derivations

July 8, 2022

1 Derivations for calculating the sample-to-detector distance from a calibration sample diffraction image

1.1 Definitions

Define q_n as

$$q_n = \frac{4\pi \sin\theta_n}{\lambda}, \tag{1}$$

where θ_n refers to the n^{th}-order Bragg peak, q_n is the wavelength-agnostic peak location, and the units of q_n and λ are inverse of each other.

We also have a triangle from our sample to the nth order peak on the detector, giving the relation

$$\tan 2\tilde{\theta}_n = \frac{\tilde{r}_n}{L}, \tag{2}$$

where $\tilde{r}_n$ is the location of the nth order peak and L is the sample-to-detector distance. The units of $\tilde{r}_n$ and L must match. We use inverse Angstroms for q_n units.

1.2 Derivations

The goal is to obtain an expression for L, the sample-to-detector distance.

Solve for θ in the expression for q_n above:

$$\theta_n = \sin^{-1}\frac{q_n\lambda}{4\pi} \tag{3}$$

Now make the assumption that our calibration sample is good and set $\tilde{\theta}_n = \theta_n$, in the second equation above, yielding

$$\frac{\tilde{r}_n}{L} = \tan 2\theta_n = \tan\left[2\sin^{-1}\left[\frac{q_n\lambda}{4\pi}\right]\right] \tag{4}$$

1.3 Linear regression

Given $\tilde{r_n}$, we need L to be able to calculate $\tilde{q}_n$. Since we have N measurements, $\tilde{r}_n$ for $n = 1, ..., N$, we can have $y = mx$, where $y = \tan 2\theta_n$, and $x = \tilde{r}_n$, and $m = 1/L$.