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Contents

SX-Description of Small- and Wide-Angle Scattering

A subset of the following parametrization of small and wide angle scattering data is currently used for monochromatic small-angle and wide angle scattering experiments at the ESRF (ID02). It is called SX-parametrization[1]. The parameter list can be expanded to adapt it to specific applications, i.e scanning diffractometry, anomalous scattering, grazing incidence scattering, tomography.

One goal of this description is to list all parameters that are needed to analyze monochromatic elastic scattering experiments. The explicit use of them or their names given here are not mandatory but it must at least be possible to calculate them from available experimental parameters. For example, in some cases it can be better to use the point as reference where the primary beam hits the detector (beam center) than the point of normal incidence (center) where the detector normal points to the scattering center, in other words, the point with the smallest distance to the scattering center. Fig. 1 shows the standard setup of a small angle scattering experiment with a flat 2D detector perpendicular to the primary beam.

Basic Geometry (concept)

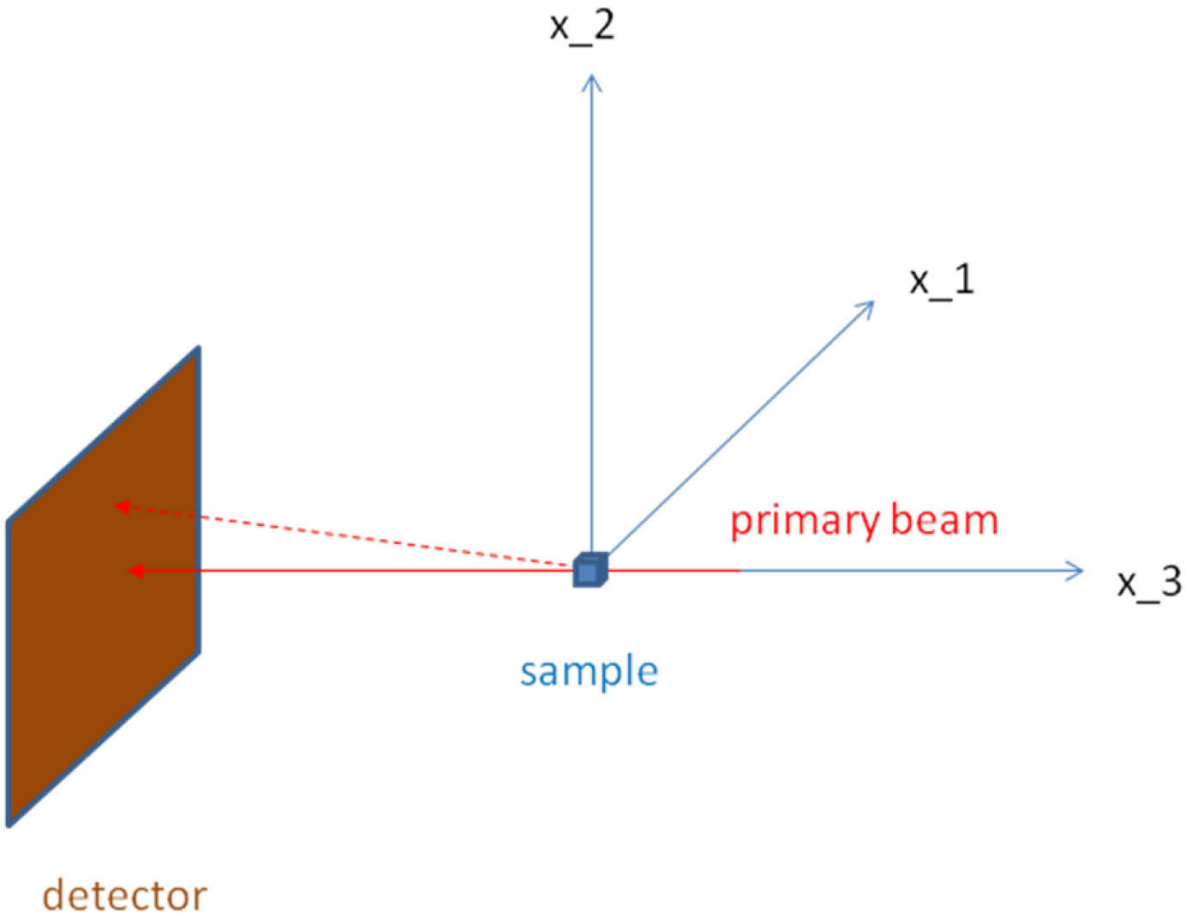

Fig. 1 Small angle scattering standard configuration: coordinate axes, primary beam (red), scattered beam (dashed red), sample (blue), detector (brown)

[1] SX shortening of SAXS for the geometry used in the SAXS programs.

A simple SAS experiment with a flat 2D detector needs the following parameters:

- *Dim_1, Dim_2* (dimensions of the array)
- *Offset_1, Offset_2* (offset of the coordinates, used for region of interest, otherwise 0)
- *PSize_1, PSize_2* (pixel sizes)
- *WaveLength* (monochromatic wavelength)
- *Center_1, Center_2* (point on the detector where the normal points to the sample)
- *SampleDistance* (distance between sample and detector *Center*)

These parameters have been defined starting with a 2D scattering pattern and performing step by step the necessary tasks, e.g. searching for the center of the scattering pattern, determining the pixel size, the distance between sample and detector and the wavelength. The viewpoint is generally the detector. Even if the parameters seem to be "self-explaining" care should be taken to use always their correct definitions.

The parametrization is based on a right-handed orthogonal coordinate system with horizontal axis 1, vertical axis 2 and longitudinal axis 3 pointing against the primary beam (see Fig. 1). The sensitive detector area with Dim_1 x Dim_2 pixels is coplanar with the x_1, x_2 plane. The distance between sample and detector (*SampleDistance*) can be changed by moving it along axis x_3. The detector can also be moved in the detector plane. Generally, all translations are given in the internal system of the element and are pointing to the origin of the translation, which is the scattering center. Rotations are sequential counter-clockwise rotations around laboratory axis 1, 2 and 3 (see Fig. 2).

A detector pattern is interpreted as observed from the front, the active side. Even if the display program flips the image it must always be interpreted using the detector axes as reference.

The scattering vectors **s** can be calculated in the following way (definition of k without 2π for convenience, $\mathbf{e_1}$, $\mathbf{e_2}$, $\mathbf{e_3}$ are unit vector along the axes x_1, x_2, x_3. i1, i2 are pixel coordinates):

(1) $\mathbf{s} = (\mathbf{s_1}, \mathbf{s_2}, \mathbf{s_3}) = \mathbf{k'} - \mathbf{k}$, where

(2) $\mathbf{k} = -1/\mathit{WaveLength} \cdot \mathbf{e_3}$

(3) $\mathbf{k'} = 1/\mathit{WaveLength} \cdot ((i1+\mathit{Offset\_1}-\mathit{Center\_1}) \cdot \mathit{PSize\_1} \cdot \mathbf{e_1} + (i2+\mathit{Offset\_2}-\mathit{Center\_2}) \cdot \mathit{PSize\_2} \cdot \mathbf{e_2} - \mathit{SampleDistance} \cdot \mathbf{e_3}) / \|(\ldots)\|$

In general, the components of **s** should be calculated along the sample axes. If the sample is not rotated (default) they are still parallel to the detector axes and the components of **s** can be approximated for small scattering angles $2\vartheta << 1$ using $\tan(2\vartheta) \approx \sin(2\vartheta)$:

(4) $\mathbf{s_1} \approx ((i1+\mathit{Offset\_1}-\mathit{Center\_1}) \cdot \mathit{PSize\_1})/(\mathit{SampleDistance} \cdot \mathit{WaveLength}) \cdot \mathbf{e_1}$

(5) $\mathbf{s_2} \approx ((i2+\mathit{Offset\_2}-\mathit{Center\_2}) \cdot \mathit{PSize\_2})/(\mathit{SampleDistance} \cdot \mathit{WaveLength}) \cdot \mathbf{e_2}$

(6) $\mathbf{s_3} \approx 0$

To facilitate calculation and comparison all parameter values use basic SI-units without prefix, e.g. WaveLength is given in meters and not in nanometers, even if this would avoid extrem small or big numbers. These transformations must be done by the analysis or display programs. The equations (4-6) are affine transformations of the pixel coordinates i1 and i2 to

approximate the scattering vector. But affine transformation are also useful for other purposes. Several other affine transformations of pixel coordinates, called reference systems, are in use. This illustrates also the general usage of these parameters:

a) *image* coordinate: pixel coordinate + *Offset*

b) *real* coordinate: image coordinate · *PSize*

c) *center* coordinate: image coordinate - *Center*

d) *normal* coordinate: center coordinate · *PSize*

e) *tangens* coordinate: normal coordinate / *SampleDistance*

f) *saxs* coordinate: tangens coordinate / (*WaveLength* · 10^9)

The factor 10^9 for saxs coordinates is used to avoid big numbers. In this way saxs-coordinates are expressed in 1/nm while *WaveLength* is given in meters.

In the reference system *image* a full image and ROIs are analyzed identically. Scattering patterns taken at different distances can be compared and easily combined in the reference systems *tangens* or *saxs*.

Even if saxs coordinates are approximations of the scattering vector **s** for small scattering angles 2ϑ (around the *Center*) they are useful for display of saxs data. The calculation of the scattering vector inside a program should always be correct for small and large scattering angles.

Reference systems help to choose an adequate set of parameters for data analysis and correction. A detector flatfield correction does not require other parameters than dim, offset and binning size (see below) to place the flatfield correctly. Pixel size, wavelength etc. are not needed here and probably not known at this step.

Prerequisites and Desired Properties

1. description of a scattering pattern taken with a monochromatic primary beam
2. scattering volume cross section << distance to detector
3. orthogonal right-handed coordinate system
4. counter-clockwise rotations around coordinate axes
5. coordinate axes are numbered starting with 1
6. upgradable to higher dimensions and additional objects
7. identical description of detector and sample movements
8. unique geometry to describe translation and rotations, applicable to the detector, sample and future objects
9. the basic detector and sample coordinate systems coincide for zero rotations and zero translations, the origin is the (ideal) scattering center, translations correspond to the translation relative to the (ideal) scattering center, rotations are counter-clockwise around the (ideal) scattering center for the given translation. They are applied sequentially starting with axis 1.
10. possibility to use several detectors in parallel

11. possibility to use or convert coordinate systems that do not coincide with the basic coordinate system, e.g. to describe in an identical way scattering patterns of detectors with different geometrical readouts.
12. the refinement of geometrical parameters (detector rotation, pixel size, distance, wavelength) is independent of the actual orientation of the coordinate system.
13. possibility to interpret small angle scattering data without need to take into account all specialities, e.g. coordinate system orientations and rotations.
14. use of basic SI-units (without prefix) when not differently specified.
15. Absolute dates and times should be saved as strings as described in ISO 8601, preferably like YYYY-MM-DDThh:mm:ss[.ssssss]+ZZZZ, where Z is the time zone offset, e.g. 2012-02-16T16:45:00+0100 or 2012-02-16T16:45:00.123456+0100 if higher precision is required.

Conventions

Arrays and Indices

Array indices are counted from 1 to length-1 in each direction. A linear array has the rank 1, a two dimensional array has the rank 2 etc. The array sizes are given by Dim_1 x ... x Dim_N where N is the rank of the array and Dim_1 to Dim_N the range of the array indices along axis_1 to axis_N. The default of Dim_1 is 0 and 1 for all others. This allows to read a lower dimensional array as an higher dimensional array. The standard sorting of array elements is: first index runs faster, e.g. for the 3D array V[Dim_1, Dim_2, Dim_3]: V_{ijk} = i+j·Dim_1+k·Dim_1·Dim_2. The sorting of the elements is given by the parameter DataRasterConfiguration (default 1).

Reserved Suffix for Indexed Parameters

An underscore at the end of a parameter followed by a number ("<key>_1") is used to label parameters along spatial directions, e.g. PSize_1 is the pixel size along axis 1, Rotation_1 is a rotation around axis 1, e.g. *Center* is a short notation for (*Center_1*, *Center_2*). Therefore, the intensities before and after the sample must not have underscores: Intensity0, Intensity1.

Units

Without a unit specification all distances are in meter.

Without a unit specification all angles are in radians.

Other units than basic SI-units are possible as long as they are specified and the conversions are linear, e.g. the conversion between the absolute scales of Kelvin and Celsius is not linear. Therefore only Kelvin (degK) can be used. The use of inches for length is possible because the conversion between meter and inches is linear.

Pixel and Image Coordinates

Coordinates are used to specify fractional positions in arrays. To avoid unwanted shifts, e.g. of the center, it is important to use a single coordinate definition. The choice is arbitrary, but to set the lower edge (p0) to zero facilitates the use of region of interests in combination with binning. In this way the position along each axis of an image array is described in the following way (see Fig. 1).

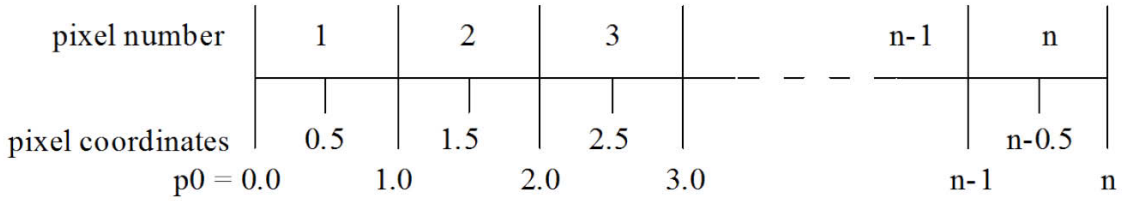

Fig. 2 Pixel coordinates (p0=0.0: pixel coordinate of lower edge, n: pixel coordinate of upper edge).

The width of each pixel is defined as one. With this definition pixel number 1 covers the pixel coordinate range between 0.0 and 1.0, pixel number 2 from 1.0 to 2.0 and the last pixel the pixel coordinate range between n-1 and n. The centers of pixels are 0.5, 1.5, etc.
To facilitate the use of region of interests image coordinates have beed defined that contain additionally the offset value:

(7) image coordinate = pixel coordinate + offset

Pixel coordinates in the full image and image coordinates in regions of interest are identical. Specific positions on the detector image are given in image coordinates, e.g. Center_1, Center_2.

Basic Small Angle Scattering Geometry

Geometrical Standard Parameters

- *Dim_1, Dim_2* (dimensions of the array)
- *Offset_1, Offset_2* (offset of the coordinates, used for region of interest, otherwise 0)
- *PSize_1, PSize_2* (pixel sizes)
- *WaveLength* (monochromatic wavelength)
- *Center_1, Center_2* (point on the detector where the normal points to the sample)
- *SampleDistance* (distance between sample and detector *Center*)

Configuration

primary beam (longitudinal)

sample

detector after sample mounted (perfectly) perpendicular to primary beam (horizontal, vertical)

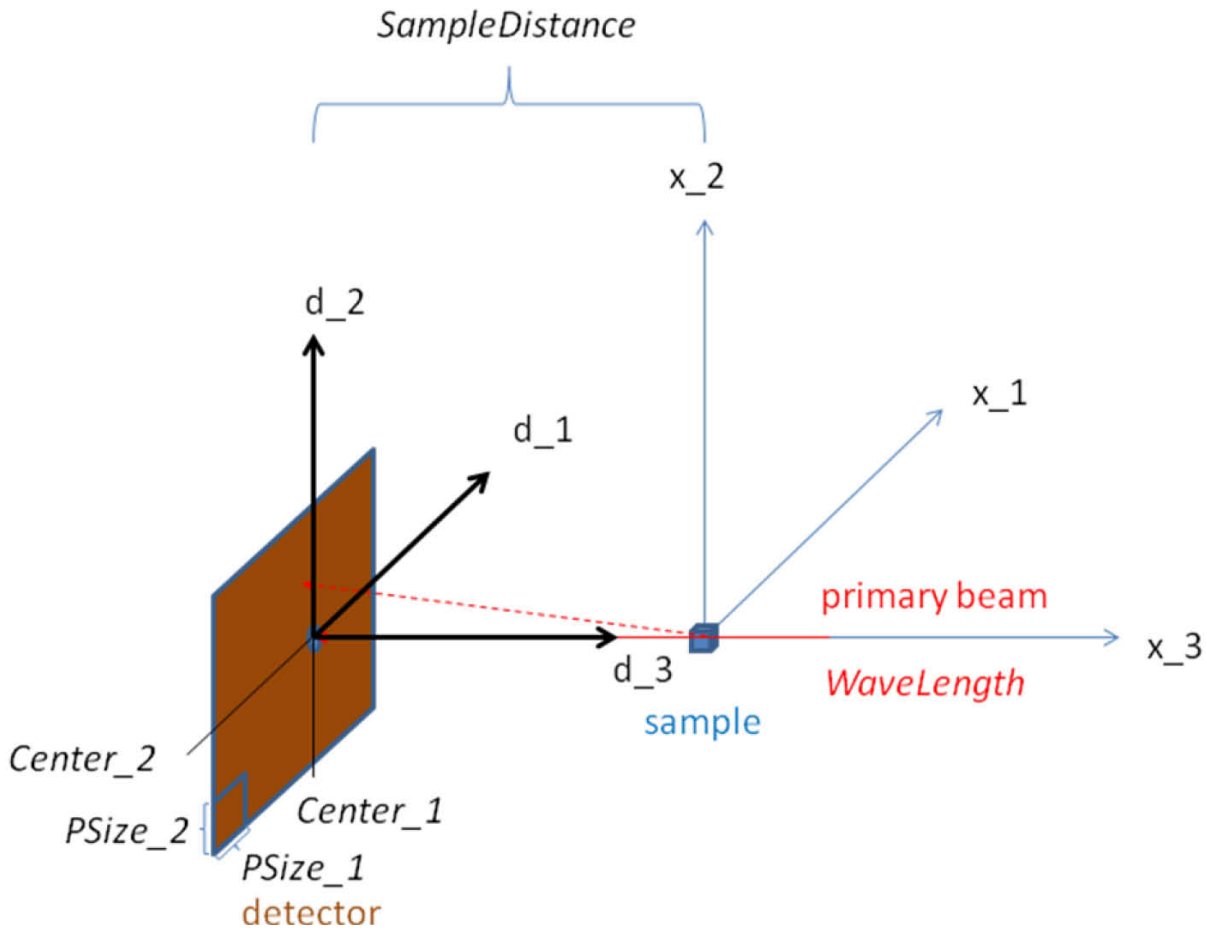

Fig. 3 Small angle scattering standard parameters (italic): *WaveLength*, *SampleDistance*, *Center_1*, *Center_2*, *PSize_1*, *PSize_2*

In the following the parameter names used for SX are given in parentheses

Basic Parameters for Rastered Detectors

actual number of pixels in each direction (*Dim_1*, *Dim_2*)

actual pixel sizes (*PSize_1*, *PSize_2*)

actual index offset of start pixel (to describe ROIs) (*Offset_1*, *Offset_2*)

actual binning size relative to unbinned detector (*BSize_1*, *BSize_2*)

Basic SAS Parameters

basic parameters for rastered detectors

wavelength

integrated photon flux during exposure before and after sample

a) POINT OF NORMAL INCIDENCE ON DETECTOR (standard set, used if available)

detector point of the normal that points to the scattering center (*Center_1*, *Center_2*)
length of the detector normal that points to the scattering center (*SampleDistance*)

b) POINT OF BEAM INCIDENCE ON DETECTOR (alternative set, only used if standard parameter set is missing)

point of incidence of primary beam on detector (*BeamCenter_1*, *BeamCenter_2*)
distance between sample and point of incidence of primary beam on detector (*BeamDistance*)

In the unrotated case (SAS geometry) (*Center_1*, *Center_2*) are identical to (*BeamCenter_1*, *BeamCenter_2*) and *SampleDistance* is identical to *BeamDistance*.

Basic Wide Angle Scattering Geometry

Geometrical Standard Parameters

- *Dim_1*, *Dim_2* (dimensions of the array)
- *Offset_1*, *Offset_2* (offset of the coordinates, used for region of interest, otherwise 0)
- *PSize_1*, *PSize_2* (pixel sizes)
- *WaveLength* (monochromatic wavelength)
- *Center_1*, *Center_2* (point on the detector where the normal points to the sample)
- *SampleDistance* (distance between sample and detector *Center*)
- *DetectorRotation_1*, *DetectorRotation_2*, *DetectorRotation_3* (detector rotations)

Configuration

The wide angle and small angle descriptions coincide for zero detector rotations. In wide angle scattering the detector can be rotated around the scattering center (sample). The point of normal incidence of a scattered beam on the detector and the point of incidence of the primary beam on the detector are in general different. The basic small angle scattering parametrization for the detector translation is kept. The small angle geometry becomes a special case of the wide angle scattering geometry for zero detector rotations.

In SX-parametrization the translation that moves the origin of the detector back to the scattering origin (sample) is implicitly given and can be calculated as (see Fig. 9):

$$DetectorTranslation = \begin{pmatrix} Center\_1 * PSize\_1 \\ Center\_2 * PSize\_2 \\ \text{SampleDistance} \end{pmatrix} \tag{8}$$

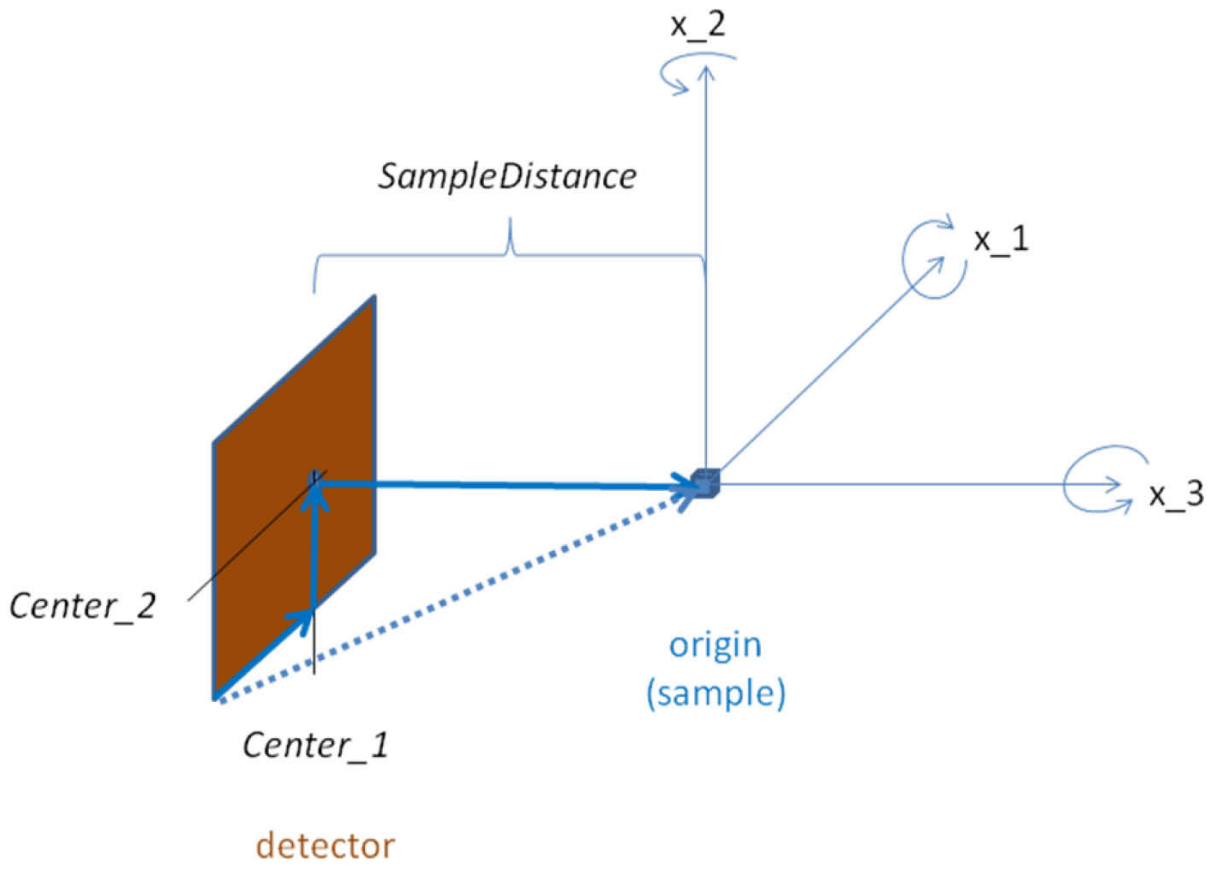

Fig. 4 Detector translation: The dotted line is the detector translation. It starts at the lower left corner (origin) and points to the sample (origin). The thick blue lines are the components along the detector axes and are used in the SX-parametrization. They must be available as parameters together with the data.

Rotations are parametrized by sequentila rotation around axis 1, 2 and 3[2]. Rotations are counter-clockwise and sequentially applied to the detector coordinates. The first rotation is around axis x_1, then around x_2 and finally around x_3. The center must now be interpreted as point of normal incidence (PoNI) and not as as the center of the primary beam.

The detector rotation matrix is:

$$(9) \qquad DetectorRotation(rot1, rot2, rot3) = \begin{pmatrix} c1\,c3 & s1\,s2\,c3 - c1\,s3 & c1\,s2\,c3 + s1\,s3 \\ c2\,s3 & c1\,c3 + s1\,s2\,s3 & c1\,s2\,s3 - s1\,c3 \\ s2 & s1\,c2 & c1\,c2 \end{pmatrix}$$

with rot1 = *DetectorRotation_1*, rot2 = *DetectorRotation_2*, rot3 = *DetectorRotation_3*, c1=cos(rot1), s1=sin(rot1), c2=cos(rot2) etc. The principal ranges are

$$(10) \qquad rot1 \;]\, -\pi \;..\; +\pi \;[,\; rot2 \;[\, -\pi/2 \;..\; +\pi/2 \,],\; rot3 \;]\, -\pi \;..\; +\pi \;[$$

In the case that the detector is rotated by a rotation R around the scattering center a pixel coordinate i1,i2 on the detector is observed from the origin as:

[2] Alternatively, the rotation matrix could be given directly. It is currently not used.

$$(11) \qquad DetectorCoordinate(i1,i2) = R^{-1} \cdot \begin{pmatrix} (i1 + Offset\_1 - Center\_1) * PSize\_1 \\ (i2 + Offset\_2 - Center\_2) * PSize\_2 \\ -\text{SampleDistance} \end{pmatrix}$$

From (11) the direction of the scattered beam and the components of the scattering vector **s** can be calculated in the laboratory (scattering center) reference system or the sample reference system when the sample rotation angles are given.

Basic WAS Parameters

Basic SAS parameter

Detector rotations (DetectorRotation_1, DetectorRotation_2, DetectorRotation_3)

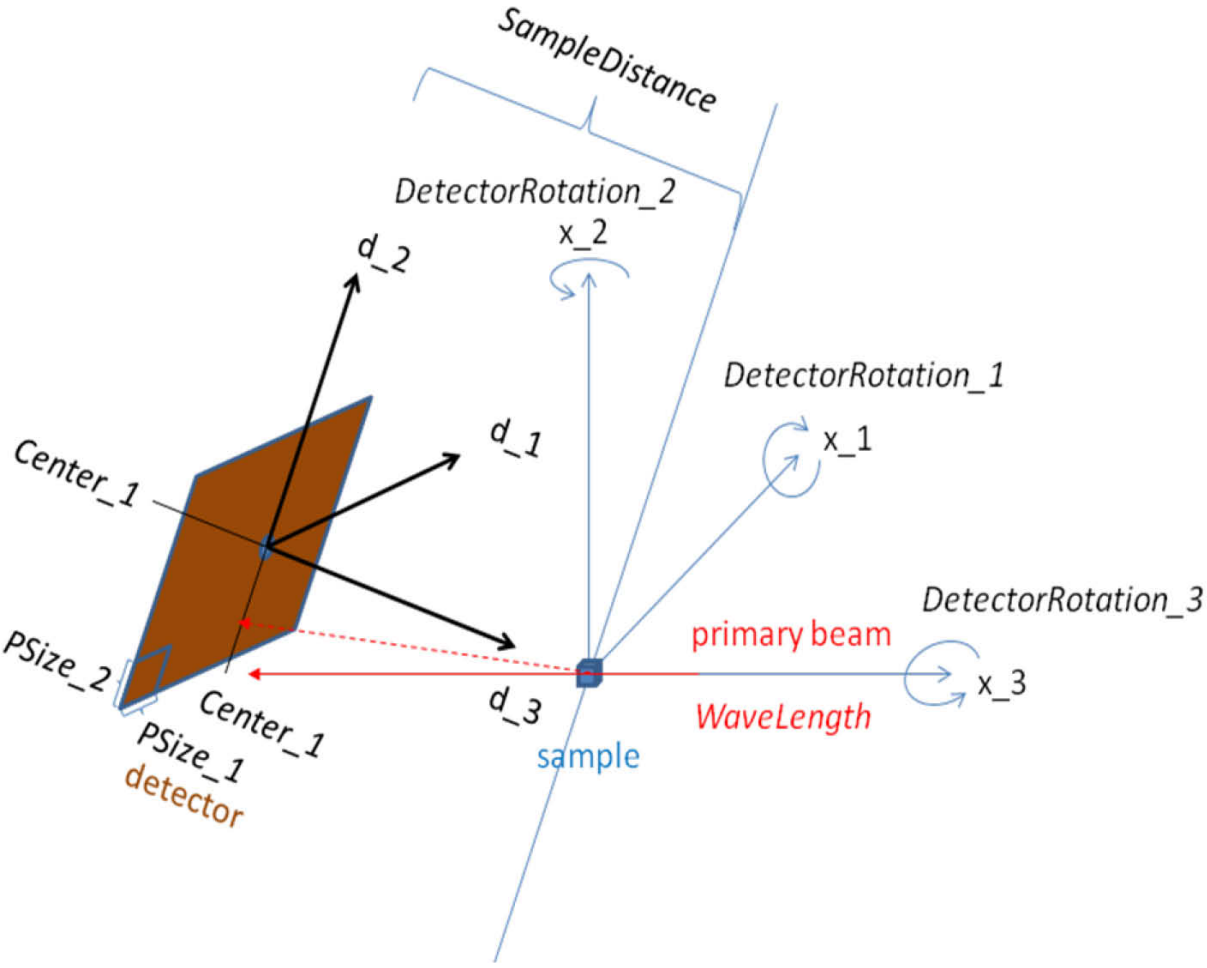

Fig. 5 Wide angle scattering standard parameters (italic): WaveLength, SampleDistance, Center_1, Center_2, PSize_1, PSize_2, DetectorRotation_1, DetectorRotation_2, DetectorRotation_3

Misalignments and GISAS Geometry

The description is adapted to scattering experiments. It uses a common reference point for translations and rotations localized at the sample position. In the ideal case the primary beam passes through the rotation center which is at the same time the center of the scattering volume. Fig. 3 to Fig. 7 illustrate possible misalignments. If in SAS geometry the sample is translated along the primary beam, only the parameters SampleDistance (SD) needs to be

changed (see Fig. 3). When the beam is scanned vertically or horizontally across a flat film that is perpendicular to the primary beam (see Fig. 4) only the center point (C) must be adjusted. In wide angle geometry (Fig. 5 and Fig. 6) usually both parameters must be adjusted.

The effect of misalignments depends on the shape of the sample and the cross section of the beam. In general, it is therefore necessary to describe the shape of the sample and its translations and rotations. Translation and rotations should be described in the same way as done for the detector, the sample shape must be described separately, e.g. as a 3d array.

Fig. 7 shows that the chosen WAS geometry can also describe experiments with an inclined primary beam, e.g. for GISAXS experiments when the angle of incidence is scanned by rotating the primary beam.

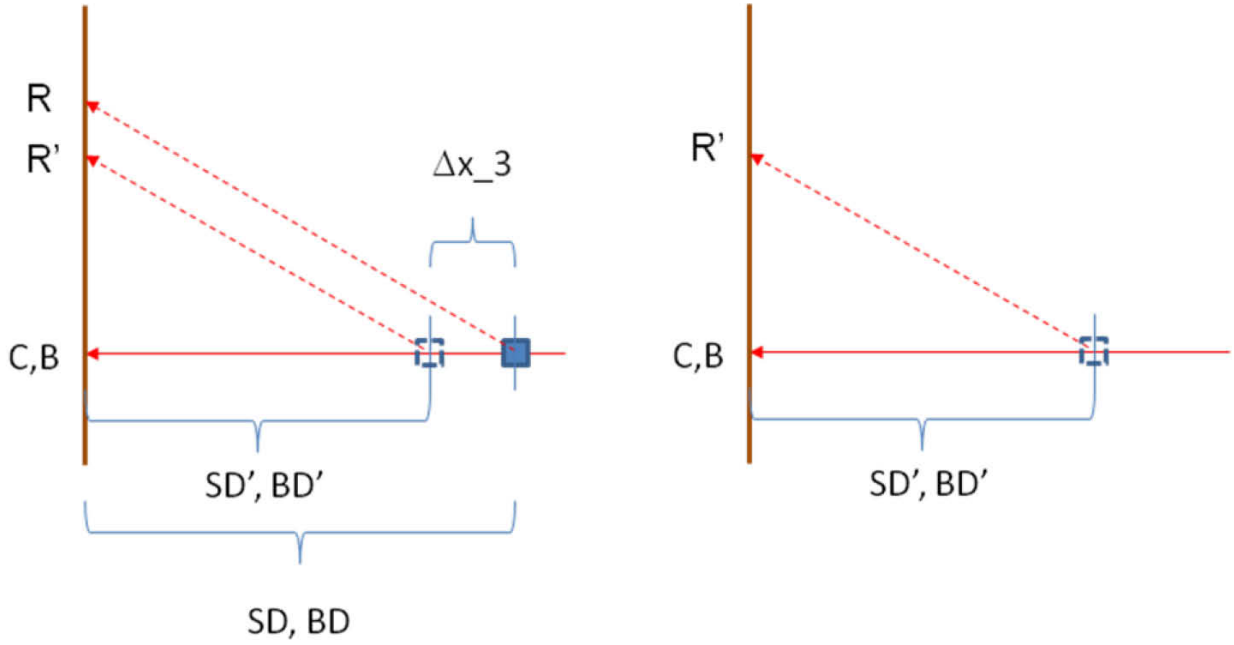

Fig. 6 SAS configuration: movement of the sample along the primary beam (Δx_3), fixed parameter: C, changing parameter: SD

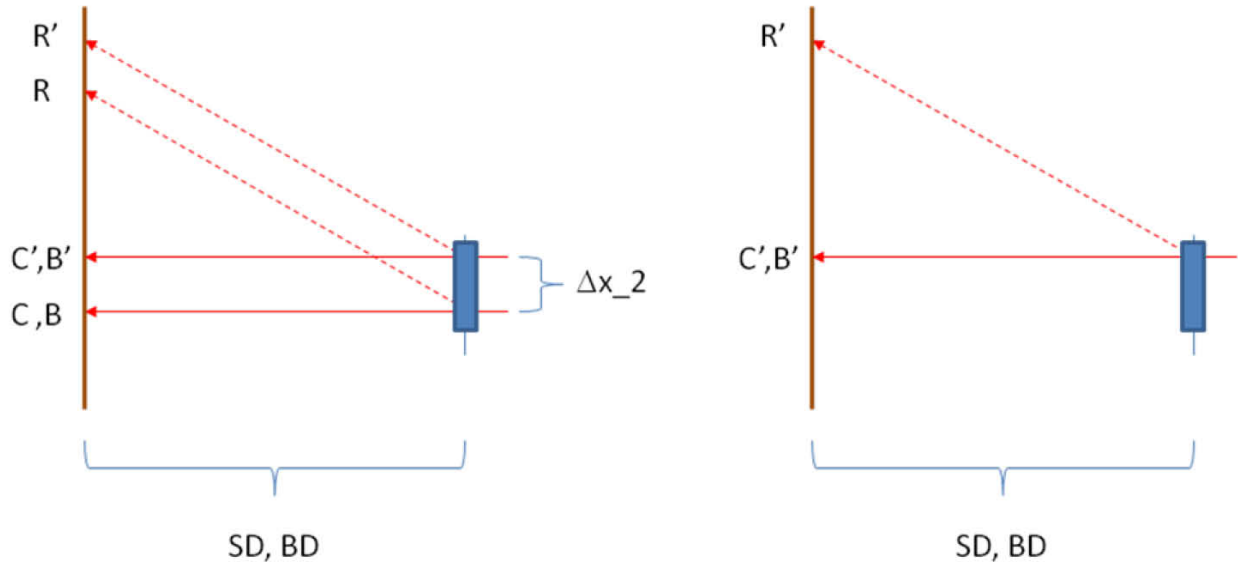

Fig. 7 SAS configuration: vertical movement of the primary beam (Δx_2), fixed parameter: SD, changing parameter: C

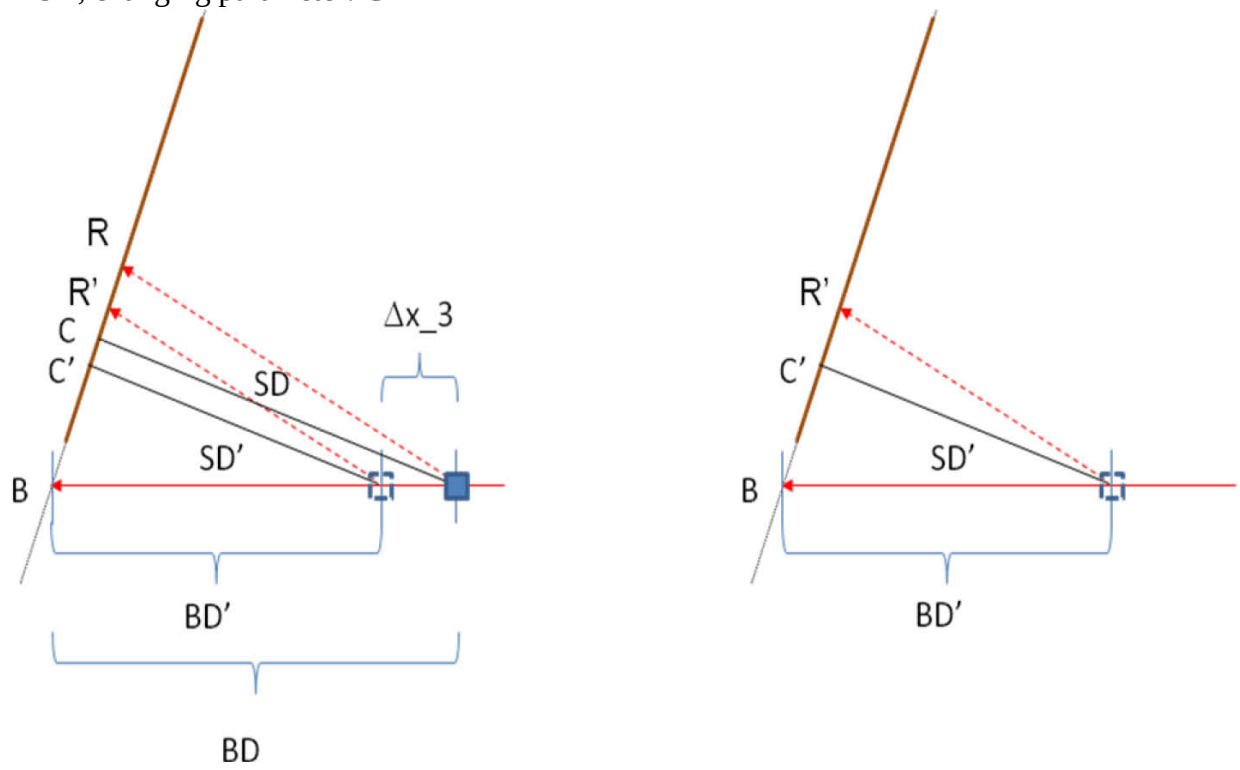

Fig. 8 WAS configuration: movement of the sample along the primary beam direction (Δx_3), fixed parameter: B, changing parameters: BD, C, SD

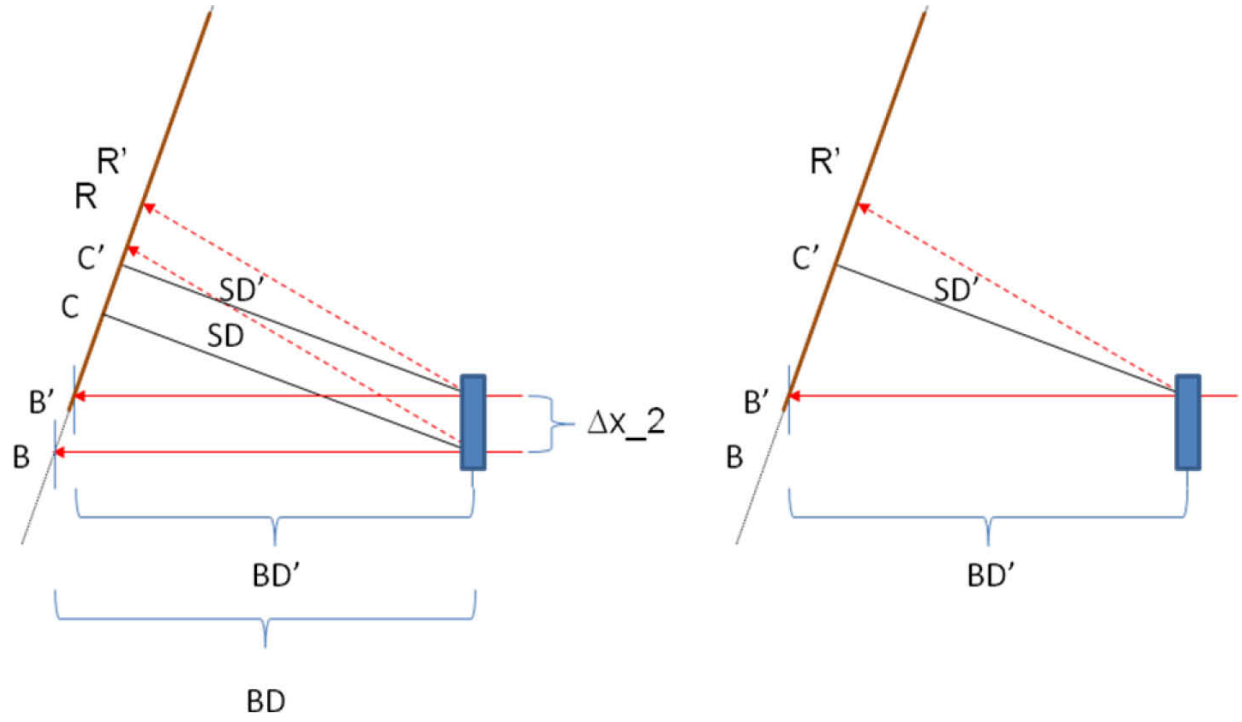

Fig. 9 WAS configuration: vertical movement of the primary beam (Δx_2), no fixed parameter: changing parameters: B, BD, C, SD,

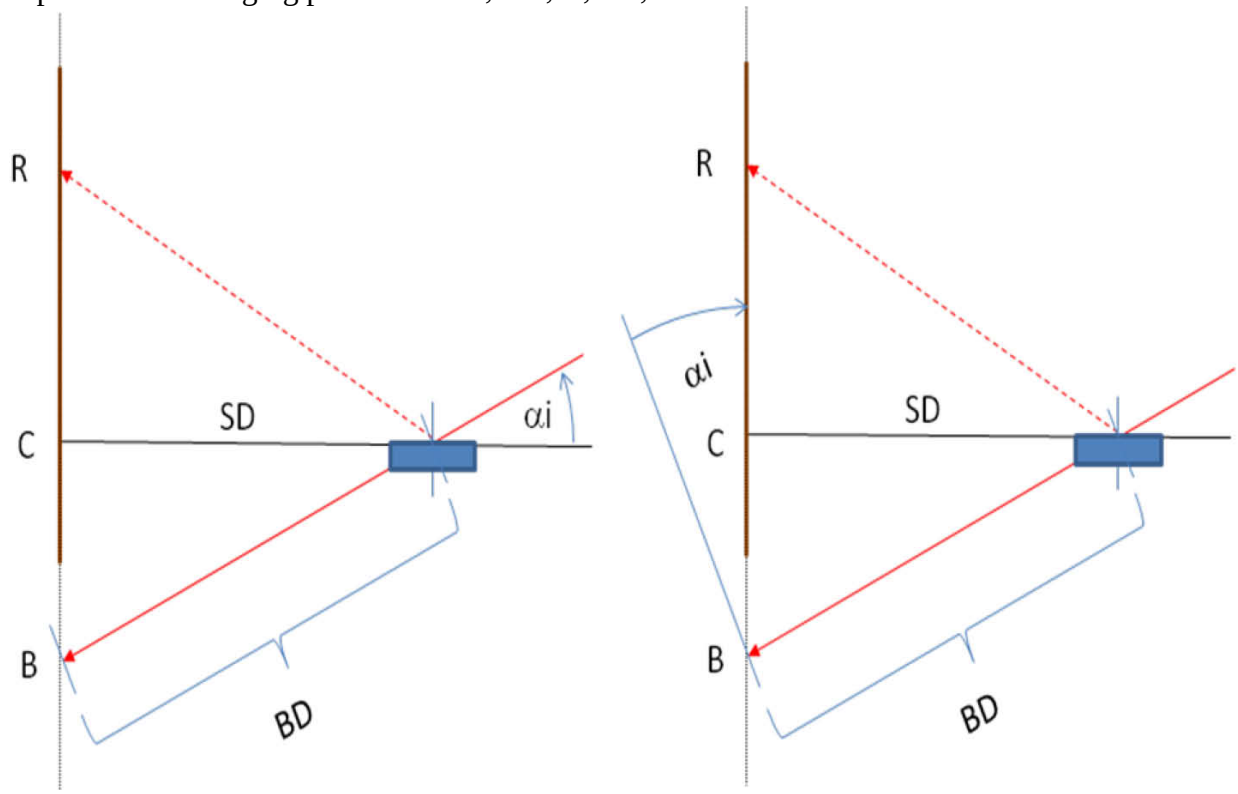

Fig. 10 GISAS configuration: rotation of the primary beam by a_i around the scattering center. A rotation of the primary beam around the scattering center by a_i can be expressed in WAS configuration as a rotation of the detector by a_i into the opposite direction.

Extensions and Generalizations

General Description of the Object Translation and Rotation

All object translations and rotations should be defined in agreement with the detector translations and rotations that are already defined. This allows to use the same formalism to avoid disagreements. The choice of these translations and rotations are independent of a specific goniometer. They are probably not the best choice for all cases. The generalized movements are given to facilitate data interpretation without knowing the mechanical details.

However, for reference the actual translations and rotations should be explicitly available as motor positions, e.g. for cross checks and to minimize calculation errors. The SX-parameters should also not be seen as fixed motor position but rather than as start values for possible refinements. Once the SX-parameters are given they should be passed through the calculation steps. The motor-positions in the experimental raw data remain always untouched, even after refinements.

The geometry is adapted to scattering experiments: primary beam, sample, detector. The origin of the laboratory coordinate system is the center of the goniometer. If it does not exist it is the ideal sample position. The coordinate axes are labelled axis 1, axis 2 and axis 3. The unrotated primary beam points against axis 3, axis 1 is horizontal and axis 2 vertical. They form a right-handed orthogonal coordinate system (axis 1, axis 2, axis 3). All objects (beam, sample, detector) are arranged around the origin of the laboratory coordinate system. The same orthogonal coordinate system is used for all objects: 3 translations and 3 rotations. Without movements (all 6 movements are zero) the object axes collapse with the laboratory axes. First the translations are applied first, then the rotations are applied sequentially in the unrotated system of the object, starting with a ccw rotation around axis_1, then ccw rotation around axis_2 etc. The defaults of all movements are zero, e.g. if no sample translation is given the sample is located at the origin. The raster orientation of the detector coordinate system can differ from the laboratory system. Scattering patterns of detectors with different raster orientations (*RasterOrientation*) can be combined by transforming them to the laboratory system. This geometrical transformation can be done at any step. Only the polarization correction needs to take into account the actual raster orientation of the detector. In analogy to the detector *RasterOrientation* specific object raster orientations could be used.

The parametrization of rotations using three angles avoids a full 3d rotation matrix with 9 elements but with only 3 degrees of freedom. However, it would also be possible to use the rotation matrices RotationMatrix_1_1, RotationMatrix_1_2, ..., RotationMatrix_3_3 instead of Rotation_1, Rotation_2, Rotation_3.

Sample Translation and Rotation

The required parameters are: *SampleTranslation_1, SampleTranslation_2, SampleTranslation_3, SampleRotation_1, SampleRotation_2, SampleRotation_3.* When all parameters are zero the reference position of the sample is at the scattering origin (scattering center).

SampleTranslation

As for the detector the sample translation should be defined as the translation that moves the sample origin (artificial point) to the scattering origin:

$$(12) \qquad SampleTranslation = \begin{pmatrix} SampleTranslation\_1 \\ SampleTranslation\_2 \\ SampleTranslation\_3 \end{pmatrix}$$

SampleRotation

The sample rotation rotates the sample around the scattering origin:

$$(13) \qquad \mathrm{SR} = SampleRotation(rot1, rot2, rot3) = \begin{pmatrix} c1\,c3 & s1\,s2\,c3 - c1\,s3 & c1\,s2\,c3 + s1\,s3 \\ c2\,s3 & c1\,c3 + s1\,s2\,s3 & c1\,s2\,s3 - s1\,c3 \\ s2 & s1\,c2 & c1\,c2 \end{pmatrix}$$

with rot1 = *SampleRotation_1*, rot2 = *SampleRotation_2*, rot3 = *SampleRotation_3*, c1=cos(rot1), s1=sin(rot1), c2=cos(rot2) etc. The principal ranges are

$\mathbf{r} = (r_1, r_2, r_3)$ is a vector in the sample coordinate system. The corresponding sample coordinaet in the laboratory coordinate system is

$$(14) \qquad SampleCoordinate(\mathbf{r}) = SR^{-1} \cdot \begin{pmatrix} r_1 - SampleTranslation\_1 \\ r_2 - SampleTranslation\_2 \\ r_3 - SampleTranslation\_3 \end{pmatrix}$$

It is now very experiment and sample specific what to do with this data. In the general case it should be assumed that the whole sample volume scatters that is illuminated by the primary beam.

Sample Surface Translation and Rotation

The surface translations and rotations should be defined in agreement with the detector and sample rotations. The additional parameters are: *SampleSurfaceTranslation_1, SampleSurfaceTranslation _2, SampleSurfaceTranslation _3, SampleSurfaceRotation_1, SampleSurfaceRotation _2, SampleSurfaceRotation _3.* The active (reflecting) surface should be perpendicular to x3, like the active detector surface. When all parameters are zero the sample surface is perpendicular to x3 and positioned at the scattering origin (scattering center). For grazing incidence scattering the sample surface must first be rotated by 90 degrees around x1 or x2.

It should be considered that surface and sample movements are linked.

Beam Translation and Rotation

In the same way beam translations and rotation can be defined. An experimental setup with a translated and rotated beam can be converted to standard WAS geometry with an inclined detector as shown in Fig. 10. The additional parameters are: *BeamTranslation_1, BeamTranslation_2, BeamTranslation_3, BeamRotation_1, BeamRotation_2, BeamRotation_3.*

Polarization

The beam polarization is taken into account by using a specific correction program. The following parameters are needed:

Pol : degree of polarization (0<=P<=1) (*BeamPolarization*)

PChi : ellipticity (after Poincaré) (-pi/4<=PChi<=+pi/4) (*BeamPolarizationEllipticity*)
PChi=-pi/4 left hand (cw) circular polarization
PChi<0 left hand polarization
PChi==0 linear polarization
PChi>0 right hand polarization
PChi=pi/4 right hand (ccw) circular polarization

PPsi : *BeamPolarizationAngle*: polarization direction (after Poincaré) (0<=PPsi<pi). PPsi is the angle between axis x_1 in RasterOrientation 1 and the polarization direction. It is measured ccw around axis x_1

The beam polarization angle PPsi is measured in the standard coordinate system of the primary beam (RasterOrientation 1).

Intensity Calibration

The normalization to absolute scattering units comprises several steps, detector correction, intensity correction and geometrical correction. The polarization correction (see above) is not mentioned here because it can be applied independently.

Because the detector flat-field and the intensity monitors are usually not calibrated to photons a normalization factor is used. In addition to the flat-field the following parameters are required:

- *NormalizationFactor*
- *Intensity0* (∝ #photons in primary beam before sample)

The sample independent corrections are:

- division by flat-field -> conversion of pixel values from ADU to #photons
- division by Intensity0 -> conversion from #photons to #photons/#incident photons
- division by spherical angle -> conversion from #photons/#incident photon to (#photons/sterad)/(#incident photon)

The absorption corrections requires knowledge about the beam cross section, the sample shape and transmission. It is most simple in SAS for samples that can be approximated as films. In these cases the scattering volume is proportional to the sample thickness and the sample transmission can be approximated by Intensity1/Intensity0. *Intensity1* is the primary beam intensity accumulated during the exposure after the sample, e.g. in the beamstop.

In addition to the flat-field the following parameters are in this case:

- *NormalizationFactor*
- *Intensity1* (∝ #photons after sample)
- *SampleThickness*

The sample dependent corrections are:

- division by flat-field -> conversion of pixel values from ADU to #photons

- division by Intensity1 -> conversion from #photons to #photons/#transmitted photons
- division by spherical angle -> conversion from #photons/#transmitted photons to (#photons/sterad)/(#transmitted photons)
- division by sample thickness conversion from (#photons/sterad)/(#transmitted photons) to 1/V ($\Delta\sigma/\Delta\Omega$)

Raster Orientation

The following section explains the concept of raster orientation.

Binary Data

Binary data formats and most compression methods are already handled by the used data container (EDF, TIFF, HDF, ...). They are not part of the SX description. The data container supplies an n-dimensional array of data values with well defined array access. All binary data are automatically transformed into a representation that is understood by the used programming environment.

The parameter DataRasterConfiguration (default 1) could describes the storage order of the data array. The raster configuration is either given as a positive integer number between 1 and 2^N*N! or as a n-tuple of index numbers: (1,2,3,...,n,n+1,...,N) is equivalent to data raster configuration 1. Raster configuration 1 means that "earlier indices run faster": A[1,j,...], A[2,j,...], ...,A[i,j,...], ..., A[I,j,...], A[1,j+1,...], A[2,j+1,...], ...,A[i,j+1,...], ..., A[I,j+1,...], A[1,j+2,...], ... Attention, DataRasterConfiguration is only used to describe array storage orders. It does not describe a coordinate system and cannot be used to swap or rotate data arrays.

SX Coordinate System

For generality, coordinate axes are numbered from 1 to N. The SX coordinate system is an orthogonal cartesian coordinate system in n-dimensions. Generally, detector axes and reference system axes do not coincide. The mapping of these axes is described with the parameter RasterOrientation (default 1) with 2^N*N! possible values. N is the dimension of the laboratory coordinate system. The value is either given as a positive integer number between 1 and 2^N*N! or a tupel of axis numbers: (1,2,3, ...n,n+1,...,N) is equivalent to raster orientation 1 and means that all axes correspond to the standard coordinate axes. This description is recursively extended to higher ranks.

- RasterOrientation

The parameter RasterOrientation allows to translate detector coordinates into SX standard coordinates (1-8). It could also be useful to translate SX coordinates to NX coordinates and vice versa (9-16)[3]. To be always well defined the standard RasterOrientation of the own description should be 1 or the n-tuple (1,2,3,...).

[3] In raster orientations 9-16 axis 3 is flipped and points along the primary beam.

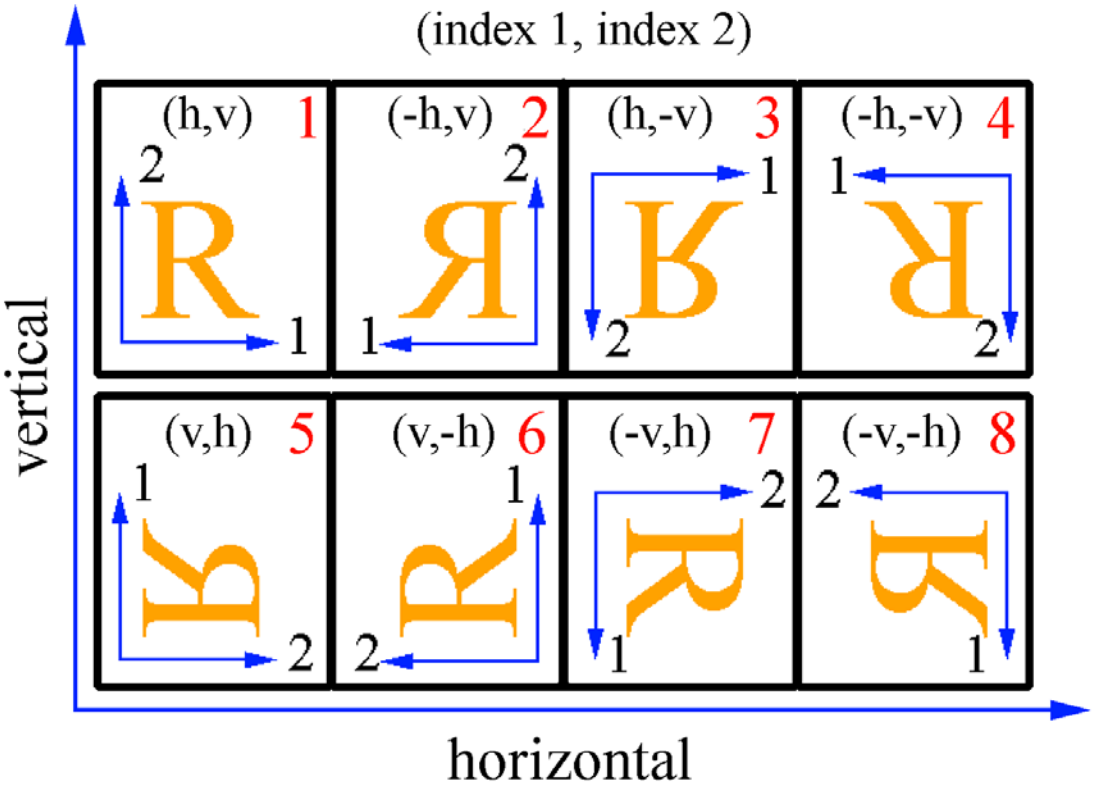

Fig. 11 Raster Orientations for N=2 (two-dimensional image). Raster orientation number 1 is used as reference. It is defined as the orientation where the geometrical origin of the image is at the lower left corner, where index 1 corresponds to the horizontal coordinate (x_1) and where index 2 corresponds to the vertical coordinate (x_2). All other orientations are derived from orientation 1 by swapping and exchanging the coordinates. In raster orientation 5 index 1 corresponds to the vertical and index 2 to the horizontal coordinate.

The utility sxparams translates parameters between raster orientations.

Using RasterOrientation the SX description and parameters are generally independent of the actual geometrical orientation in space when only the array axes have been taken as reference. Only the polarization correction uses this parameter to determine the polarization direction. Apart from that the raster orientation of an image can be changed at any time. This includes a pixel by pixel rearrangement of the 2D data and an update of the rotation angles to match the new geometry.

SX Parameters (Summary)

SX General Parameters

- *Dim_1, Dim_2, ...* (Dim_1 default is 0, all others are 1)
- *RasterOrientation* (1 to 8 possible, 9-16 for compatibility, needs to be tested, default 1)

SX Image Parameters

These parameters describe a region of interest of an N-dimensional array with respect to the original. The rank N of the array is not specified explicitly. It is derived from the Dim_n key with the highest n.

- *Offset_1, Offset_2, ...* (default: 0)
- *BSize_1, BSize_2, ...* (default: 1)
- *RasterRegion_1, RasterRegion_2, ...* (no default)

RasterRegion_1, RasterRegion_2, ... are the dimensions of the original data array (no binning, no ROI). It can be useful to keep this information for the case that the *RasterOrientation* of a ROI must be changed, e.g by swapping the image. It is currently not used and not strictly required.

SX Scattering Parameters

The parameters of this paragraph describe an image as a scattering pattern. Some of these parameters can be extended to higher dimensions. They are marked with three periods.

- *PSize_1, PSize_2, ...* (no default) [m]
- *Center_1, Center_2, ...* (PoNI in image reference system including offsets, no default)
- *SampleDistance* (no default) [m]
- *WaveLength* (no default) [m]
- *DetectorRotation_1, DetectorRotation_2, DetectorRotation_3, ...* (default: 0) [rad]

Alternative set of SX Scattering Parameters (only used in case that the above standard parameters are not available)

- *PSize_1, PSize_2, ...* (no default) [m]
- *BeamCenter_1, BeamCenter_2, ...* (no default)
- *BeamDistance* (no default) [m]
- *WaveLength* (no default) [m]
- *DetectorRotation_1, DetectorRotation_2, DetectorRotation_3, ...* (default: 0) [rad]

Additional SX Scattering Parameters

- *ProjectionType* (Saxs|Waxs, default: Saxs: distances proportional to tan(2ϑ))
- *AxisType_1, AxisType_2, ...*(Distance, Angle, Numerator, default: Distance)

SX Intensity Calibration and Normalization Parameters[4]

- *Intensity0* (no default), *Intensity1* (*Intensity0*)
- *NormalizationFactor* (default 1)
- *SampleThickness* (no default)

[4] For details see normalization program

SX Sample Parameters (proposed)

- *SampleTranslation_1*,
  SampleTranslation_2,
  SampleTranslation_3 [m]
- *SampleRotation_1*,
  SampleRotation_2,
  SampleRotation_3 [rad]

SX Surface Parameters (proposed)

- *SampleSurfaceTranslation_1*,
  SampleSurfaceTranslation_2,
  SampleSurfaceTranslation _3 [m]
- *SampleSurfaceRotation _1*,
  SampleSurfaceRotation _2,
  SampleSurfaceRotation _3 [rad]

SX Beam Parameters (proposed)

- *BeamTranslation_1*,
  BeamTranslation _2,
  BeamTranslation _3 [m]
- *BeamRotation_1*,
  BeamRotation _2,
  BeamRotation _3 [rad]

SX Beam Polarization (proposed)

- *BeamPolarization* (0.0<=P<=1.0)
  BeamPolarizationEllipticity (-pi/4<=PChi<=+pi/4)
  BeamPolarizationAngle (0<=PPsi<pi)