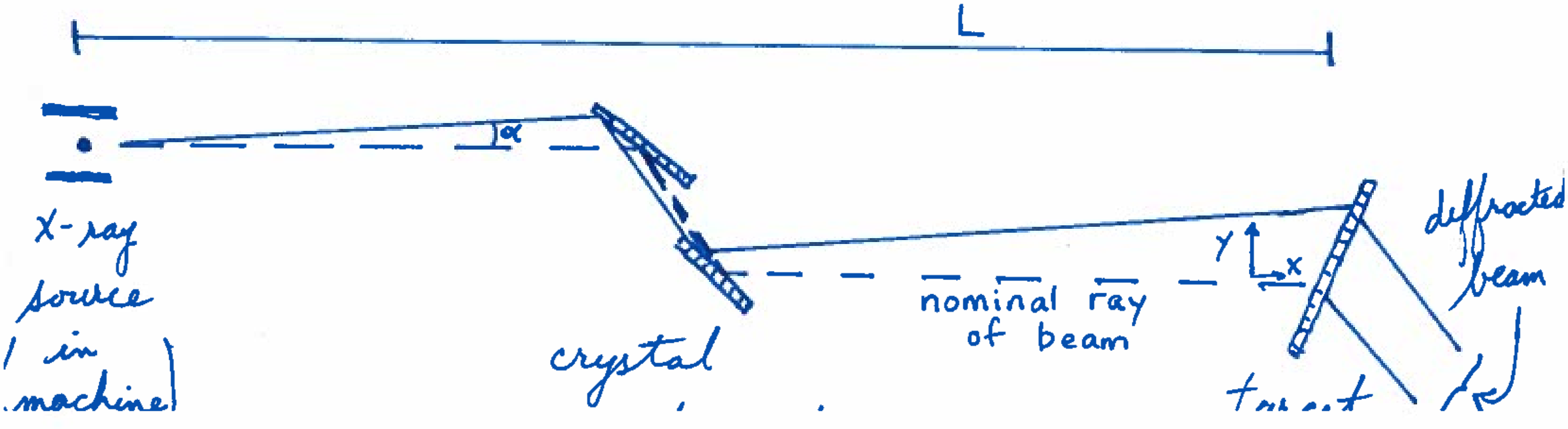
Dispersion Correction in X-Ray Topography R. Jones

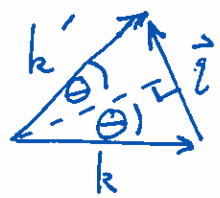
Sept 22, 2016 Because the X-ray beam from a synchrotron light source is highly parallel, to a first approximation all of the area of a diffraction sample that is illuminated by the beam should light up at once, once the diffraction condition is met. This is assuming that the entire sample is a perfect crystal. However, for crystals with very narrow rocking curves, this approximations breaks down, with different parts of the crystal reaching the diffraction maximum at slightly different angles. The reason for this is that the X-ray beam exhibits dispersion along the direction of the monochromator deflection plane. This is illustrated below.



The nominal ray indicated by the dashed line is presumably the center of the beam, and all other rays accepted by the beam slits are indicated by values of $\alpha \neq 0$. At the position of the target, a ray of angle α strikes the target at height y from the beam axis, where

$$y = L \tan\alpha \cong L\alpha \quad , \quad L \gg y$$

The general condition for diffraction from a set of planes with reciprocal lattice vector $\vec{q}$ is given by the Bragg triangle, where k is the momentum of the X-ray



$$q = 2k \sin\theta \leftarrow \text{Bragg diffraction condition}$$

at the monochromator, this condition becomes

$$q_m = 2k \sin(\theta_M + \alpha)$$

which becomes a constraint between k and α, the range of α being constrained by the beam slits and ultimately by the size of the mono crystal.

θ_m is the "monochromator setting" which is the angle between the $\vec{q}_m$ vector planes and the nominal beam ray, which is adjusted so that the mono beam has a maximum intensity at some desired X-ray momentum k_0 given by

$$q_m = 2k_0 \sin\theta_m$$

During the measurement, the equivalent angle to θ_m at the diamond target for vector $\vec{q}_D$ is defined as θ_D

$$q_D = 2k_0 \sin\theta_D$$

However the whole diamond <u>does</u> <u>not</u> diffract when the target $\theta = \theta_D$, just the part at $\alpha = 0$, because more generally, the Bragg condition for the target is:

$$q_D = 2k \sin(\theta + \alpha)$$

So how does the beam dispersion cause the angle θ_{max} to shift away from θ_D, as a function of Y? That is what this derivation sets out to find.

$$q_D = 2(k_0 + dk)(\sin\theta + \alpha\cos\theta)$$

where here I treat the dispersion shift Δk and the angle shift α as first-order differentials in dy. To find $dk(dy)$, see that

$$q_m = 2(k_0 + dk)(\sin\theta_m + \alpha\cos\theta_m)$$

$$(q_m - 2k_0\sin\theta_m) = 0 = 2\sin\theta_m dk + 2k_0\alpha\cos\theta_m$$

$$dk = -k_0\cot\theta_m\,\alpha = \left(-\frac{k_0\cot\theta_m}{L}\right)y$$

Putting that into the above equation for q_D:

$$q_D = 2k_0(1 - \alpha\cot\theta_m)(\sin\theta + \alpha\cos\theta)$$

$$q_D - 2k_0\sin\theta = 2k_0\,\alpha\,(\cos\theta - \sin\theta\cot\theta_m)$$

$$-\cancel{2k_0}(\sin\theta - \sin\theta_D) = -\cancel{2k_0}(\sin\theta\cot\theta_m - \cos\theta)\alpha$$

$$\tan\theta - \underbrace{\left(\frac{\sin\theta_D}{\cos\theta}\right)}_{\simeq\tan\theta_D} = (\underbrace{\tan\theta}_{\simeq\tan\theta_D}\cot\theta_m - 1)\alpha$$

$$\boxed{\tan\theta = \tan\theta_D + \alpha(\tan\theta_D\cot\theta_m - 1)}$$