NRSF2 Design Document Appendix

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Construct 2 orthogonal q vectors from y-direction and x-direction respectively with rotation by θ along z-axis

$$\begin{aligned}\vec{q_1} &= R_z(-\frac{2\theta}{2})(010)\\ \vec{q_2} &= R_z(-\frac{2\theta}{2})(100)\end{aligned}$$

where

- $2\theta_{peak}$ = position of peak (which is in plane)

In order to convert $\vec{q}$ from instrument coordinate to sample coordinate, the ration will be done on ω, χ and ϕ respectively.

The rotation matrix R_p is defined as

$$R_p = R_x(\phi + 90^o) \times R_y(\chi) \times R_z(-\omega)$$

where

- ω = incident angle
- $\chi = \chi$ rotation about (100) of sample
- $\phi = \phi$ rotation about sample normal

Thus, $\vec{q_1}$ and $\vec{q_2}$ are rotated by R_p such as

$$\begin{aligned}\vec{q\prime}_1 &= R_p \times \vec{q_1}\\ \vec{q\prime}_2 &= R_p \times \vec{q_2}\end{aligned}$$

Finally angle α and β are between $\vec{q_1}$, $\vec{q\prime}_1$, $\vec{q_2}$ and $\vec{q\prime}_2$. Such that

$$\alpha = \cos^{-1}(\vec{q\prime}_2 \cdot \vec{q_2})$$

It is a little complicated for β:

- If $(\vec{q_1})_z >= 0$: $beta = 360^o - \cos^{-1}(\vec{q\prime}_1 \cdot \vec{q_1})$;
- if $(\vec{q_1})_z < 0$: $beta = \cos^{-1}(\vec{q\prime}_1 \cdot \vec{q_1})$

Then

- If $\beta <= 90^o$: $beta = 360^o + (\beta - 90^o)$;
- if $\beta > 90^o$: $beta = (\beta - 90^o)$

Such that β is between 0^o and 360^o.