ψ angle, firstly one finds the corresponding rotation matrix $\mathbf{\Psi}$:

$$\mathbf{\Psi} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & -\sin\psi \\ 0 & \sin\psi & \cos\psi \end{bmatrix}$$

Then, for the desired scattering vector $\boldsymbol{v_b}$ and the reference vector $\boldsymbol{n_b}$ in reciprocal-lattice system, one finds the corresponding $\boldsymbol{v_\phi}$ and $\boldsymbol{n_\phi}$ in ϕ-stage system. A 3×3 matrix could be easily obtained:

$$\boldsymbol{T_\phi} = [\boldsymbol{u_1} \quad \boldsymbol{u_2} \quad \boldsymbol{u_3}]$$

where u_1, u_2, and u_3 are unit column vectors of v_ϕ, $(v_\phi \times n_\phi) \times v_\phi$, and $v_\phi \times n_\phi$, respectively. Therefore, the basic equation of six-circle calculation is:

$$\mathbf{\Theta\Omega X\Phi T_\phi} = \boldsymbol{D\Psi I}$$

In four-circle calculation, $\boldsymbol{D} = \boldsymbol{I}$, therefore $\mathbf{\Theta\Omega X\Phi T_\phi} = \mathbf{\Psi}$. This is the same as Ref [1].

2.2.4 Incident angle α and exit angle β

One can relate incident angle α and exit angle β to the azimuth angle ψ when the reference vector is surface normal. The relation is clarified in Figure 2 below.

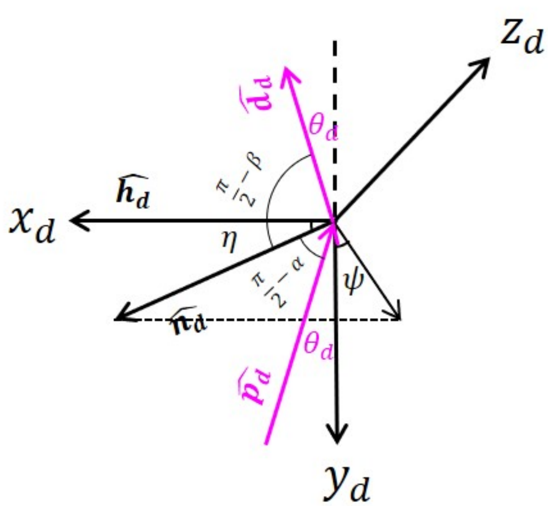

Figure 3. Relations between α, β, and ψ. Subscript 'd' represents the diffraction-plane coordinate system. Unit vectors of primary X-ray beam $\widehat{\boldsymbol{p_d}}$ and deflected X-ray beam $\widehat{\boldsymbol{d_d}}$ are in the x_d-y_d plane. Angle η is between the scattering vector $\widehat{\boldsymbol{h_d}}$ and the reference vector $\widehat{\boldsymbol{n_d}}$.

One then has

$$\widehat{\boldsymbol{n_d}} = \begin{bmatrix} \cos\eta \\ \sin\eta\cos\psi \\ \sin\eta\sin\psi \end{bmatrix} \qquad -\widehat{\boldsymbol{p_d}} = \begin{bmatrix} \sin\theta_d \\ \cos\theta_d \\ 0 \end{bmatrix} \qquad \widehat{\boldsymbol{d_d}} = \begin{bmatrix} \sin\theta_d \\ -\cos\theta_d \\ 0 \end{bmatrix}$$

Therefore, for a specified α,

$$\sin\alpha = \cos(90-\alpha) = \frac{\boldsymbol{n_d}\cdot(-\boldsymbol{p_r})}{|\boldsymbol{n_d}||-\boldsymbol{p_d}|}$$

$$\cos\psi = \frac{\sin\alpha - \sin\theta_d\cos\eta}{\cos\theta_d\sin\eta}$$

$$\psi_1 = atan\left(\sqrt{1-\cos^2\psi}, \cos\psi\right) \qquad \psi_2 = atan\left(-\sqrt{1-\cos^2\psi}, \cos\psi\right)$$

For a specified β,

$$\sin\beta = \cos(90-\beta) = \frac{\boldsymbol{n_d}\cdot\boldsymbol{d_d}}{|\boldsymbol{n_d}||\boldsymbol{d_d}|}$$

$$\cos\psi = \frac{\cos\eta\sin\theta_d - \sin\beta_d}{\cos\theta_d\sin\eta}$$

$$\psi_1 = atan2\left(\sqrt{1-\cos^2\psi}, \cos\psi\right) \qquad \psi_2 = atan2\left(-\sqrt{1-\cos^2\psi}, \cos\psi\right)$$

In this way, six-circle calculation with fixed α or fixed β could be converted to calculation with fixed ψ.

From Figure 2 it is easy to find the range of α and β as

$$\left[max\left(-\frac{\pi}{2}, \theta_d - \eta\right), min\left(\frac{\pi}{2}, \theta_d + \eta\right)\right]$$

3. Implementation

3.1 Frozen modes

The present software uses numerical approximation to do calculation. Direct inverse equations are also possible in some special frozen modes, as displayed in Appendix (to be continued).

3.2 Extension

The present open-source software provides convenience for users to develop their own toolkits, to deal with problems like multi-domain samples, etc.

4. References

Baron, A. Q. . (2016). "Introduction to High Resolution Inelastic X-ray Scattering I&II" *Synchrotron Light Sources and Free-Electron Lasers: Accelerator Physics, Instrumentation and Science Applications*, , edited by E. Jaeschke, S. Khan, J.R. Schneider, & J.B. Hastings, pp. 1643-1757 See also arXiv 1504.01098. Cham: Springer International Publishing. http://arxiv.org/abs/1504.01098.

Busing, W. R. & Levy, H. A. (1967). "Angle Calculations for 3- and 4- Circle X-ray and Neutron Diffraetometers" *Acta Crystallogr.* **22**, 467.

Lohmeier, M. & Vlieg, E. (1993). "Angle calculations for a six-circle surface X-ray diffractometer" *J. Appl. Crystallogr.* **26**, 706–716. DOI: 10.1107/S0021889893004868.

Appendix. Analytical equations of specific frozen modes

For BL43LXU at SPring-8, μ and γ are frequently fixed and cannot be changed arbitrarily: μ is fixed by upstream optical components like KB mirrors, and γ is fixed by the installation location of analyzers. Here examples are given to show analytical equations of specific frozen modes with μ and γ fixed.

Knowing lattice parameters and X-ray wavelength, we obtain θ_d and θ when μ and γ are fixed (Eq. Red). Knowing matrix UB, it is easy to obtain the scattering vector in ϕ-system. Let

$$h_b = \begin{bmatrix} H \\ K \\ L \end{bmatrix}$$

Then the scattering vector $\boldsymbol{h_\phi}$ in ϕ-system:

$$\boldsymbol{h_\phi} = \boldsymbol{UBh_b} \qquad \frac{\boldsymbol{h_\phi}}{|\boldsymbol{h_\phi}|} = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix}$$

h_ϕ may also be expressed as:

$$\boldsymbol{h_\phi} = \boldsymbol{\Phi^{-1}X^{-1}\Omega^{-1}\Theta^{-1}D} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Taking

$$\boldsymbol{\mu} = \boldsymbol{\Theta^{-1}D} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \text{ and } \frac{\boldsymbol{\mu}}{|\boldsymbol{\mu}|} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{bmatrix}$$

And

$$\boldsymbol{\Phi^{-1}X^{-1}\Omega^{-1}} = \boldsymbol{\Phi^T X^T \Omega^T}$$
$$= \begin{bmatrix} \cos\phi\cos\chi\cos\omega - \sin\phi\sin\omega & \cos\phi\cos\chi\sin\omega + \sin\phi\cos\omega & \cos\phi\sin\chi \\ -\sin\phi\cos\chi\cos\omega - \cos\phi\sin\omega & -\sin\phi\cos\chi\sin\omega + \cos\phi\cos\omega & -\sin\phi\sin\chi \\ -\sin\chi\cos\omega & -\sin\chi\sin\omega & \cos\chi \end{bmatrix}$$

gives:

$$h_1 = u_1(\cos\phi\cos\chi\cos\omega - \sin\phi\sin\omega) + u_2(\cos\phi\cos\chi\sin\omega + \sin\phi\cos\omega) + u_3\cos\phi\sin\chi \quad (1)$$

$$h_2 = u_1(-\sin\phi\cos\chi\cos\omega - \cos\phi\sin\omega) + u_2(-\sin\phi\cos\chi\sin\omega + \cos\phi\cos\omega) + u_3(-\sin\phi\sin\chi) \quad (2)$$

$$h_3 = u_1(-\sin\chi\cos\omega) + u_2(-\sin\chi\sin\omega) + u_3\cos\chi \quad (3)$$

This is the equation set (1), (2), (3) used in A1 and A2.

A1. Solving χ, ϕ when ω is fixed

From (3):

$$\cos\chi = \frac{1}{\mu_3}[h_3 + (\mu_1\cos\omega + \mu_2\sin\omega)\sin\chi]$$

As

$$\sin^2\chi + \cos^2\chi = 1$$

a simple one-variable quadratic equation could be obtained:

$$[u_3^2 + (u_1\cos\omega + u_2\sin\omega)^2]\sin^2\chi + 2h_3(u_1\cos\omega + u_2\sin\omega)\sin\chi + (h_3^2 - u_3^2) = 0$$

Let

$$a = u_3^2 + (u_1\cos\omega + u_2\sin\omega)^2,\ b = 2h_3(u_1\cos\omega + u_2\sin\omega),\ c = (h_3^2 - u_3^2)$$

Then

$$\sin\chi_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \qquad \sin\chi_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}$$

If $u_3 \neq 0$,

$$\cos\chi_1 = \frac{1}{\mu_3}[h_3 + (\mu_1\cos\omega + \mu_2\sin\omega)\sin\chi_1]$$

$$\cos\chi_2 = \frac{1}{\mu_3}[h_3 + (\mu_1\cos\omega + \mu_2\sin\omega)\sin\chi_2]$$

If $u_3 = 0$,

$$b^2 - 4ac = 0,\ \sin\chi_1 = \sin\chi_2$$

$$\cos\chi_1 = \sqrt{1 - \sin^2\chi_1} \qquad \cos\chi_2 = -\sqrt{1 - \sin^2\chi_2}$$

Then

$$\chi = atan(\sin\chi, \cos\chi)$$

From (1) and (2):

$$\cos\phi\,(u_1\cos\chi\cos\omega + u_2\cos\chi\sin\omega + u_3\sin\chi) + \sin\phi\,(-u_1\sin\omega + u_2\cos\omega) = h_1$$

$$\cos\phi\,(-u_1\sin\omega + u_2\cos\omega) + \sin\phi\,(-u_1\cos\chi\cos\omega - u_2\cos\chi\sin\omega - u_3\sin\chi) = h_2$$

Let:

$$m = u_1\cos\chi\cos\omega + u_2\cos\chi\sin\omega + u_3\sin\chi$$

$$n = -u_1\sin\omega + u_2\cos\omega$$

$$p = -u_1 \sin\omega + u_2 \cos\omega$$

$$q = -u_1 \cos\chi \cos\omega - u_2 \cos\chi \sin\omega - u_3 \sin\chi$$

Then

$$\sin\phi = \frac{mh_2 - ph_1}{mq - pn} \qquad \cos\phi = \frac{qh_1 - nh_2}{mq - pn}$$

$$\phi = atan(\sin\phi, \cos\phi)$$

Specially, when $\delta = \gamma = 0$, six-circle calculation degenerates to four-circle calculation. In this case,

$$\sin\chi = -\frac{h_3}{\cos\omega}$$

$$\chi_1 = atan\left(\sin\chi, \sqrt{1 - \sin^2\chi}\right) \qquad \chi_2 = atan\left(\sin\chi, -\sqrt{1 - \sin^2\chi}\right)$$

$$\sin\phi = -\frac{h_1 \sin\omega + h_2 \cos\omega \cos\chi}{\sin^2\omega + \cos^2\chi \cos^2\omega} \qquad \cos\phi = \frac{h_1 \cos\chi \cos\omega - h_2 \sin\omega}{\sin^2\omega + \cos^2\chi \cos^2\omega}$$

$$\phi = atan(\sin\phi, \cos\phi)$$

A2. Solving ω, ϕ when χ is fixed

From (3):

$$\cos\omega = -\frac{u_2 \sin\chi \sin\omega + h_3 - u_3 \cos\chi}{u_1 \sin\chi}$$

As

$$\sin^2\omega + \cos^2\omega = 1$$

a simple one-variable quadratic equation can be obtained:

$$(u_1^2 + u_2^2)\sin^2\chi \sin^2\omega + 2u_2 \sin\chi (h_3 - u_3 \cos\chi)\sin\omega + (h_3 - u_3\cos\chi)^2 - u_1^2 \sin^2\chi = 0$$

Again, let

$a = (u_1^2 + u_2^2)\sin^2\chi$, $b = 2u_2 \sin\chi(h_3 - u_3\cos\chi)$, and $c = (h_3 - u_3\cos\chi)^2 - u_1^2\sin^2\chi$

Then the solution of $\sin\omega$:

$$\sin\omega_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \qquad \sin\omega_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}$$

If $u_1 \neq 0$:

$$\cos\omega_1 = -\frac{u_2 \sin\chi \sin\omega_1 + h_3 - u_3\cos\chi}{u_1 \sin\chi}$$

$$\cos\omega_2 = -\frac{u_2 \sin\chi \sin\omega_2 + h_3 - u_3\cos\chi}{u_1 \sin\chi}$$

If $u_1 = 0$:

$$b^2 - 4ac = 0, \qquad \sin\omega_1 = \sin\omega_2:$$

$$\cos\omega_1 = \sqrt{1-\sin^2\omega_1} \qquad \cos\omega_2 = -\sqrt{1-\sin^2\omega_2}$$

Then

$$\omega = atan(sin\,\omega\,, cos\,\omega)$$

Again, similar to A1, from (1) and (2):

$$\cos\phi\,(u_1\cos\chi\cos\omega + u_2\cos\chi\sin\omega + u_3\sin\chi) + \sin\phi\,(-u_1\sin\omega + u_2\cos\omega) = h_1$$

$$\cos\phi\,(-u_1\sin\omega + u_2\cos\omega) + \sin\phi\,(-u_1\cos\chi\cos\omega - u_2\cos\chi\sin\omega - u_3\sin\chi) = h_2$$

Let:

$$\mathrm{m} = u_1\cos\chi\cos\omega + u_2\cos\chi\sin\omega + u_3\sin\chi$$

$$n = -u_1\sin\omega + u_2\cos\omega$$

$$p = -u_1\sin\omega + u_2\cos\omega$$

$$q = -u_1\cos\chi\cos\omega - u_2\cos\chi\sin\omega - u_3\sin\chi$$

Then:

$$\sin\phi = \frac{mh_2 - ph_1}{mq - pn} \qquad \cos\phi = \frac{qh_1 - nh_2}{mq - pn}$$

$$\phi = atan(\sin\phi\,, \cos\phi)$$

Specially, when $\delta = \gamma = 0$, six-circle calculation degenerates to four-circle calculation. In this case:

$$\cos\omega = -\frac{\mu_3}{\sin\chi}$$

Therefore:

$$\omega_1 = atan\left(\sqrt{1-\cos^2\omega}\,, \cos\omega\right) \qquad \omega_2 = atan\left(-\sqrt{1-\cos^2\omega}\,, \cos\omega\right)$$

And also

$$\sin\phi = -\frac{h_1 \sin\omega + h_2 \cos\omega \cos\chi}{\sin^2\omega + \cos^2\chi \cos^2\omega}$$

$$\cos\phi = \frac{h_1 \cos\chi \cos\omega - h_2 \sin\omega}{\sin^2\omega + \cos^2\chi \cos^2\omega}$$

$$\phi = atan(\sin\phi, \cos\phi)$$

A3. Solving ω, χ when ϕ is fixed

The equation set (1), (2), and (3) could be simplified. This time let's use the unit scattering vector in χ-system.

$$\mathbf{X^{-1}\Omega^{-1}}\boldsymbol{u} = \boldsymbol{h_\chi}$$

Here

$$\boldsymbol{h_\chi} = \boldsymbol{\Phi U B h_b} \qquad \frac{\boldsymbol{h_\chi}}{|\boldsymbol{h_\chi}|} = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix}$$

As

$$\mathbf{X^{-1}\Omega^{-1}} = \widetilde{\boldsymbol{X}}\widetilde{\boldsymbol{\Omega}} = \begin{bmatrix} \cos\chi \cos\omega & \cos\chi \sin\omega & \sin\chi \\ -\sin\omega & \cos\omega & 0 \\ -\sin\chi \cos\omega & -\sin\chi \sin\omega & \cos\chi \end{bmatrix}$$

An equation set is obtained:

$h_1 = u_1 \cos\chi \cos\omega + u_2 \cos\chi \sin\omega + u_3 \sin\chi$ …(1*)

$h_2 = -u_1 \sin\omega + u_2 \cos\omega$ …(2*)

$h_3 = -u_1 \sin\chi \cos\omega - u_2 sin\chi \sin\omega + u_3 \cos\chi$ …(3*)

From (2*):

$$\cos\omega = \frac{h_2 + u_1 \sin\omega}{u_2}$$

As

$$\sin^2\omega + \cos^2\omega = 1$$

a one-variable quadratic equation could be obtained:

$$a \sin^2\omega + b \sin\omega + c = 0$$

where $a = u_1^2 + u_2^2,\ b = 2u_1 h_2, c = h_2^2 - u_2^2$

Therefore

$$\sin\omega_1 = \frac{-b+\sqrt{b^2-4ac}}{2a} \quad \sin\omega_2 = \frac{-b-\sqrt{b^2-4ac}}{2a}$$

If $u_2 \neq 0$,

$$\cos\omega_1 = \frac{h_2+u_1\sin\omega_1}{u_2} \qquad \cos\omega_2 = \frac{h_2+u_1\sin\omega_2}{u_2}$$

If $u_2 = 0$,

$$b^2-4ac = 0, \qquad \sin\omega_1 = \sin\omega_2$$

$$\cos\omega_1 = \sqrt{1-\sin^2\omega_1} \qquad \cos\omega_2 = -\sqrt{1-\sin^2\omega_2}$$

Then

$$\omega = atan(\sin\omega, \cos\omega)$$

From (1*) (2*):

$$u_3\sin\chi + (u_1\cos\omega + u_2\sin\omega)\cos\chi = h_1$$

$$-(u_1\cos\omega + u_2\sin\omega)\sin\chi + u_3\cos\chi = h_3$$

So we get:

$$\cos\chi = \frac{h_3m+h_1n}{m^2+n^2} \qquad \sin\chi = \frac{h_1m-h_3b}{m^2+n^2}$$

where

$$m = u_3, n = u_1\cos\omega + u_2\sin\omega$$

Therefore

$$\chi = \text{atan}\,(\sin\chi, \cos\chi)$$

Specially, when $\delta = \gamma = 0$, six-circle calculation degenerates to four-circle calculation. In this case:

$$\sin\chi\cos\omega = -h_3$$

$$\cos\chi\cos\omega = h_1\cos\phi - h_2\sin\phi$$

Therefore

$$\chi_1 = atan(sin\chi\, cos\,\omega, cos\,\chi\, cos\,\omega)$$

$$\chi_2 = atan(-\sin\chi\cos\omega, -\cos\chi\cos\omega)$$

Then

$$\cos\omega = -\frac{h_3}{\sin\chi}$$

$$\sin\omega = -\frac{h_1 + h_2 + \cos\omega\cos\chi\,(\sin\phi - \cos\phi)}{\cos\phi + \sin\phi}$$

and

$$\omega = atan(\sin\omega\,, \cos\omega)$$