derivations

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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:

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

where $\tilde{r}_n$ is the location of the nth order peak and L is the sample-to-detector distance. The units of r_n and L must match.

1.2 Derivations

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

Solve for θ in both equations above:

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

$$\theta_n = \frac{1}{2}\tan^{-1}\frac{\tilde{r}_n}{L}. \tag{4}$$

Now set these two equations equal,

$$\sin^{-1}\frac{q_n\lambda}{4\pi} = \frac{1}{2}\tan^{-1}\frac{\tilde{r}_n}{L}, \tag{5}$$

and, finally, solve for L:

$$L = \frac{\tilde{r}_n}{\tan\left[2\sin^{-1}\frac{q_n\lambda}{4\pi}\right]} \tag{6}$$

1.3 Linear regression

If we plot $\tan\left[2\sin^{-1}\frac{q_n\lambda}{4\pi}\right]$ vs. $\tilde{r}_n$, the slope will be L.