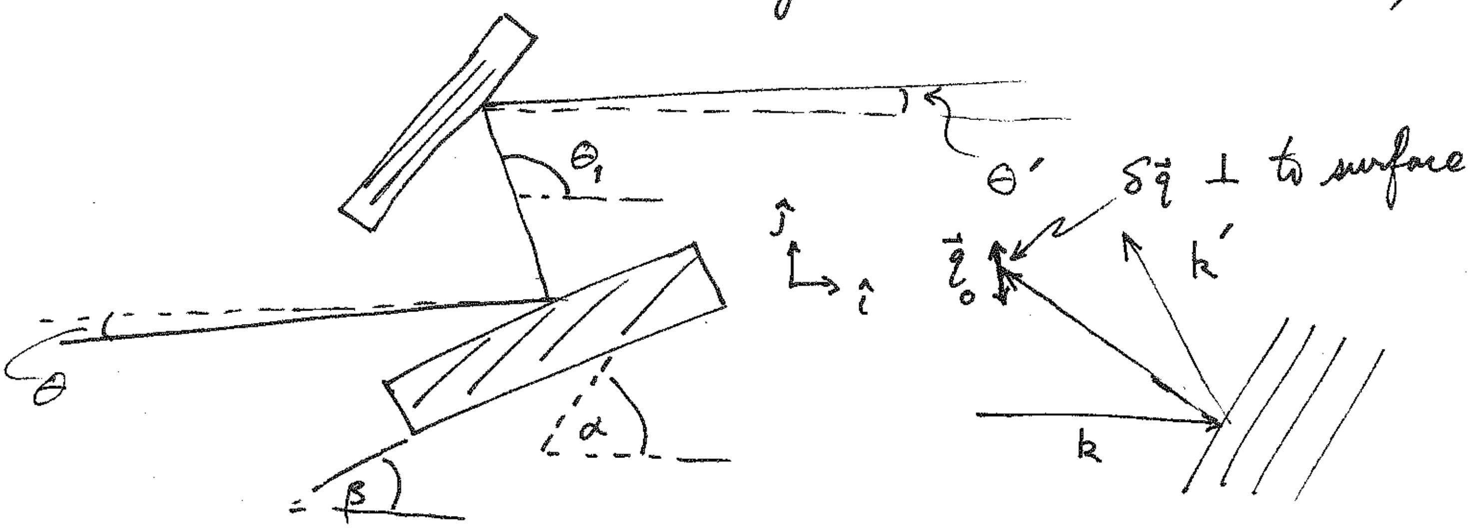
Chess Monochromator Simulation

R. Jones

(Notes made trying to recover the geometry of this simulation based on memory and code comments.)



1) energy conservation : $|\vec{k}| = |\vec{k}'|$

2) momentum " : $\vec{k}' = \vec{k} + \vec{q}_0$ (Bragg) $+ \delta\vec{q}$ (uncert.)

$$\vec{q}_0 = q_0 \left(\cos\alpha \, \hat{j} - \sin\alpha \, \hat{i} \right)$$

$$\delta\vec{q} = \delta q \left(\cos\beta \, \hat{j} - \sin\beta \, \hat{i} \right)$$

<u>case</u> 1: symmetric crystal $\alpha = \beta$

$$\vec{k}' = \vec{k} + (q_0 + \delta q) \underbrace{\left(\cos\alpha \, \hat{j} - \sin\alpha \, \hat{i} \right)}_{\hat{n} \text{ : normal to planes}}$$

$$\cancel{k'^2} = \cancel{k^2} + 2 (q_0 + \delta q)(\vec{k} \cdot \hat{n}) + (q_0 + \delta q)^2$$

$$\vec{k} \cdot \hat{n} = -\frac{1}{2} (q_0 + \delta q) = -\vec{k}' \cdot \hat{n}$$

angle of incidence = angle of reflection $\theta = \theta'$

<u>case 2</u> : asymmetric crystal

$k = k'$ still holds, but not $\theta = \theta'$

because δq creates some broadening $\Delta\theta = \theta - \theta'$

This is a good time to apply Monte Carlo methods.

What is Δq? Estimate from <u>Darwin width</u>

$$\vec{k}' = \vec{k} + q_0(\hat{n}) + \delta q(\hat{s}) \qquad \begin{aligned} \hat{n} &= \cos\alpha\,\hat{j} - \sin\alpha\,\hat{i} \\ \hat{s} &= \cos\beta\,\hat{j} - \sin\beta\,\hat{i} \end{aligned}$$

$$\hat{n}\cdot\vec{k}' = \hat{n}\cdot\vec{k} + q_0 + \delta q\cos(\alpha-\beta)$$

But $\hat{n}\cdot\vec{k}' \cong -\hat{n}\cdot\vec{k}$ to a good approximation

$$-2\underbrace{\hat{k}\cdot\hat{n}}_{k\sin(\alpha+\delta\alpha)} = q_0 + \delta q\cos(\alpha-\beta)$$

(rocking curve width $\delta\alpha$)

(a) $q_0 = 2k\sin\alpha$

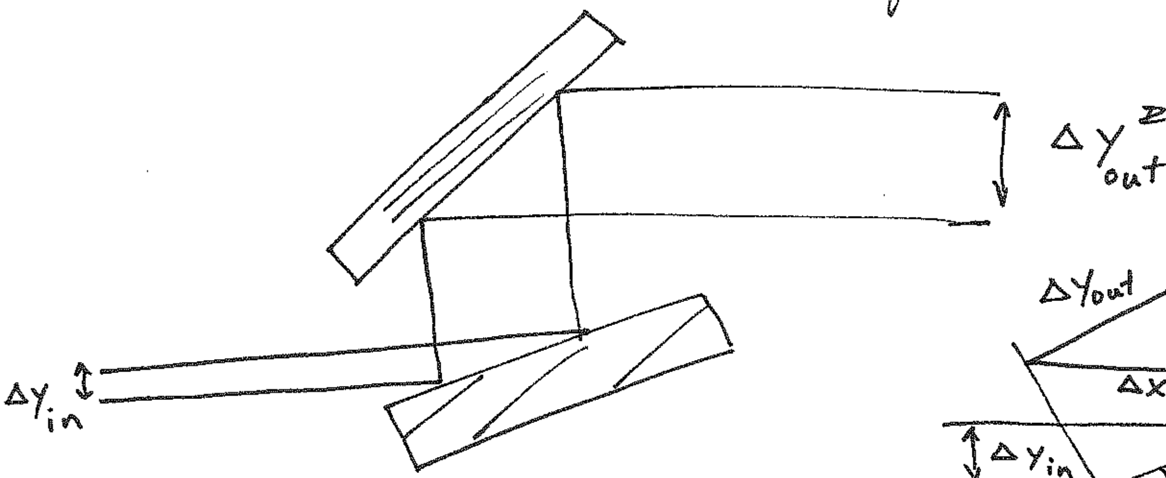
(b) $\delta q = \dfrac{2k\cos\alpha\,\delta\alpha}{\cos(\alpha-\beta)}$

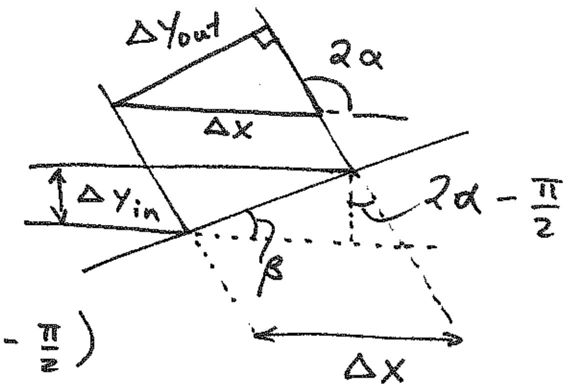
If I take the miscut angle $\alpha - \beta$ to be small

$$\delta q_{FWHM} \simeq 2k\cos\alpha\,\delta\alpha_{FWHM}$$

Darwin width symmetric refl.

What is the beam expansion factor?





$$\Delta x = \frac{\Delta y_{in}}{\tan\beta} + \Delta y_{in} \tan\left(2\alpha - \frac{\pi}{2}\right)$$

$$\Delta y_{out} = \Delta x \sin 2\alpha$$

$$\therefore\ b \equiv \frac{\Delta y_{out}}{\Delta y_{in}} = \sin 2\alpha \left(\frac{1}{\tan\beta} + \tan\left(2\alpha - \frac{\pi}{2}\right) \right)$$

$$= \sin 2\alpha \left(\frac{1}{\tan\beta} - \frac{1}{\tan 2\alpha} \right)$$

consider $\frac{b-1}{b+1}$:

$$\frac{b-1}{b+1} = \frac{\frac{1}{\tan\beta} - \frac{1}{\tan 2\alpha} - \frac{1}{\sin 2\alpha}}{\frac{1}{\tan\beta} - \frac{1}{\tan 2\alpha} + \frac{1}{\sin 2\alpha}}$$

$$= \frac{\frac{1}{\tan\beta} - \frac{\cos 2\alpha + 1}{\sin 2\alpha}}{\frac{1}{\tan\beta} - \frac{\cos 2\alpha - 1}{\sin 2\alpha}} = \frac{\frac{1}{\tan\beta} - \frac{\cancel{2}\cos^{\cancel{2}}\alpha}{\cancel{2}\cancel{\cos\alpha}\sin\alpha}}{\frac{1}{\tan\beta} - \frac{\cancel{2}\sin^{\cancel{2}}\alpha}{\cancel{2}\cos\alpha\cancel{\sin\alpha}}}$$

$$\frac{b-1}{b+1} = \frac{\frac{1}{\tan\beta} - \frac{1}{\tan\alpha}}{\frac{1}{\tan\beta} - \tan\alpha} = \frac{1 - \frac{\tan\beta}{\tan\alpha}}{1 - \tan\alpha\tan\beta}$$

$$\tan\alpha\left(\frac{b-1}{b+1}\right) = \frac{\tan\alpha - \tan\beta}{1 - \tan\alpha\tan\beta} = \tan(\alpha-\beta)$$

$$\tan(\alpha-\beta) = \tan\alpha\left(\frac{b-1}{b+1}\right)$$

Can be used to find b from β or β from b, given α.

★ Simulation

The simulation found in xraymono.f has tools built in to generate θ, k and compute θ' based on the equations above, and also the transmitted intensity. For θ, I use a Gaussian model based on

$$\theta \sim \text{Gauss}\left(0, \frac{1}{\gamma}\right) \quad \text{where } \gamma = 10^4$$

for a CHESS beam energy ~ 5 GeV and a bending magnet field ~ 1.5 T.

$$\underset{\text{keV}}{\mathcal{E}_{crit}} = \frac{2}{3}\,\underset{\text{GeV}}{E_{beam}^2}\,\underset{\text{T}}{B(T)} \cong 25\text{ keV}$$

For $k = 15\text{ keV} = 0.6\,\mathcal{E}_{crit}$ we are close to $\sigma_\theta = \frac{1}{\gamma} = 10^{-4}$ rad.

To do the ray reflections from an asymmetric crystal we need to solve the problem

$$\vec{k}' - \vec{k} = \vec{q} = \vec{q}_0 + \vec{\delta q}$$

$$\vec{k}' = k(\cos\theta'\,\hat{i} + \sin\theta'\,\hat{j}) \qquad \vec{q}_0 = q_0(\cos\alpha\,\hat{j} - \sin\alpha\,\hat{i})$$

$$\vec{k} = k(\cos\theta\,\hat{i} + \sin\theta\,\hat{j}) \qquad \delta\vec{q} = \delta q(\cos\beta\,\hat{j} - \sin\beta\,\hat{i})$$

$$k(\cos\theta' - \cos\theta) = -q_0\sin\alpha - \delta q\sin\beta$$

$$k(\cancel{\sin}\,\theta' - \sin\theta) = q_0\cos\alpha + \delta q\cos\beta$$

Eliminate the δq term:

$$k\left(\cos\theta' - \cos\theta + (\sin\theta' - \sin\theta)\tan\beta\right) = q_0(-\sin\alpha + \cos\alpha\tan\beta)$$

$$\cos\theta' + \sin\theta'\tan\beta = \cos\theta + \sin\theta\tan\beta - \frac{q_0}{k}\sin\alpha + q_0\cos\alpha\tan\beta$$

$$\underbrace{\cos\theta'\cos\beta + \sin\theta'\sin\beta}_{\cos(\theta'-\beta)} = \underbrace{\cos\theta\cos\beta + \sin\theta\sin\beta}_{\cos(\theta-\beta)} - \frac{q_0}{k}\underbrace{(\sin\alpha\cancel{\cos}\cos\beta - \cos\alpha\sin\beta)}_{\sin(\alpha-\beta)}$$

$$\cos(\theta'-\beta) = \cos(\theta-\beta) - \frac{q_0}{k}\sin(\alpha-\beta)$$

Based on this, one can go back and substitute for θ' in the earlier equations to solve for δq.