Derivation: broadening of a rocking curve from curvature of the crystal

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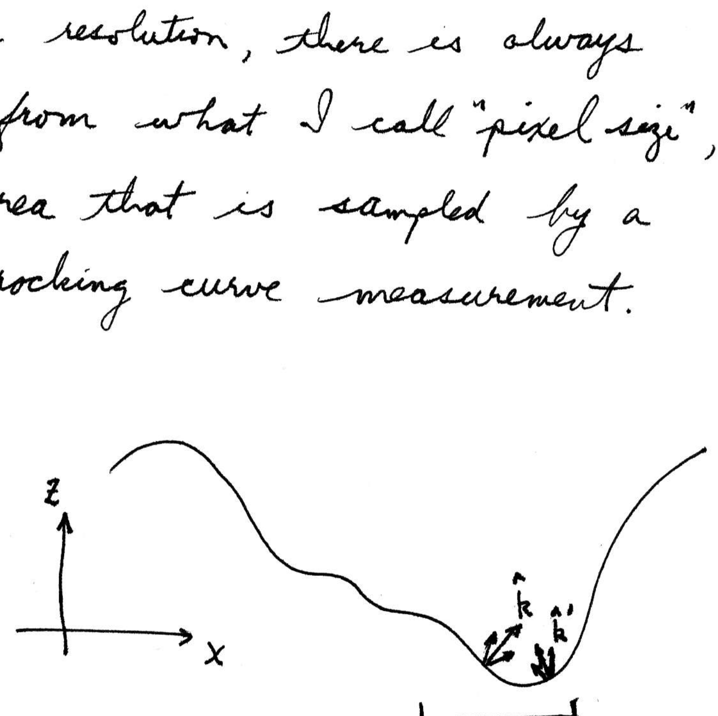
In regions of a crystal with large curvature, the rocking curve has a contribution to its width from the size of the crystal illuminated by the beam. This contribution goes to zero as the beam slits are closed, or as the spatial resolution of the rocking curve image improves. At finite resolution, there is always a non-zero contribution from what I call "pixel size", the size of the crystal area that is sampled by a single channel in the rocking curve measurement.

Let $z(x,y)$ represent the elevation function of a continuous plane in an extended crystal.



Let $I_0(\alpha, x, y)$ be the rocking curve for vanishing pixel size, and $I(\alpha, x, y)$ be the actual observed rocking curve for a pixel of size $(\Delta x)(\Delta y)$. Here I take x to measure displacement in the rocking plane and y $\perp$ to the rocking plane, α is rocking angle.

$$I(\alpha, \vec{x}) = \int d^2x' \; S(\vec{x} - \vec{x}') \; I_0(\alpha, \vec{x}')$$

where $S(\vec{x})$ is the "point-spread function" of the camera + beam optics for the given geometry. I take the "twisted sheet" view of the dependence of $I_0(\alpha, \vec{x})$ on position $\vec{x}$, that it mainly just shifts the central value of α (rocking curve peak position)

$$I_0(\alpha, \vec{x}) = I_1(\alpha - \alpha_0(\vec{x}))$$

at least in some local neighborhood of $\vec{x}$, the shape of I_0 just shifts without significant distortion. In this same spirit, I expand the function α_0 about the point $\vec{x}$, as

$$\alpha_0(\vec{x}') \cong \alpha_0(\vec{x}) + \vec{\alpha}_1(\vec{x}) \cdot (\vec{x}' - \vec{x}) \;, \quad |\vec{x}' - \vec{x}| \lesssim \Delta x$$

$$\therefore \quad I(\alpha, \vec{x}) = \int d^2x' \; S(\vec{x} - \vec{x}') \; I_1(\alpha - \alpha_0(\vec{x}) - \vec{\alpha}_1(\vec{x}) \cdot (\vec{x}' - \vec{x}))$$

where $\vec{\alpha}_1 = \vec{\nabla}\alpha$. Redefine $\vec{x}' \to \vec{x}' - \vec{x}$, integration becomes

$$I(\alpha, \vec{x}) = \int d^2x' \; S(\vec{x}') \; I_1(\alpha - \alpha_0(\vec{x}) - \vec{\alpha}_1(\vec{x}) \cdot \vec{x}')$$

$$\cancel{= \int d^2a \; S'(\vec{a}) \; I_1(\alpha - \alpha_0(\vec{x}) - \vec{a})}$$

Now let $a = \vec{\alpha}_1(\vec{x}) \cdot \vec{x}'$ be the relevant spatial axis of integration and integrate $S(x, y)$ over the other direction.

$$I(\alpha, \vec{x}) = \int da \;\; S'(a) \;\; I_1(\alpha - \alpha_0(\vec{x}) - a)$$

which is a convolution between S' and I_1 where I_1 is the intrinsic rocking curve at $(\vec{x})$

and
$$S'(a) = \int d^2x' \;\; S(\vec{x}') \; \delta(a - \vec{\alpha}_1(\vec{x}) \cdot \vec{x}')$$

is the point spread function projected onto the direction of $\vec{\alpha}_1$.

Take $S(\vec{x})$ to be a Gaussian with 2 widths:

$$S(\vec{x}) = \frac{1}{2\pi(\Delta x)(\Delta y)} \, e^{-\frac{1}{2}\left(\left[\frac{x}{\Delta x}\right]^2 + \left[\frac{y}{\Delta y}\right]^2\right)}$$

$$S'(a) = \frac{1}{2\pi(\Delta x)(\Delta y)} \int dx' \;\; e^{-\frac{1}{2}\left(\left[\frac{x'}{\Delta x}\right]^2 + \left[\frac{y'}{\Delta y}\right]^2\right)} \delta(a - \vec{\alpha}_1 \cdot \vec{x}')$$

Let $\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x' \\ y' \end{pmatrix}$ such that $\tan\theta = \dfrac{\alpha_{1y}}{\alpha_{1x}}$

$$S'(a) = \frac{1}{2\pi(\Delta x)(\Delta y)} \int du\, dv \;\; e^{-\frac{1}{2}\left(\left[\frac{u\cos\theta - v\sin\theta}{\Delta x}\right]^2 + \left[\frac{u\sin\theta + v\cos\theta}{\Delta y}\right]^2\right)} \delta(a - \alpha_1 u)$$

(after several steps) $= \dfrac{\alpha_1}{\sqrt{2\pi}\,\sigma_a} \displaystyle\int du \;\; e^{-\frac{1}{2}\left(\frac{\alpha_1 u}{\sigma_a}\right)^2} \delta(a - \alpha_1 u)$, $\quad \sigma_a = \sqrt{\alpha_{1x}^2 \Delta x^2 + \alpha_{1y}^2 \Delta y^2}$

$$S'(a) = \frac{1}{\sqrt{2\pi}\,\sigma_a} \, e^{-\frac{1}{2}\left(\frac{a}{\sigma_a}\right)^2}$$, gaussian of r.m.s. $= \sqrt{\alpha_{1x}^2 \Delta x^2 + \alpha_{1y}^2 \Delta y^2}$

Therefore, to find $I_0(\alpha, x, y)$ I first measure $I(\alpha, x, y)$ and use it to find an estimate for $\alpha_0(x,y)$ by finding the peak centroid at each pixel. I then differentiate $\alpha_0(x,y)$ to find the vector function $\vec{\alpha}_1 = \vec{\nabla}\alpha_0$ at each pixel.

Then I compute $\sigma_a = \sqrt{\alpha_{1x}^2 \Delta x^2 + \alpha_{1y}^2 \Delta y^2}$ for each pixel.

Then I take a Gaussian of width σ_a and unit norm and de-convolve it with the $I(\alpha, x, y)$ rocking curve to get an estimate for $I_0(\alpha, x, y)$ at each pixel. Alternately, I can fit each pixel $I(\alpha, x, y)$ curve to a Gaussian and take the widths $\sigma_\alpha(x,y)$ for each fit and correct for pixel size as:

$$\sigma_{\alpha 0}^2(x,y) = \sigma_\alpha^2(x,y) - \sigma_a^2(x,y)$$

and take $\sigma_{\alpha 0}^2$ as the estimate for the width squared of $I_0(\alpha, x, y)$ at each pixel.