In the component, the integral in (5.14) is computed using a 15-order Gaussian quadrature formula, with the integral restricted to an inteval 5 times wider than the mosaic width σ.

The input parameters for Mosaic_simple are *zmin*, *zmax*, *ymin*, and *ymax* to define the surface of the crystal in the Y-Z plane; *mosaic* to give the FWHM of the mosaic spread; *R0* to give the reflectivity at the Bragg angle, and *Qx*, *Qy*, and *Qz* to give the scattering vector.

5.6.2 The crystal with anisotropic mosaic

The component **Mosaic_anisotropic** is a modified version of the Mosaic_simple component, intended to replace the Monocromator component from previous releases. It restricts the scattering vector to be perpendicular to the crystal surface, but extends the Mosaic_simple component by allowing different mosaics in the horizontal and vertical direction.

The code is largely similar to that for Mosaic_simple, and the documentation for the latter should be consulted for details. The differences are mainly for two reasons:

- Some simplifications have been done since two of the components of the scattering vector are known to be zero.
- The computation of the Gaussian for the mosaic is done done using different mosaics for the two axes.

The input parameters for the component Mosaic_anisotropic are *zmin*, *zmax*, *ymin*, and *ymax* to define the size of the crystal (in meters); *mosaich* and *mosaicv* to define the mosaic (in minutes of arc); *r0* to define the reflectivity (no unit); and Q to set the length of the scattering vector (in Å^{-1}).

5.6.3 The single crystal component

The physical model

The textbook expression for the scattering cross-section of a crystal is [10]:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh.el.}} = N\frac{(2\pi)^3}{V_0}\sum_{\boldsymbol{\tau}}\delta(\boldsymbol{\tau}-\boldsymbol{\kappa})|F_{\boldsymbol{\tau}}|^2$$

Here $|F_{\boldsymbol{\tau}}|^2$ is the structure factor, N is the number of unit cells, V_0 is the volume of an individual unit cell, and $\boldsymbol{\kappa} = \mathbf{k}_i - \mathbf{k}_f$ is the scattering vector. $\delta(\boldsymbol{x})$ is a 3-dimensional delta function in reciprocal space, so for given incoming wave vector $\mathbf{k}_i$ and lattice vector $\boldsymbol{\tau}$, only a single final wave vector $\mathbf{k}_f$ is allowed. In a real crystal, however, reflections are not perfectly sharp. Because of imperfection and finite-size effects, there will be a small region around $\boldsymbol{\tau}$ in reciprocal space of possible scattering vectors.

The Single_crystal component simulates a crystal with a mosaic spread η and a lattice plane spacing uncertainty $\Delta d/d$. In such crystals the reflections will not be completely sharp; there will be a small region around each reciprocal lattice point of the crystal that contains valid scattering vectors.

We model the mosaicity and $\Delta d/d$ of the crystal with 3-dimensional Gaussian functions in reciprocal space (see figure 5.10). Two of the axes of the Gaussian are perpendicular

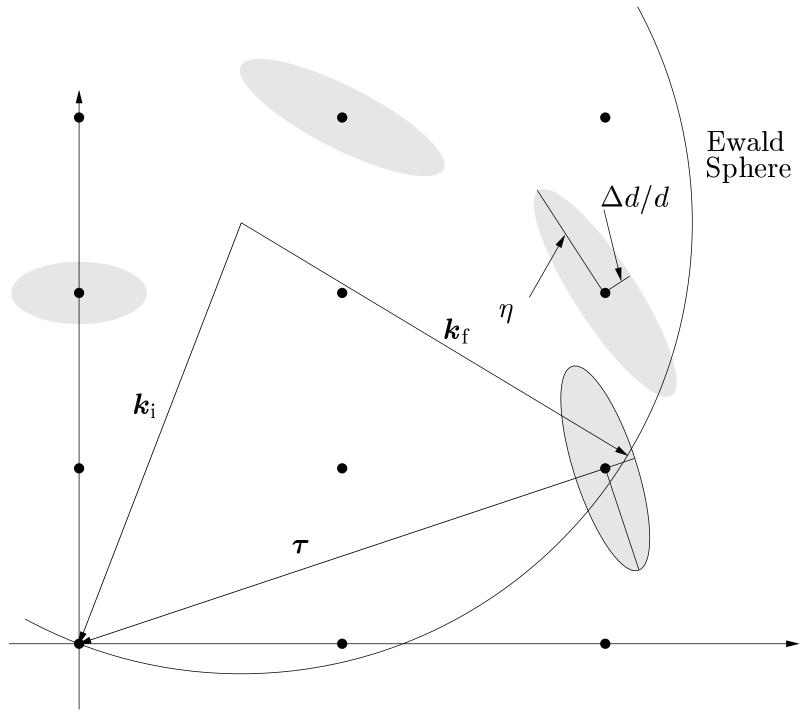

Figure 5.10: Ewald sphere construction for a single neutron showing the Gaussian broadening of reciprocal lattice points in their local coordinate system.

to the reciprocal lattice vector $\boldsymbol{\tau}$ and model the mosaicity. The third one is parallel to $\boldsymbol{\tau}$ and models $\Delta d/d$. We use an isotropic mosaicity, so the two axes perpendicular to $\boldsymbol{\tau}$ are of equal length η. We assume that the mosaicity is small so that the possible directions of the scattering vector may be approximated with a Gaussian in rectangular coordinates.

We now derive a quantitative expression for the scattering cross-section of the crystal in the model. For this, we introduce a *local coordinate system* for each reciprocal lattice point $\boldsymbol{\tau}$ and use $\boldsymbol{x}$ for vectors written in local coordinates. The origin is $\boldsymbol{\tau}$, the first axis is parallel to $\boldsymbol{\tau}$ and the other two axes are perpendicular to $\boldsymbol{\tau}$. In the local coordinate system, the 3-dimensional Gaussian is given by

$$G(x_1, x_2, x_3) = \frac{1}{(\sqrt{2\pi})^3} \frac{1}{\sigma_1\sigma_2\sigma_3} e^{-\frac{1}{2}(\frac{x_1^2}{\sigma_1^2} + \frac{x_2^2}{\sigma_2^2} + \frac{x_3^2}{\sigma_3^2})} \tag{5.15}$$

The axes of the Gaussian are $\sigma_1 = \tau\Delta d/d$ and $\sigma_2 = \sigma_3 = \eta\tau$. Here we used the assumption that η is small, so that $\tan\eta \approx \eta$ (with η given in radians). By introducing the diagonal matrix

$$D = \begin{pmatrix} \frac{1}{2}\sigma_1^2 & 0 & 0 \\ 0 & \frac{1}{2}\sigma_2^2 & 0 \\ 0 & 0 & \frac{1}{2}\sigma_3^2 \end{pmatrix}$$

equation (5.15) can be written as

$$G(\boldsymbol{x}) = \frac{1}{(\sqrt{2\pi})^3} \frac{1}{\sigma_1\sigma_2\sigma_3} e^{-\boldsymbol{x}^\mathrm{T} D \boldsymbol{x}} \tag{5.16}$$

again with $\boldsymbol{x} = (x_1, x_2, x_3)$ written in local coordinates.

To get an expression in the coordinates of the reciprocal lattice of the crystal, we introduce a matrix U such that if $\boldsymbol{y} = (y_1, y_2, y_3)$ are the global coordinates of a point in the crystal reciprocal lattice, then $U(\boldsymbol{y} + \boldsymbol{\tau})$ are the coordinates in the local coordinate system for $\boldsymbol{\tau}$. The matrix U is given by

$$U^{\mathrm{T}} = (\hat{u}_1, \hat{u}_2, \hat{u}_3),$$

where $\hat{u}_1$, $\hat{u}_2$, and $\hat{u}_3$ are the axes of the local coordinate system, written in the global coordinates of the reciprocal lattice. Thus $\hat{u}_1 = \boldsymbol{\tau}/\tau$, and $\hat{u}_2$ and $\hat{u}_3$ are unit vectors perpendicular to $\hat{u}_1$ and to each other. The matrix U is unitarian, that is $U^{-1} = U^{\mathrm{T}}$. The translation between global and local coordinates is

$$\boldsymbol{x} = U(\boldsymbol{y} + \boldsymbol{\tau}) \qquad \boldsymbol{y} = U^{\mathrm{T}}\boldsymbol{x} - \boldsymbol{\tau}$$

The expression for the 3-dimensional Gaussian in global coordinates is

$$G(\boldsymbol{y}) = \frac{1}{(\sqrt{2\pi})^3} \frac{1}{\sigma_1 \sigma_2 \sigma_3} e^{-(U(\boldsymbol{y}+\boldsymbol{\tau}))^{\mathrm{T}} D (U(\boldsymbol{y}+\boldsymbol{\tau}))} \tag{5.17}$$

The elastic coherent cross-section is then given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh.el.}} = N \frac{(2\pi)^3}{V_0} \sum_{\boldsymbol{\tau}} G(\boldsymbol{\tau} - \boldsymbol{\kappa}) |F_{\boldsymbol{\tau}}|^2 \tag{5.18}$$

The user must specify a list of reciprocal lattice vectors $\boldsymbol{\tau}$ to consider along with their structure factors $|F_{\boldsymbol{\tau}}|^2$. The user must also specify the coordinates (in direct space) of the unit cell axes $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$, from which the reciprocal lattice will be computed.

In this version of the Single_crystal component, no account is taken of extinction (the sample is assumed to be so thin that extinction is not important). A future version will include secondary extinction and multiple scattering.

The algorithm

The overview of the algorithm used in the Single_crystal component is as follows:

1. Check if the neutron intersects the crystal, and if so, select at random a point of scattering inside the crystal.
2. Search through a list of reciprocal lattice points of interest, selecting those that are close enough to the Ewald sphere to have a non-vanishing scattering probability.
3. Of the selected reciprocal lattice points, choose one at random for this scattering event.
4. Select an outgoing wave vector $\boldsymbol{k}_{\mathrm{f}}$ from the intersection between the Ewald sphere and the Gaussian ellipsoid.
5. Adjust the neutron weight to get the correct cross-section in (5.18).

For point 1, since no extinction is considered the scattering point is chosen uniformly on the potential flight path through the crystal. For point 2, the distance *dist* between a reciprocal lattice point and the Ewald sphere is considered small enough to allow scattering if it is less than five times the maximum axis of the Gaussian, $dist \leq 5 \max(\sigma_1, \sigma_2, \sigma_3)$.

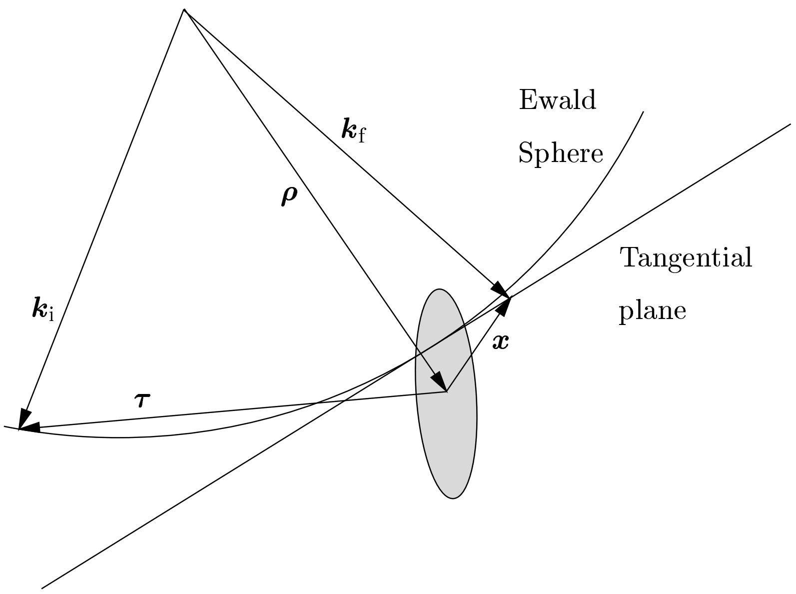

Figure 5.11: The scattering triangle in the single crystal.

Choosing the outgoing wave vector The final wave vector $\boldsymbol{k}_\mathrm{f}$ must lie on the intersection between the Ewald sphere and the Gaussian ellipsoid. Since η and $\Delta d/d$ are assumed small, the intersection can be approximated with a plane tangential to the sphere, see figure 5.11. The tangential point is taken to lie on the line between the center of the Ewald sphere $-\boldsymbol{k}_\mathrm{i}$ and the reciprocal lattice point $\boldsymbol{\tau}$. Since the radius of the Ewald sphere is k_i, this point is

$$\boldsymbol{o} = (1 - k_\mathrm{i}/\rho)\boldsymbol{\rho} - \boldsymbol{\tau}$$

where $\rho = \boldsymbol{k}_\mathrm{i} - \boldsymbol{\tau}$.

The equation for the plane is

$$\boldsymbol{P}(\boldsymbol{t}) = \boldsymbol{o} + B\boldsymbol{t}, \qquad \boldsymbol{t} \in \mathbb{R}^2 \tag{5.19}$$

Here $B = (\boldsymbol{b}_1, \boldsymbol{b}_2)$ is a 3×2 matrix with the two generators for the plane $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. These are (arbitrary) unit vectors in the plane, being perpendicular to each other and to the plane normal $\boldsymbol{n} = \boldsymbol{\rho}/\rho$.

Each $\boldsymbol{t}$ defines a potential final wave vector $\boldsymbol{k}_\mathrm{f}(\boldsymbol{t}) = \boldsymbol{k}_\mathrm{i} + \boldsymbol{P}(\boldsymbol{t})$. The value of the 3-dimensional Gaussian for this $\boldsymbol{k}_\mathrm{f}$ is

$$G(\boldsymbol{x}(\boldsymbol{t})) = \frac{1}{(\sqrt{2\pi})^3} \frac{1}{\sigma_1\sigma_2\sigma_3} e^{-\boldsymbol{x}(\boldsymbol{t})^\mathrm{T} D \boldsymbol{x}(\boldsymbol{t})} \tag{5.20}$$

where $\boldsymbol{x}(\boldsymbol{t}) = \boldsymbol{\tau} - (\boldsymbol{k}_\mathrm{i} - \boldsymbol{k}_\mathrm{f}(\boldsymbol{t}))$ is given in local coordinates for $\boldsymbol{\tau}$. It can be shown that equation (5.20) can be re-written as

$$G(\boldsymbol{x}(\boldsymbol{t})) = \frac{1}{(\sqrt{2\pi})^3} \frac{1}{\sigma_1\sigma_2\sigma_3} e^{-\alpha} e^{-(\boldsymbol{t}-\boldsymbol{t}_0)^\mathrm{T} N (\boldsymbol{t}-\boldsymbol{t}_0)} \tag{5.21}$$

where $N = B^{\mathrm{T}}DB$ is a 2×2 symmetric and positive definite matrix, $\boldsymbol{t}_0 = -N^{-1}B^{\mathrm{T}}D\boldsymbol{o}$ is a 2-vector, and $\alpha = -\boldsymbol{t}_0^{\mathrm{T}}N\boldsymbol{t}_0 + \boldsymbol{o}^{\mathrm{T}}D\boldsymbol{o}$ is a real number. Note that this is a two-dimensional Gaussian (not necessarily normalized) in $\boldsymbol{t}$ with center $\boldsymbol{t}_0$ and axis defined by N.

To choose $\boldsymbol{k}_{\mathrm{f}}$ we sample $\boldsymbol{t}$ from the 2-dimensional Gaussian distribution (5.21). To do this, we first construct the Cholesky decomposition of the matrix $(\frac{1}{2}N^{-1})$. This gives a 2×2 matrix L such that $LL^{\mathrm{T}} = \frac{1}{2}N^{-1}$ and is possible since N is symmetric and positive definite. It is given by

$$L = \begin{pmatrix} \sqrt{\nu_{11}} & 0 \\ \frac{\nu_{12}}{\sqrt{\nu_{11}}} & \sqrt{\nu_{22} - \frac{\nu_{12}^2}{\nu_{11}}} \end{pmatrix} \qquad \text{where } \frac{1}{2}N^{-1} = \begin{pmatrix} \nu_{11} & \nu_{12} \\ \nu_{12} & \nu_{22} \end{pmatrix}$$

Now let $\boldsymbol{g} = (g_1, g_2)$ be two random numbers drawn form a Gaussian distribution with mean 0 and standard deviation 1, and let $\boldsymbol{t} = L\boldsymbol{g} + \boldsymbol{t}_0$. The probability of a particular $\boldsymbol{t}$ is then

$$\begin{aligned} P(\boldsymbol{t})d\boldsymbol{t} &= \frac{1}{2\pi}e^{-\frac{1}{2}\boldsymbol{g}^{\mathrm{T}}\boldsymbol{g}}d\boldsymbol{g} && (5.22) \\ &= \frac{1}{2\pi}\frac{1}{\det L}e^{-\frac{1}{2}(L^{-1}(\boldsymbol{t}-\boldsymbol{t}_0))^{\mathrm{T}}(L^{-1}(\boldsymbol{t}-\boldsymbol{t}_0))}d\boldsymbol{t} && (5.23) \\ &= \frac{1}{2\pi}\frac{1}{\det L}e^{-(\boldsymbol{t}-\boldsymbol{t}_0)^{\mathrm{T}}N(\boldsymbol{t}-\boldsymbol{t}_0)}d\boldsymbol{t} && (5.24) \end{aligned}$$

where we used that $\boldsymbol{g} = L^{-1}(\boldsymbol{t} - \boldsymbol{t}_0)$ so that $d\boldsymbol{g} = \frac{1}{\det L}d\boldsymbol{t}$. This is just the normalized form of (5.21). Finally we set $\boldsymbol{k}'_{\mathrm{f}} = \boldsymbol{k}_{\mathrm{i}} + \boldsymbol{P}(\boldsymbol{t})$ and $\boldsymbol{k}_{\mathrm{f}} = (k_{\mathrm{i}}/k'_f)\boldsymbol{k}'_{\mathrm{f}}$ to normalize the length of $\boldsymbol{k}_{\mathrm{f}}$ to correct for the (small) error introduced by approximating the Ewald sphere with a plane.

Adjusting the neutron weight We now calculate the correct neutron weight adjustment. The probability of a neutron with initial wave vector $\boldsymbol{k}_{\mathrm{i}}$ that hits the crystal within a small area A being scattered with a wave vector $\boldsymbol{k}_{\mathrm{f}}$ within a small solid angle $d\Omega$ is $n_{\mathrm{in}}/n_{\mathrm{out}}$, where n_{in} and n_{out} are the number of incident and scattered neutrons, respectively. The definition of the cross-section is

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh.el.}} = n_{\mathrm{out}}/\phi_{\mathrm{in}}$$

where $\phi_{\mathrm{in}} = n_{\mathrm{in}}/A$ is the incoming flux. We can thus express the scattering probability in terms of the cross-section as follows:

$$\Pi(\boldsymbol{\tau}, \boldsymbol{k}_{\mathrm{f}}) = \frac{n_{\mathrm{out}}}{\phi_{\mathrm{in}}A} = \frac{1}{A}\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh.el.}}$$

The volume of the crystal as seen by a beam with cross-section A is $\ell A = NV_0$ where ℓ is the path length of the beam all the way through the crystal. The probability of scattering in the physical model is thus

$$\begin{aligned} \Pi(\boldsymbol{\tau}, \boldsymbol{k}_{\mathrm{f}}) &= \frac{\ell}{NV_0}\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh.el.}} && (5.25) \\ &= \frac{\ell(2\pi)^3}{V_0^2}|F_{\boldsymbol{\tau}}|^2\frac{1}{(\sqrt{2\pi})^3}\frac{1}{\sigma_1\sigma_2\sigma_3}e^{-\boldsymbol{x}^{\mathrm{T}}D\boldsymbol{x}} && (5.26) \end{aligned}$$

where $\boldsymbol{x} = \boldsymbol{\tau} - (\boldsymbol{k}_\mathrm{i} - \boldsymbol{k}_\mathrm{f})$.

The Monte Carlo probability $f(\boldsymbol{\tau}, \boldsymbol{k}_\mathrm{f})$ of the scattering event taking place in the simulation is the product of the probability of selecting the particular reciprocal lattice point $\boldsymbol{\tau}$ and the probability of selecting the particular $\boldsymbol{k}_\mathrm{f}$. Let a be the number of reciprocal lattice vectors closer than *dist* to the Ewald sphere. From (5.24) we then have

$$f(\boldsymbol{\tau}, \boldsymbol{k}_\mathrm{f}) d\Omega = \frac{1}{a}\frac{1}{2\pi}\frac{1}{\det L} e^{-(\boldsymbol{t}-\boldsymbol{t}_0)^\mathrm{T} N(\boldsymbol{t}-\boldsymbol{t}_0)} d\boldsymbol{t} \tag{5.27}$$

$$= \frac{1}{a}\frac{1}{2\pi}\frac{k_\mathrm{i}^2}{\det L} e^{\alpha} e^{-\boldsymbol{x}^\mathrm{T} D \boldsymbol{x}} d\Omega \tag{5.28}$$

where we used equations (5.20) and (5.21), as well as the fact that $d\boldsymbol{t} = k_\mathrm{i}^2 d\Omega$.

We can now use equation (4.8) to get the correct weight adjustment:

$$\pi(\boldsymbol{\tau}, \boldsymbol{k}_\mathrm{f}) = \frac{\Pi(\boldsymbol{\tau}, \boldsymbol{k}_\mathrm{f})}{f(\boldsymbol{\tau}, \boldsymbol{k}_\mathrm{f})} \tag{5.29}$$

$$= \frac{\ell}{V_0^2} |F_{\boldsymbol{\tau}}|^2 (2\pi)^{5/2} \frac{\det L}{k_\mathrm{i}^2} a \frac{e^{-\alpha}}{\sigma_1\sigma_2\sigma_3} \tag{5.30}$$

The implementation

The equations describing the Single_crystal simulation are quite complex, and consequently the code is fairly sizeable. Most of it is just the expansion of the vector and matrix equations in individual coordinates, and should thus be straightforward to follow.

The implementation pre-computes a lot of the necessary values in the `INITIALIZE` section. It is thus actually very efficient despite the complexity. If the list of reciprocal lattice points is big, however, the search through the list will be slow. The precomputed data is stored in the structures `hkl_info` and in an array of `hkl_data` structures (one for each reciprocal lattice point in the list). In addition, for every neutron event an array of `tau_data` is computed with one element for each reciprocal lattice point close to the Ewald sphere. Except for the search for possible $\boldsymbol{\tau}$ vectors, all computations are done in local coordinates using the matrix U to do the necessary transformations.

The list of reciprocal lattice points is specified in an ASCII data file. Each line contains seven numbers, separated by white space. The first three numbers are the (h, k, l) indices of the reciprocal lattice point, and the last number is the value of the structure factor $|F_{\boldsymbol{\tau}}|^2$, in barns. The middle three numbers are not used; they are nevertheless required since this makes the file format compatible with the output from the Crystallographica program [11].

The input parameters for the components are *xwidth*, *yheight*, and *zdeflth* to define the dimensions of the crystal in meters; *delta_d_d* and *mosaic* to give the value of $\Delta d/d$ (no unit) and η (in minutes of arc); (ax, ay, az), (bx, by, bz), and (cx, cy, cz) to define the axes of the direct lattice of the crystal (the sides of the unit cell) in units of Ångstrøm; and *reflections*, a string giving the name of the file with the list of structure factors to consider.

5.6.4 The Monochromator

The component **Monochromator** is obsolete as from McStas version 1.2. Use the component **Mosaic_anisotropic** instead.