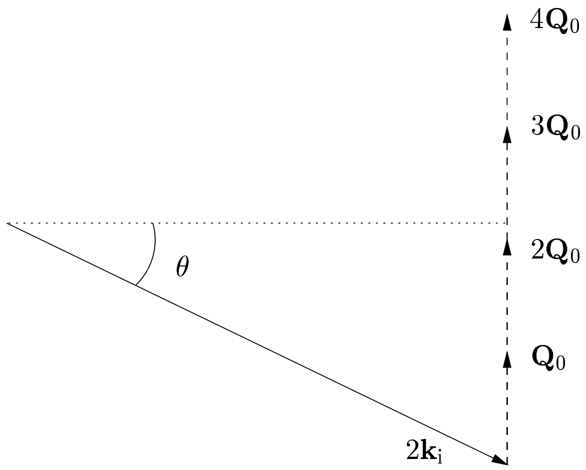

Figure 8: Selection of the Bragg order ("2" in this case).

5.6.1 An infinitely thin mosaic crystal with a single scattering vector

The component **Mosaic_simple** simulates an infinitely thin single crystal with a single scattering vector and a mosaic spread. A typical use for this component is to simulate a monocromator or an analyzer.

The physical model used in the component is a rectangular piece of material composed of a large number of small micro-crystals. **Skriv referencer her til bger mv.** The orientation of the microcrystals deviates from the nominal crystal orientation so that the probability of a given microcrystal orientation is proportional to a gaussian of the angle between the given and the nominal orientation. The width of the gaussian is given by the mosaic spread of the crystal. The mosaic spread is assumed to be large compared to the Bragg width of the scattering vector.

As a further simplification, the crystal is assumed to be infinitely thin. This means that multiple scattering effects are not simulated. It also means that the total reflectivity can be used as a parameter for the model rather than the atomic scattering cross section.

When a neutron trrajectory intersecs the crystal, the first step in the computation is to determine the probability of scatttering. This probability is then used in a Monte Carlo choice desiding whether to scatter or transmit the neutron. The scattering probability is the sum of the probabilities of first-order scattering, second-order, ..., up to the highest order that permits Bragg scattering at the given neutron wave length. However, in most cases at most one order will have a significant scattering probability, and the computation thus considers only the order that best matches the neutron wavelength. Bragg's law is

$$n\mathbf{Q}_0 = 2\mathbf{k}_i \sin\theta$$

Thus, the scattering order is obtained simply as the integer multiple n of the nominal scattering vector $\mathbf{Q}_0$ which is closest to the projection of $2\mathbf{k}_i$ onto $\mathbf{Q}_0$ (see figure 8). Once n has been determined, the Bragg angle θ can be computed. The angle d that the nominal scattering vector $\mathbf{Q}_0$ makes with the closest scattering vector $\mathbf{q}$ that admits Bragg

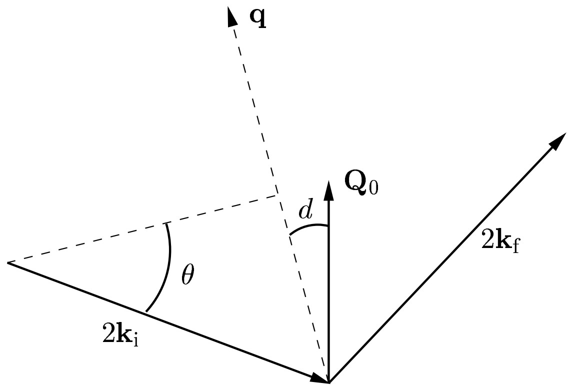

Figure 9: Computing the deviation d from the nominal scattering direction.

scattering is then used to compute the probability of reflection from the mosaic

$$p_{\text{reflect}} = R_0 e^{-d^2/2\sigma^2},$$

where R_0 is the reflectivity at the Bragg angle (see figure 9). The probability p_{reflect} is used in a Monte Carlo choice to decide whether the neutron is transmitted or reflected.

In the case of reflection, the neutron will be scattered into the Debye-Scherrer cone, with the probability of each point on the cone being determined by the mosaic. The Debye-Scherrer cone can be described by the equation

$$\mathbf{k}_\mathrm{f} = \mathbf{k}_\mathrm{i} \cos 2\theta + \sin 2\theta (\mathbf{c} \cos \varphi + \mathbf{b} \sin \varphi), \qquad \varphi \in [-\pi; \pi], \tag{23}$$

where $\mathbf{b}$ is a vector perpendicular to $\mathbf{k}_\mathrm{i}$ and $\mathbf{Q}_0$, $\mathbf{c}$ is perpendicular to $\mathbf{k}_\mathrm{i}$ and $\mathbf{b}$, and both $\mathbf{b}$ and $\mathbf{c}$ have the same length as $\mathbf{k}_\mathrm{i}$ (see figure 10). In the component, φ is sampled from a gaussian distribution with the mosaic width, and the final wave vector is computed as

$$\mathbf{k}_\mathrm{f} = \mathbf{q} + \mathbf{k}_\mathrm{i}$$

defining the final neutron state.

What remains is to get the neutron weight right. The distribution from which the scattering event is sampled is a gaussian in φ,

$$f_{\mathrm{MC}}(\varphi) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\varphi^2/2\sigma^2}$$

In the physical model, the probability of the scattering event is proportional to a gaussian in the angle between the nominal scattering vector $\mathbf{Q}_0$ and the actual scattering vector $\mathbf{q}$. The normalisation condition is that the integral over all φ should be 1. Thus the probability of the scattering event in the physical model is

$$\Pi(\varphi) = e^{\frac{-d(\varphi)^2}{2\sigma^2}} \Big/ \int_{-\pi}^{\pi} e^{\frac{-d(\varphi)^2}{2\sigma^2}} d\varphi \tag{24}$$

where $d(\varphi)$ denotes the angle between the nominal scattering vector and the actual scattering vector corresponding to φ. According to equation (8), the weight adjustment π_j is then given by

$$\pi_j = \Pi(\varphi)/f_{\mathrm{MC}}(\varphi).$$

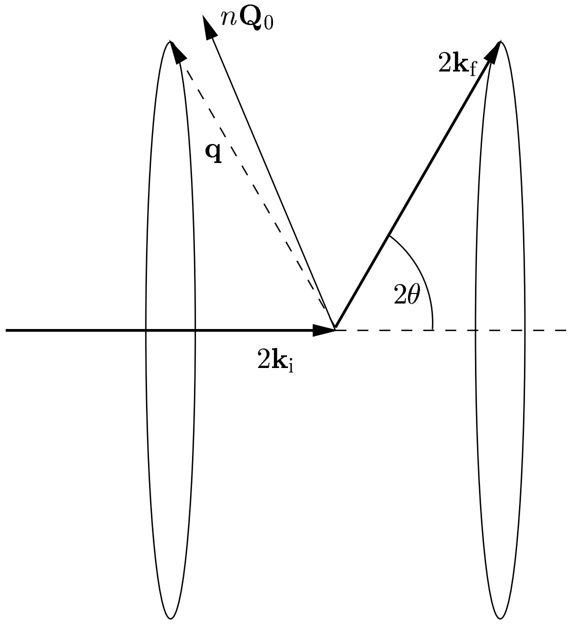

Figure 10: Scattering into the part of the Debye-Scherrer cone covered by the mosaic.

In the component, the integral in (24) 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 Monochromator

The component **Monochromator** describes a rectangular single crystal, which is described by its measures $(z_{\rm min}, z_{\rm max}, y_{\rm min}, y_{\rm max})$, a scattering vector, $\mathbf{Q}$, and a corresponding maximum reflectivity, R_0. This component is also used for simulating analyser crystals, and it may be used for simple single-crystal samples.

The component has two additional input parameters: A vertical and a horizontal mosaicity, η_h and η_v. This means that the little crystallites constituting the crystal are assumed to have a small, Gaussian distributed, misorientation from the main crystal direction. It is further assumed that the two directions of misorientations are independent. The shape of the rocking curve (*i.e.* the results of a scan where the horisontal crystal orientation is varied with respect to the incoming neutrons) will thus for a perfectly collimated monochromatic beam be a Gaussian with a width determined by η_h. No extinction corrections are being made.

The effect of the monochromator is that each neutron is being Bragg scattered according to the Bragg law

$$Q = 2k \sin\theta, \tag{25}$$