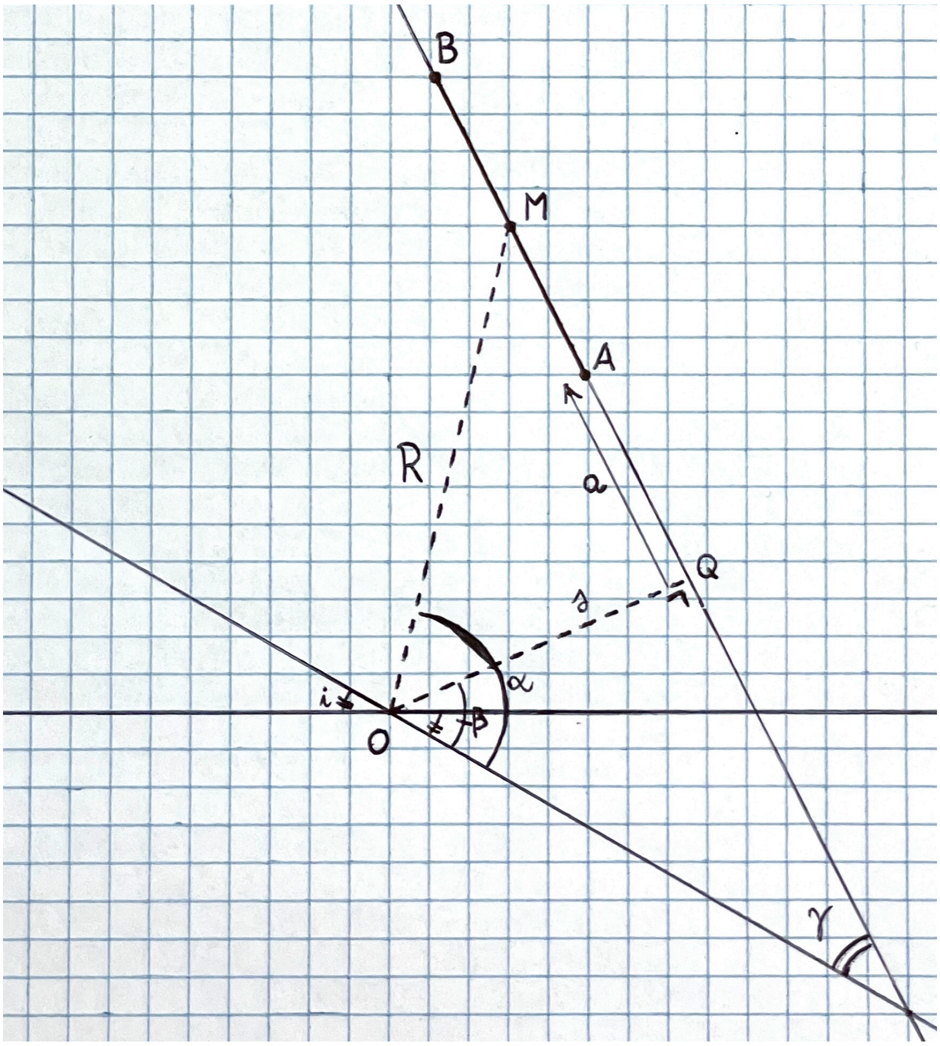
Angular error using linear detector

Compare different descriptions of detector positioning



The incident ray hits the sample in point O. The detector is represented by segment AB, with length $L = \overline{AB}$. The middle point of the detector is called M. We indicate as Q the point in the line of the detector such that OQ is perpendicular to the line of the detector.

When we deal with calibration procedure, we indicate position and orientation of the detector by means of 3 parameters:

- a: distance $\overline{QA}$, taken as positive if Q and M lie in opposite semilines with respect to A, taken as negative if Q and M lie in the same semiline with respect to A;
- s: distance $\overline{OQ}$ between the hit point of the sample and the line of the detector;
- β: angle between the prolongation of incident ray and segment OQ.

On the other hand, when we deal with experimental setting, we indicate position and orientation of the detector by means of 3 other parameters:

- R: distance $\overline{OM}$ between the hit point of the sample and the middle point of the detector;
- α: angle between the prolongation of incident ray and segment OM;
- γ: angle between the prolongation of incident ray and the line of the detector.

With some calculations, we can obtain the formulas to transform between the two sets of coordinates:

$$(a, s, \beta) \longleftrightarrow (R, \alpha, \gamma)$$

$$\begin{cases} R = \sqrt{s^2 + \left(\frac{L}{2} + a\right)^2} \\ \alpha = \beta + \arctan\left(\dfrac{\frac{L}{2} + a}{s}\right) \\ \gamma = 90^\circ - \beta \end{cases}$$

$$\begin{cases} a = -\left[\frac{L}{2} + R\cos(\alpha + \gamma)\right] \\ s = R\sin(\alpha + \gamma) \\ \beta = 90^\circ - \gamma \end{cases}$$

Positioning detector with fixed θ_{min} and θ_{max}

Position and orientation of the detector are given by a, s, β. Knowing these parameters, the calibration is given by

$$\theta = \arctan\left(\frac{x + a}{s}\right) + \beta$$

If we fix θ_{min} and θ_{max}, the detector has some constraints and the parameters a, s, β must satisfy some relationships. In particular we can see that, for given θ_{min} and θ_{max}, if we choose a value of β (orientation of the detector), the distances a and s are determined as a consequence of that. The mathematical solution is

$$\begin{aligned} a &= s\tan(\theta_{\text{min}} - \beta) \\ s &= \frac{L}{\tan(\theta_{\text{max}} - \beta) - \tan(\theta_{\text{min}} - \beta)} \end{aligned}$$

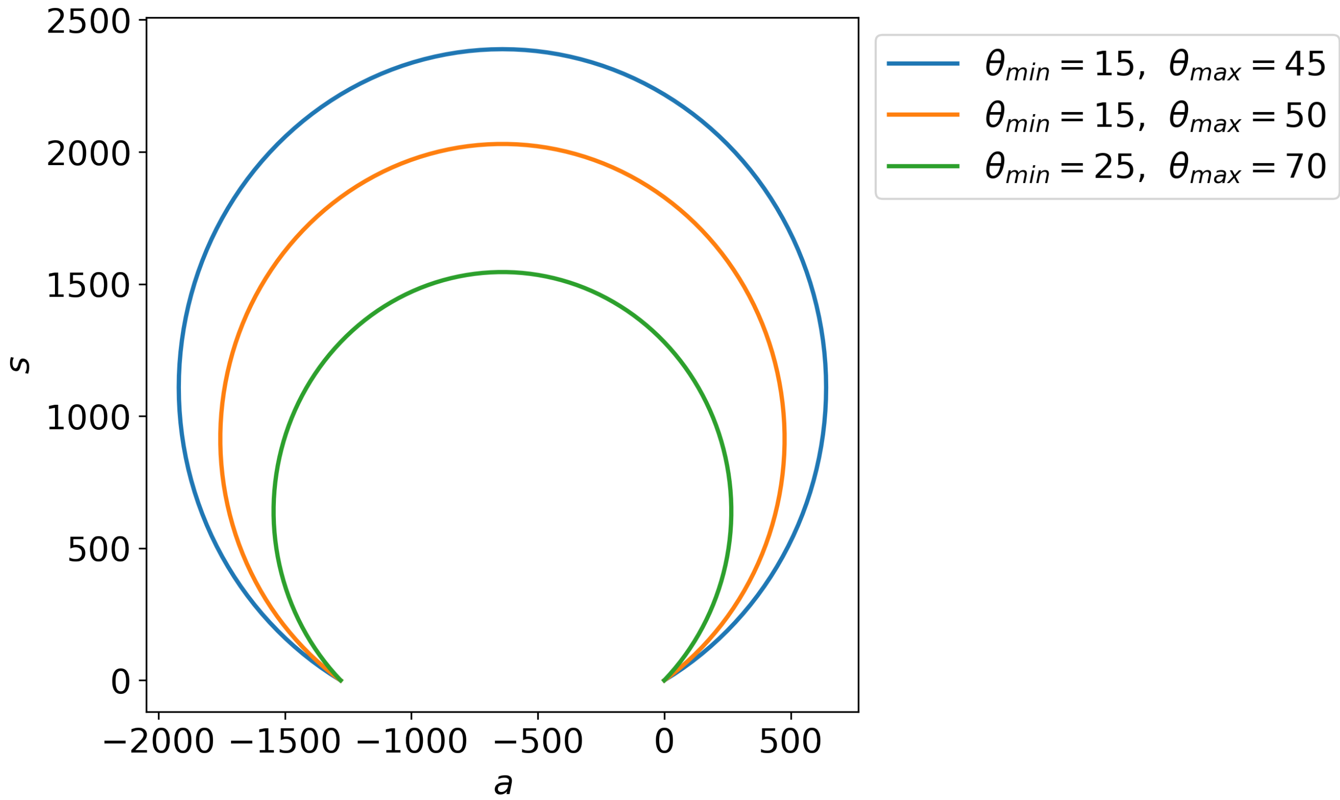
which can be rewritten as

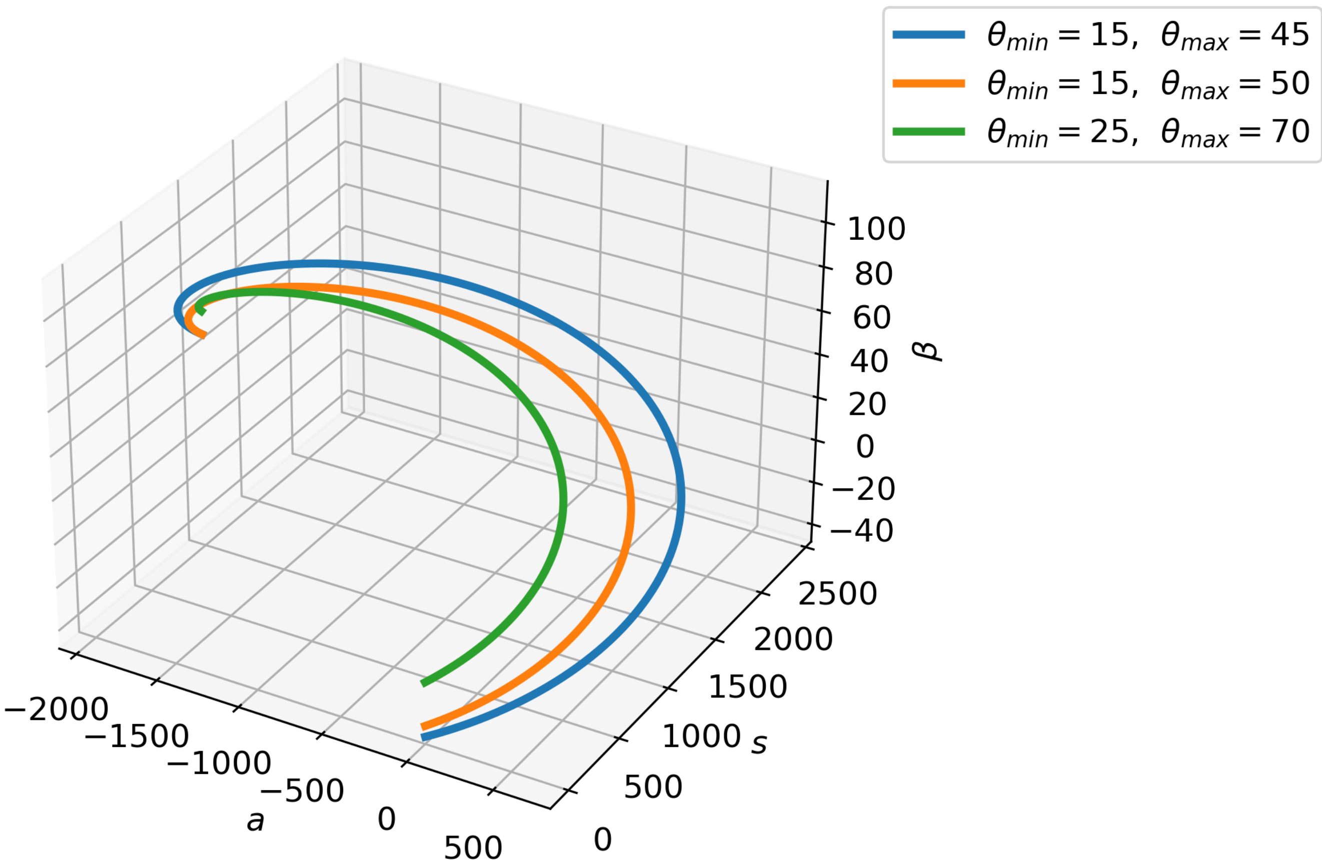
$$a = \frac{\cos(\theta_{\max} - \beta)\sin(\theta_{\min} - \beta)}{\sin(\theta_{\max} - \theta_{\min})} L = \left[\frac{\sin(\theta_{\max} + \theta_{\min} - 2\beta)}{\sin(\theta_{\max} - \theta_{\min})} - 1\right] \frac{L}{2}$$

$$s = \frac{\cos(\theta_{\max} - \beta)\cos(\theta_{\min} - \beta)}{\sin(\theta_{\max} - \theta_{\min})} L = \left[\frac{\cos(\theta_{\max} + \theta_{\min} - 2\beta)}{\sin(\theta_{\max} - \theta_{\min})} + \frac{1}{\tan(\theta_{\max} - \theta_{\min})}\right] \frac{L}{2}$$

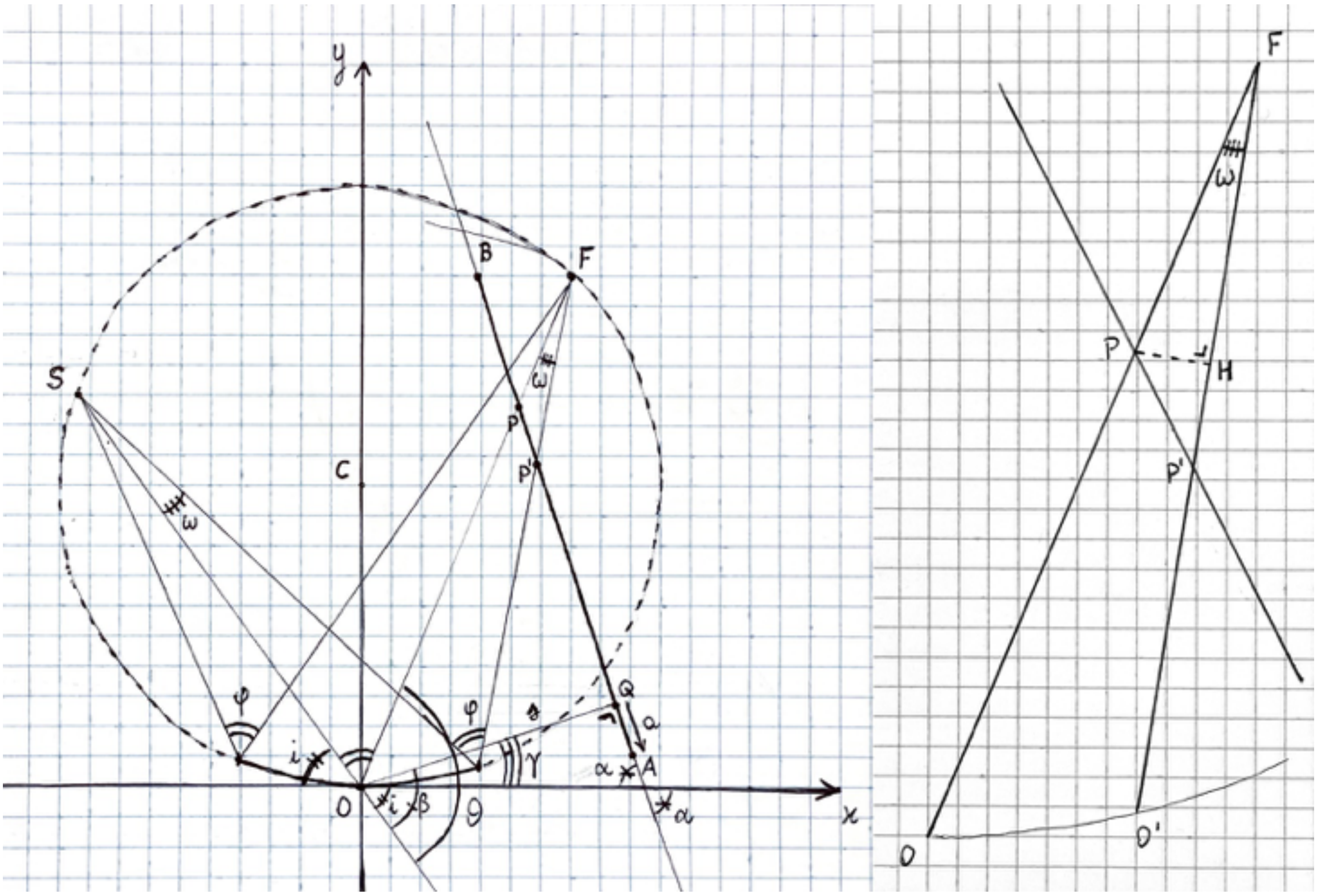
We remind that L is the length of the detector.

To select solutions that are physically meaningful, we need to limit the values of β. It is easy to see that the condition is $\theta_{\max} - 90^\circ < \beta < \theta_{\min} + 90^\circ$.





Analytical description (circular sample approximation)



In our construction, S is the focus of the beam coming from the source. In the approximation of circular sample, the sample is an arc of circle and all the rays of the incident beam that are diffracted with the same angle will converge on a point F in the same circle. That's why this circle is called *focussing circle*. We indicate it as $\mathcal{C}$.
We choose a coordinate system with origin O in the center of the sample. The x axis is tangent to the focussing circle. As a consequence, the center C of the focussing circle $\mathcal{C}$ lays on y axis.

Regarding the incident beam, we indicate as d the distance $\overline{OS}$ and as i the incident angle. We indicate as θ the diffraction angle (which in some sources is indicated as 2θ). The detector is represented by segment AB, with channels increasing from A to B. Parameters a, s, β express position and orientation of the detector.

The central ray of the beam hits the sample in point O, is diffracted with angle θ and hits the detector in point P. We also follow the path of another ray of the beam, coming from S with deviation ω with respect to the central ray. We choose deviation angle ω as positive in case of anti-clockwise deviation. The second ray hits the sample in point O', is diffracted with the same angle θ and hits the detector in P'.

So far, we have described deviation on the plane of the figure, described by angle ω. Deviation can also happen perpendicularly to that plane and we describe it with angle ψ.

Some relations between the angles in the figure:

$$\theta + \varphi = 180^\circ \quad ; \quad \gamma = \beta - i \quad ; \quad \alpha = 90^\circ - \gamma = 90^\circ - (\beta - i)$$

We can easily express the coordinates of points S and Q:

$$S\,(-d\cos i, d\sin i) \quad ; \quad Q\,(s\cos\gamma, s\sin\gamma) = (s\cos(\beta - i), s\sin(\beta - i))$$

OF line

We can easily see that its equation is

$$y = x\tan(\theta - i)$$

Focussing circle C

We impose that its center is in y axis and that it contains points O and S. With easy calculations we find that its equation is

$$x^2 + y^2 - \frac{d}{\sin i}y = 0$$

Its radius is $R = \frac{d}{2\sin i}$

Point F

We find it as the intersection between OF line and focussing circle C. Excluding the trivial solution in point O, the other solution is

$$F\left(\frac{\sin(\theta - i)\cos(\theta - i)}{\sin i}d, \frac{\sin^2(\theta - i)}{\sin i}d\right)$$

Point O'

$$O'\,(R\sin(2\omega), R\,[1 - \cos(2\omega)]) = \left(\frac{\sin\omega\cos\omega}{\sin i}d, \frac{\sin^2\omega}{\sin i}d\right)$$

Footprint

The footprint of the incident beam on the sample is given by 2 times the arc OO':

$$M = 4\omega R = \frac{2d\omega}{\sin i}$$

$P'F$ line

Slope: $\tan(\theta - i + \omega)$
If we impose that the line contains point F, after some calculations we can find the equation of the line:

$$y = x\tan(\theta - i + \omega) - \frac{\sin\omega\sin(\theta - i)}{\sin i\cos(\theta - i + \omega)}d$$

AB line

Slope: $-\tan\alpha = -\tan(90^\circ - \gamma) = -\frac{1}{\tan\gamma} = -\frac{1}{\tan(\beta - i)}$
Y-intercept q: $s = q\sin\gamma = q\sin(\beta - i) \quad ; \quad q = \frac{s}{\sin(\beta - i)}$
Its equation is

$$y = -\frac{1}{\tan(\beta - i)}x + \frac{1}{\sin(\beta - i)}s$$

Also, from calibration formula we know that

$$\overline{QP} = s\tan(\theta - \beta)$$

Points A, B

They have simple coordinates in the reference system $Ox'y'$ with x' axis parallel to s. If we apply to this system a clockwise rotation of angle $\gamma = \beta - i$, we find the coordinates of the points A, B in the reference system Oxy.

$$A(s\cos(\beta - i) - a\sin(\beta - i), a\cos(\beta - i) + s\sin(\beta - i))$$
$$B(s\cos(\beta - i) - (L - a)\sin(\beta - i), (L - a)\cos(\beta - i) + s\sin(\beta - i))$$

Point P

We find it as the intersection between OF and AB. After some calculations, we find that

$$P\left(\frac{\cos(\theta - i)}{\cos(\theta - \beta)}s, \frac{\sin(\theta - i)}{\cos(\theta - \beta)}s\right)$$

Distance $\overline{OP}$

$$\overline{OP} = \frac{s}{\cos(\theta - \beta)}$$

Point P'

We find it as the intersection between $P'F$ and AB. After some calculations, we find that

$$\begin{cases} x_{P'} = \dfrac{1}{\cos(\theta-\beta+\omega)}\left[s\cos(\theta-i+\omega)+d\dfrac{\sin(\beta-i)\sin\omega\sin(\theta-i)}{\sin i}\right] \\ y_{P'} = \dfrac{1}{\cos(\theta-\beta+\omega)}\left[s\sin(\theta-i+\omega)-d\dfrac{\cos(\beta-i)\sin\omega\sin(\theta-i)}{\sin i}\right] \end{cases}$$

Error given by defocus

Defocus distance

Let's define the defocus distance as $\Delta f = \overline{FP}$.
After some calculations, it can be found that

$$\Delta f = \frac{1}{\cos(\theta-\beta)}s - \frac{\sin(\theta-i)}{\sin i}d$$

This distance is positive if P and O lie in opposite semilines with respect to F, while it is negative if P lies between O and F. In other words, Δf is positive if the beam hits the detector after converging in F and starting to diverge; it is negative if the beam hits the detector before converging in F.

Defocus in the detector

Defocus in the detector is given by $\Delta p = \overline{PP'}$.

$$\begin{aligned} O\hat{P}P' &= 90^\circ - (\theta-\beta) \\ F\hat{P}P' &= 180^\circ - O\hat{P}P' = 90^\circ + \theta - \beta \\ P\hat{P'}F &= 180^\circ - F\hat{P}P' - \omega = 90^\circ - (\theta-\beta+\omega) \\ \overline{PH} &= \overline{FP}\sin\omega = \Delta f \sin\omega \\ \overline{PH} &= \overline{PP'}\sin\left(P\hat{P'}F\right) = \overline{PP'}\cos(\theta-\beta+\omega) \end{aligned}$$

$$\begin{aligned} \Delta p(\omega) = \overline{PP'} &= \frac{\sin\omega}{\cos(\theta-\beta+\omega)}\Delta f \\ &= \frac{\sin\omega}{\cos(\theta-\beta+\omega)}\left[\frac{1}{\cos(\theta-\beta)}s - \frac{\sin(\theta-i)}{\sin i}d\right] \end{aligned}$$

Δp can be positive or negative, depending on the signs of ω and Δf. If $\Delta p > 0$, it means that P' is in a higher channel than P in the detector. On the other hand, if $\Delta p < 0$, P' is in a lower channel than P.

Error in position

Experimentally, we detect a diffraction peak and we measure the position p of the peak in the detector. In other words, we measure the distance between the peak and the first channel of the detector.

The central ray of the beam, after a diffraction of angle θ, hits the detector in point P. We measure $p = \overline{AP}$. On the other hand, the ray of the beam with deviation ω hits the detector in point P'. This would give us a biased measure of the position of the peak: $p' = \overline{AP'}$.

We suppose that the beam coming out from focus point S has a uniform distribution of deviation angles in the range $[-\omega, \omega]$. Let's call $(\Delta p)_{\text{defocus}}$ the error in the measure of position p produced by defocus. We take it as the average of the two errors produced by the extreme rays with deviations ω and $-\omega$.

$$(\Delta p)_{\text{defocus}} = \frac{|\Delta p\,(\omega)| + |\Delta p\,(-\omega)|}{2}$$

Error given by diffraction cone

We need to take into account that the incident ray diffracted in point O produces not only a single diffracted ray OP, but a diffraction cone whose axis is the prosecution of the incident ray and whose aperture is 2θ.

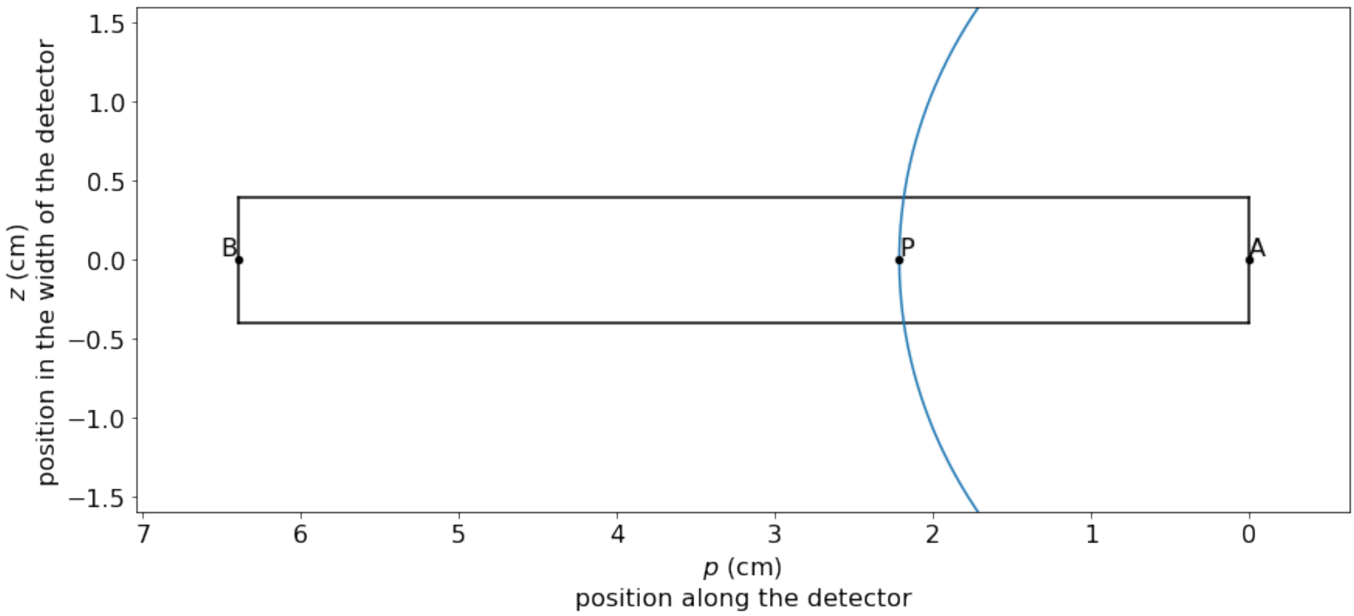
We have approximated the detector as segment AB, but in reality it has a non-negligible height h perpendicular to AB. So, the detector needs to be described as a rectangular contained in the plane of the detector. This plane is perpendicular to both x and y axes and parallel to AB. We want to find the conic given by the intersection between the diffraction cone and the plane of the detector. In general, this conic can span more than one channel in the detector.

A right circular conical surface with apex at the origin, axis parallel to the vector $\boldsymbol{v}$ and aperture 2θ is described by the implicit equation

$$(\boldsymbol{v} \cdot \boldsymbol{x})^2 - (\boldsymbol{v} \cdot \boldsymbol{v})\,(\boldsymbol{x} \cdot \boldsymbol{x}) \cos^2 \theta = 0$$

We analyse the diffraction cone in a convenient reference system $Ox'y'z$ with origin in O and with axes x' and y' parallel to OQ and AB respectively. In this system, the plane of the detector has equation $x' = s$. We want to find the conic curve in the plane of the detector. We call $p = y' - a$ the distance of the generic point of the conic from channel 0. This distance is measured along the detector axis. For example, point

P has $p = \overline{AP}$. Also, we remember that z is the distance of the generic point of the conic from the detector axis AB. We describe the conic by the two coordinates p and z.



Central ray

The axis of the cone is parallel to vector $\boldsymbol{v} = (\cos\beta, -\sin\beta, 0)$. After some calculations, we can find the equation of the conic curve in the plane of the detector.

$$z^2 = \left(\frac{\sin^2\beta}{\cos^2\theta} - 1\right)(p+a)^2 - 2s\frac{\sin\beta\cos\beta}{\cos^2\theta}(p+a) + \left(\frac{\cos^2\beta}{\cos^2\theta} - 1\right)s^2$$

We can calculate p as a function of z. There are two solutions:

$$p_1 = p_1\,(z; a, s, \beta, \theta) = s\tan(\theta - \beta) - a - \frac{z^2\cos\theta}{s\sin\theta + \sqrt{\left(s^2 + z^2\right)\sin^2\theta - z^2\cos^2\beta}}$$

$$p_2 = p_2\,(z; a, s, \beta, \theta) = -s\tan(\theta + \beta) - a + \frac{z^2\cos\theta}{s\sin\theta + \sqrt{\left(s^2 + z^2\right)\sin^2\theta - z^2\cos^2\beta}}$$

We are interested in solution p_1. Point P has $p = p_1\,(0; a, s, \beta, \theta) = s\tan(\theta - \beta) - a$. If we move along the conic curve, where $z \neq 0$ the value of p is shifted by a quantity dependent on z. The maximum shift occurs at the edge of the detector ($z = h/2$), where $p = p_1\,(h/2; a, s, \beta, \theta)$.

Deviation ω

If we consider a ray with deviation ω parallel to the plane of figure, in a first approximation we can just horizontally traslate the conic curve so that its vertex is in P' instead of P. The shifting $\overline{PP'}$ is already calculated in the section about defocus error.

Deviation ψ

If we consider a ray with deviation ψ perpendicular to the plane of figure, in a first approximation we can just vertically traslate the conic by an amount

$$\Delta z = \left(d + \overline{OP}\right) \tan \psi = \left[d + \frac{s}{\cos(\theta - \beta)}\right] \tan \psi$$

Total error given by cone and defocus

Let's call $p\,(z; a, s, \beta, \theta, d, i, \omega, \psi)$ the function describing the diffraction conic in the plane of the detector, for some given detector positioning (a, s, β), diffraction angle (θ), focus-sample distance (d), incident angle of the beam axis (i) and deviation of the incident ray (ω, ψ).

Rays of the beam have deviations ω spanning in the interval $\Omega = [-\omega^*, \omega^*]$ and ψ spanning in the interval $\Psi = [-\psi^*, \psi^*]$. Also, to describe the conic we need to span the detector in its height $[-h/2, h/2]$. Each ray of the beam generates a diffraction conic in the detector. We consider the interval between minimum and maximum p among all these conics and take the error $(\Delta p)_{\text{cone}}$ as half of that interval.

$$(\Delta p)_{\text{cone}} = \frac{1}{2}\left(\max_{\substack{\forall z \in [-h/2, h/2] \\ \forall \omega \in \Omega \\ \forall \psi \in \Psi}} p - \min_{\substack{\forall z \in [-h/2, h/2] \\ \forall \omega \in \Omega \\ \forall \psi \in \Psi}} p \right)$$

Angular error

Once we measure the position p of the diffraction peak in the detector, we can convert position to angle by using the calibration formula

$$\theta = \arctan\left(\frac{p + a}{s}\right) + \beta$$

If the measure of p is affected by error Δp, the propagated error $\Delta\theta$ in the measure of θ is given by

$$\Delta\theta = \left|\frac{d\theta}{dp}\right| \Delta p = \frac{|s|}{s^2 + (p+a)^2} \Delta p$$

Resolution error

Measurements performed with detector have a limited resolution, because the length of the detector is divided into a certain number of channels. In our case, the resolution error is

$$(\Delta p)_{\text{resolution}} = 50 \mu m$$

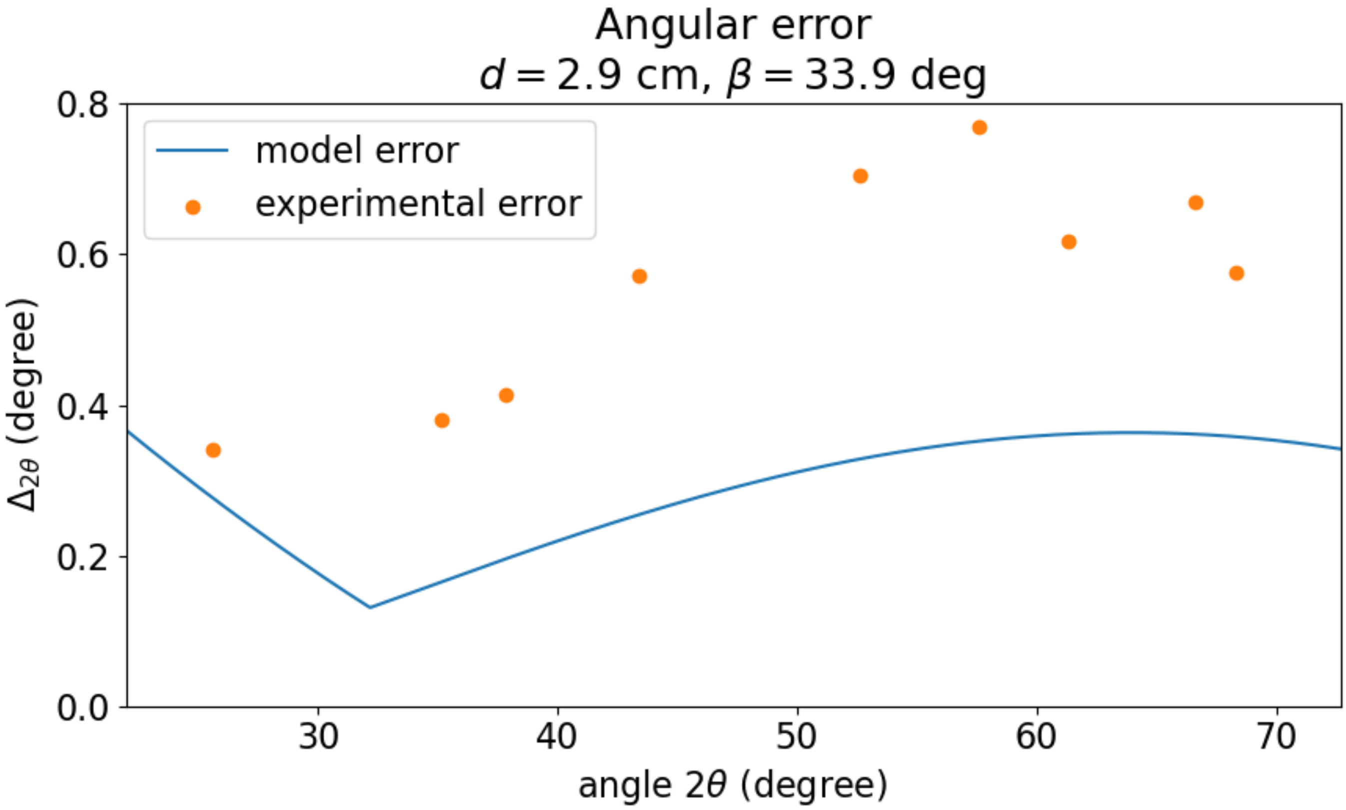
The corresponding resolution error on angle varies along the detector and is given by

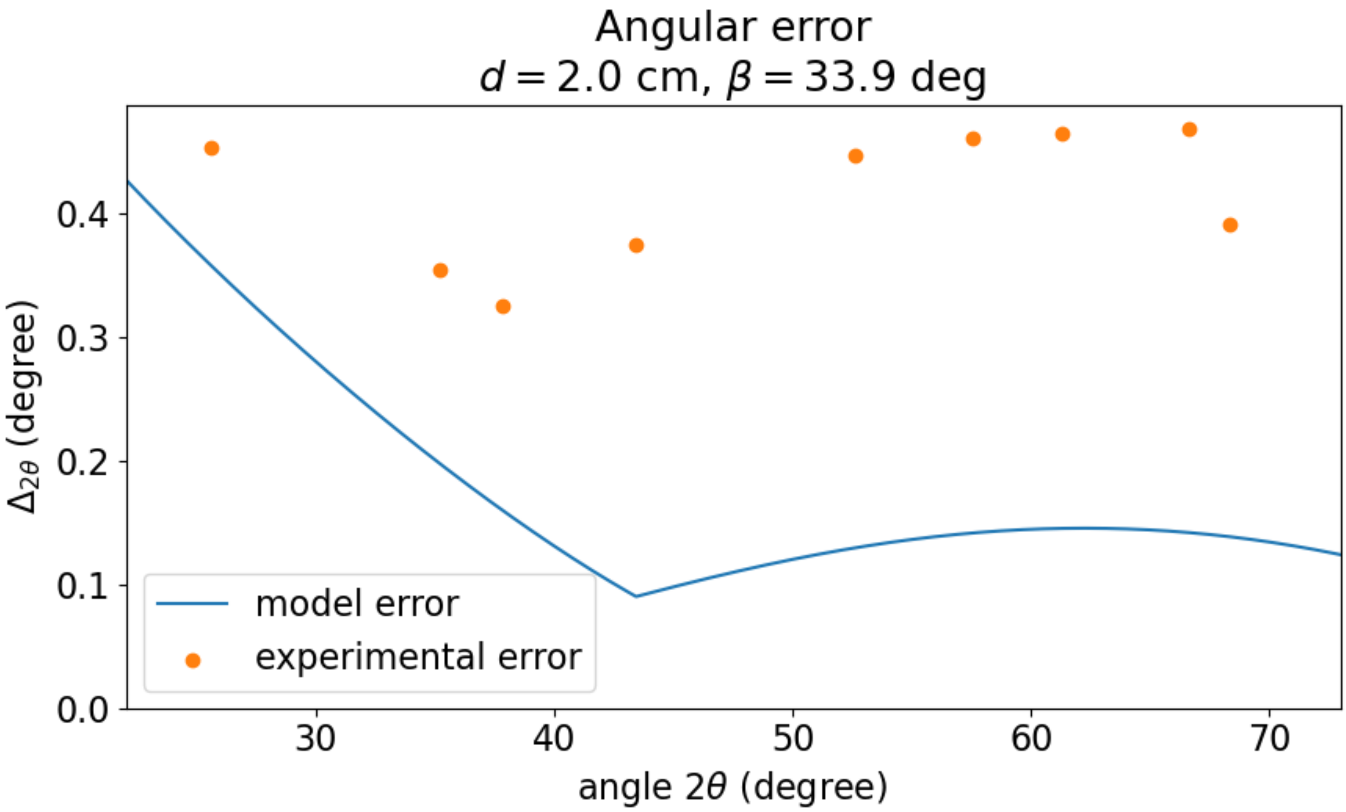
$$(\Delta\theta)_{\text{resolution}} = \frac{|s|}{s^2 + (p+a)^2} (\Delta p)_{\text{resolution}}$$

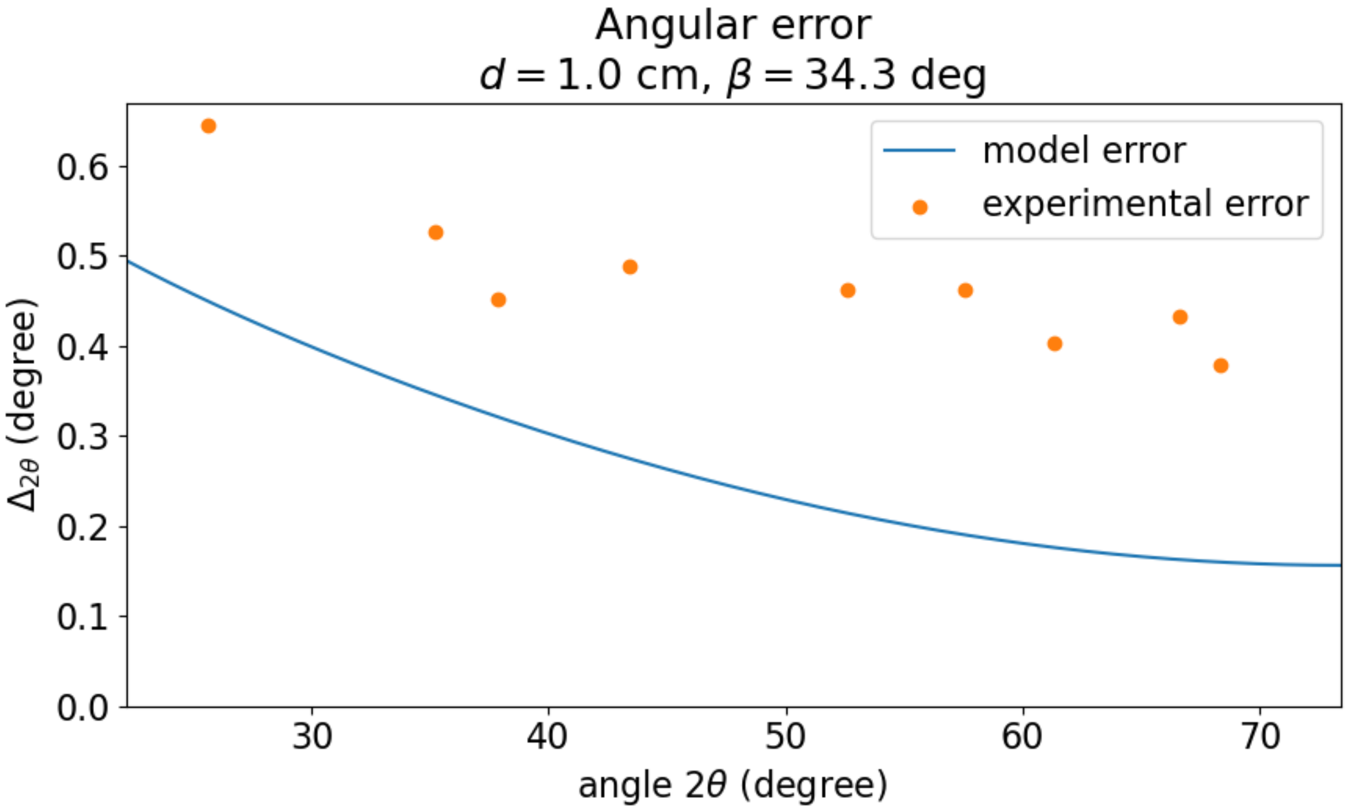
Compare model with experimental data

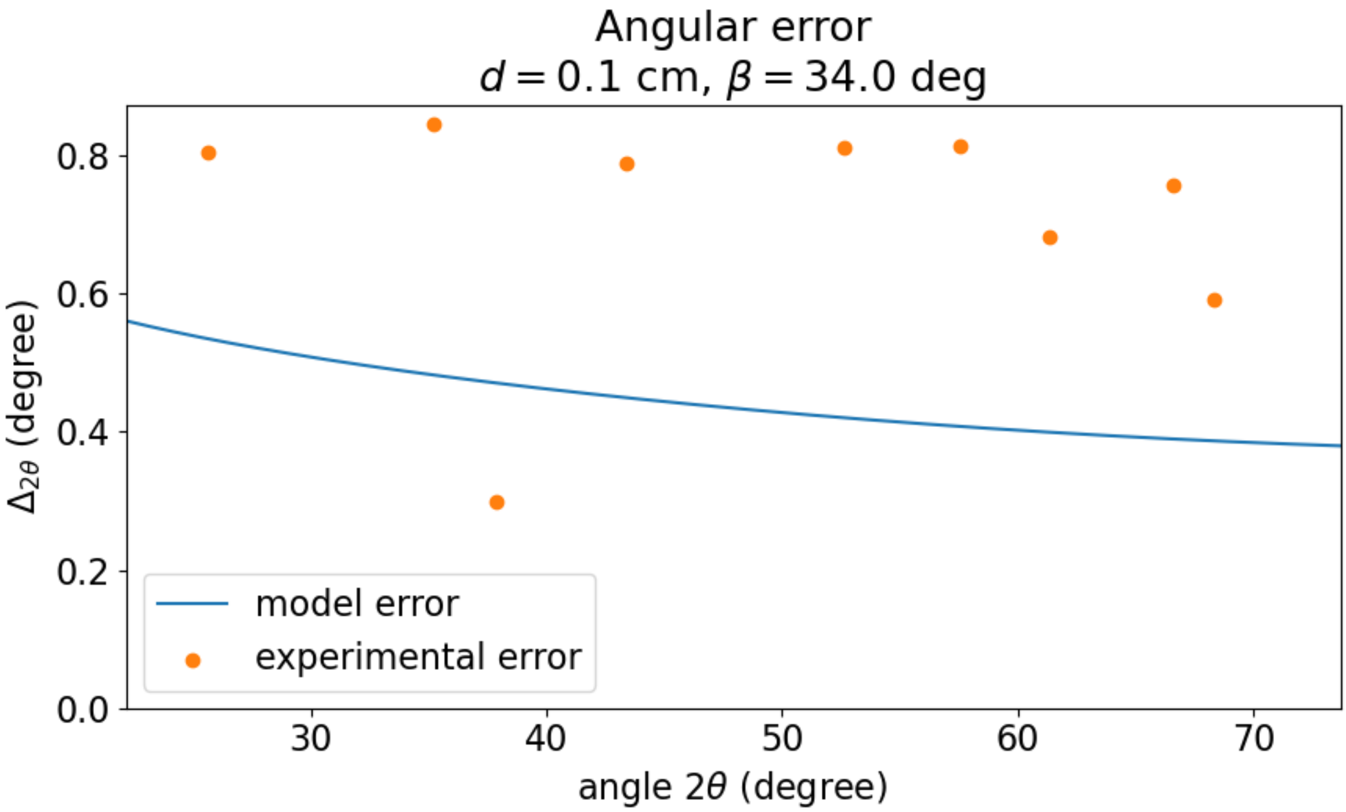
No slit

We have some measures of X-ray diffraction on alumina, performed roughly in the angular range of $22° - 73°$, for d varying between 0.1 cm and 2.9 cm. No slit is put in the path of the incident ray. We detect peaks of alumina at different angles and, through a fit with gaussian curve, we can determine position and standard deviation of each peak. Then, we compare these experimental points with the model that gives the angular error as a function of diffraction angle.


Angular error
$d = 2.9$ cm, $\beta = 33.9$ deg
model error
experimental error
$\Delta_{2\theta}$ (degree)
angle 2θ (degree)
0.0
0.2
0.4
0.6
0.8
30
40
50
60
70

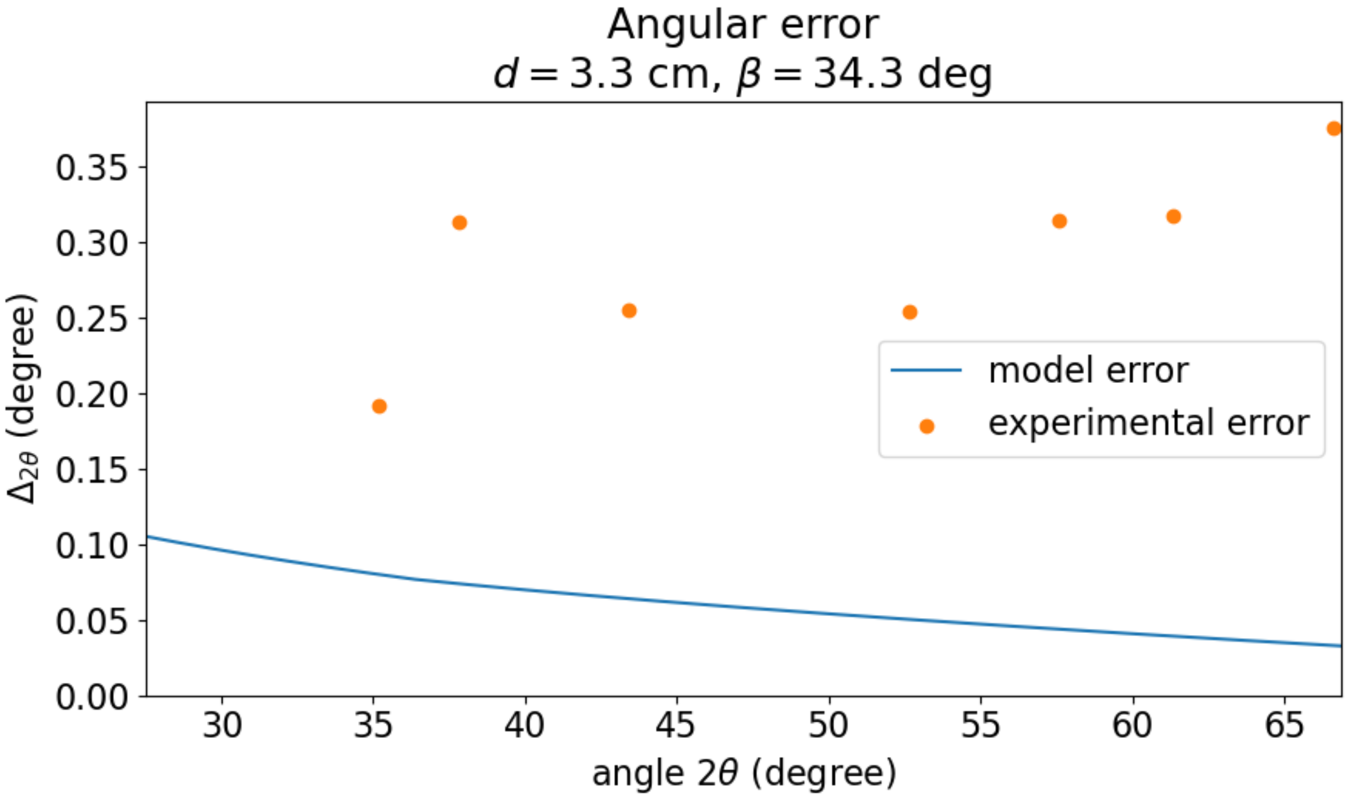

Angular error
$d = 2.0$ cm, $\beta = 33.9$ deg
model error
experimental error
$\Delta_{2\theta}$ (degree)
angle 2θ (degree)
0.0
0.1
0.2
0.3
0.4
30
40
50
60
70

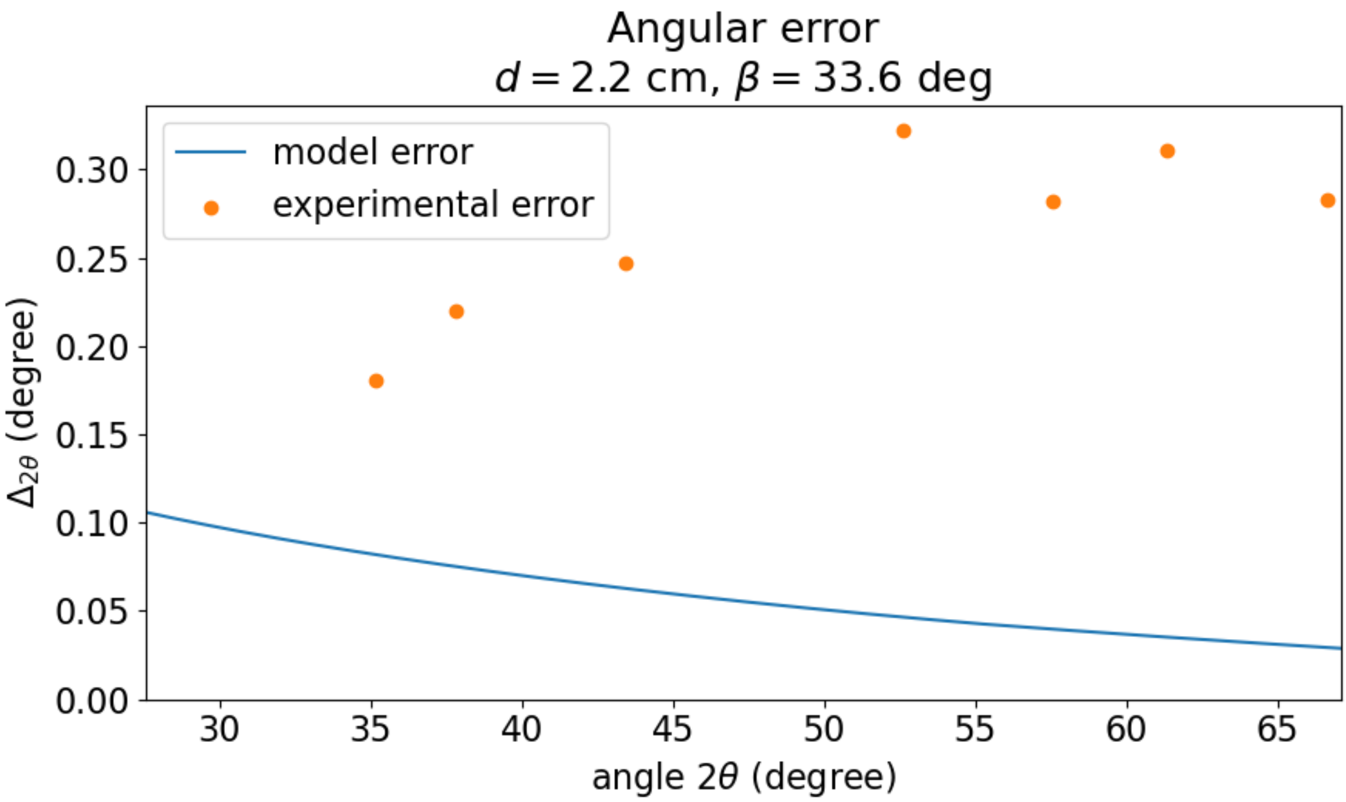


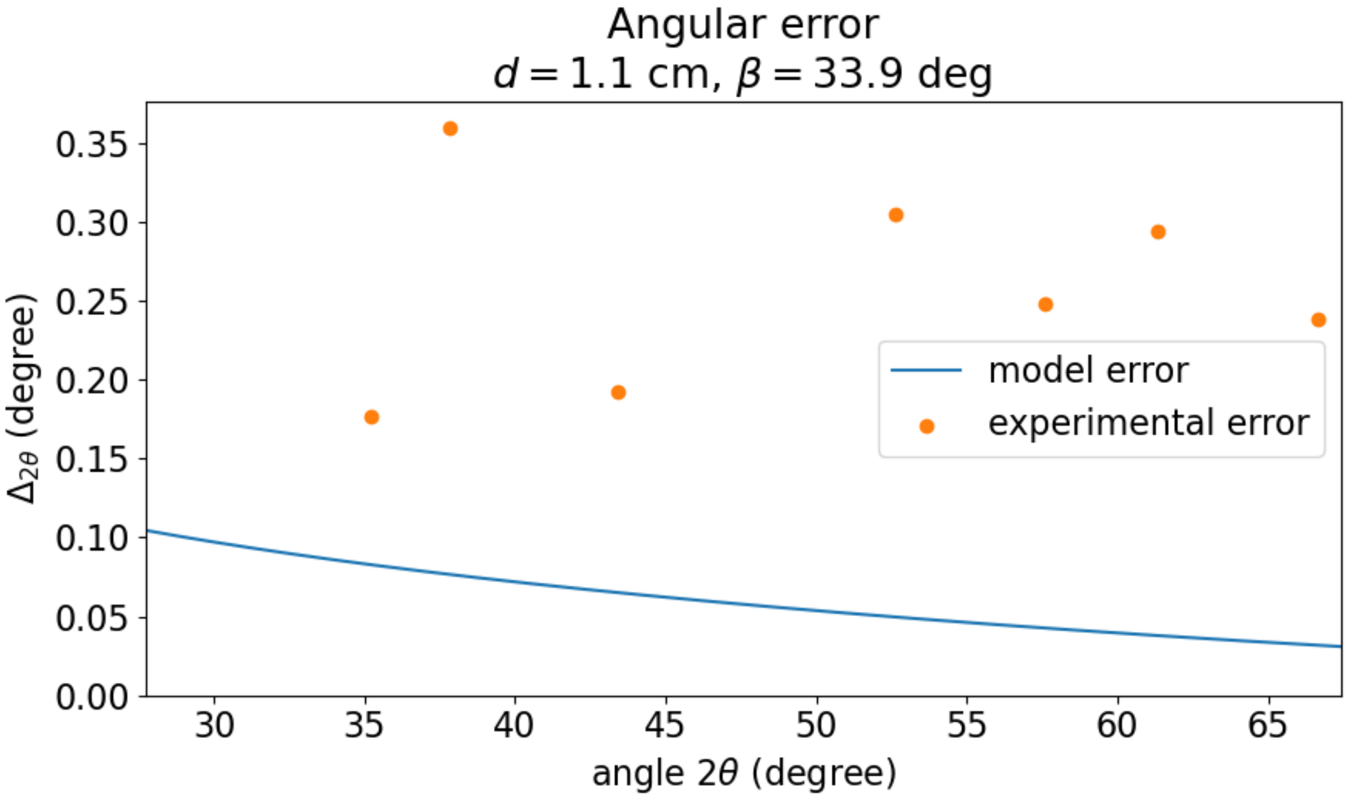


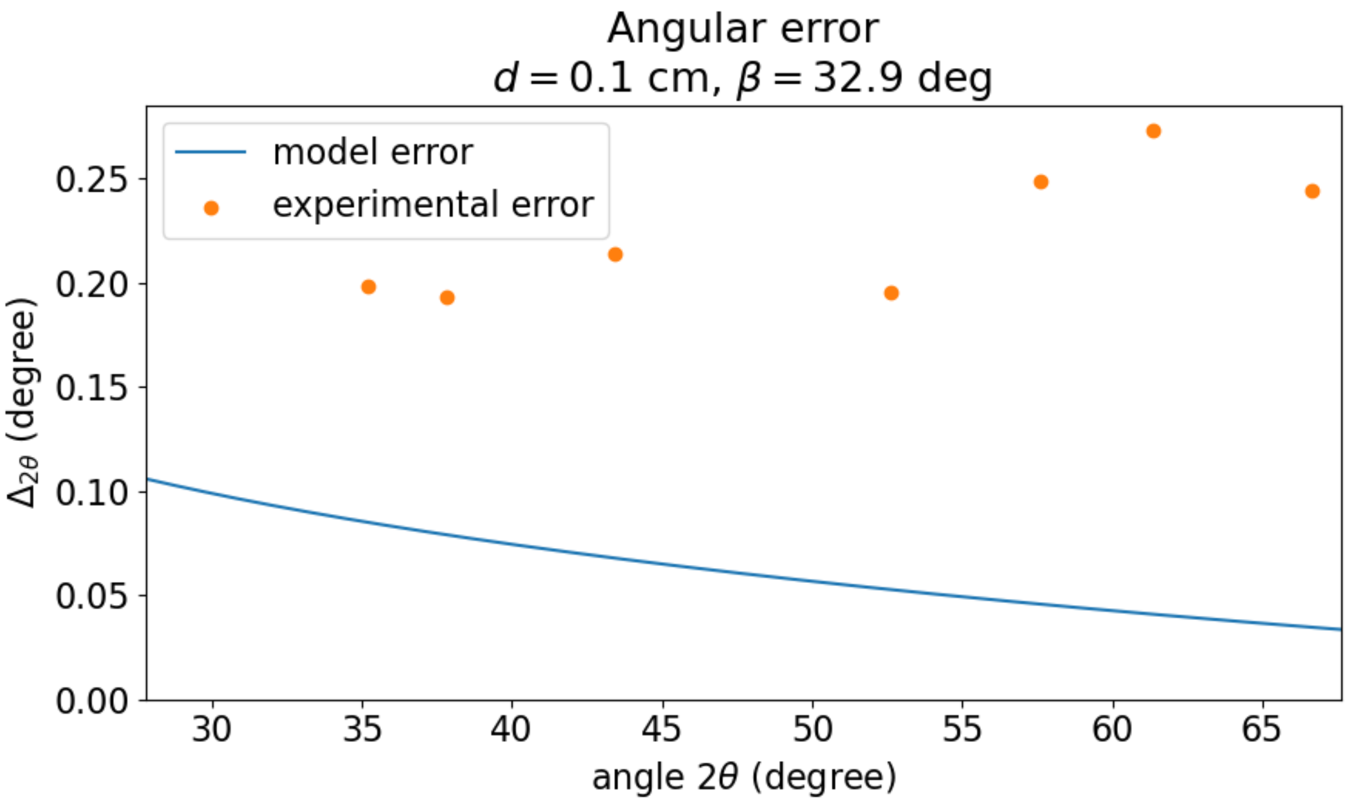
Slit

We perform the same experiment and analysis with a slit of $600\ \mu\mathrm{m}$ in the path of incident ray.


Angular error
$d = 3.3$ cm, $\beta = 34.3$ deg
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$\Delta_{2\theta}$ (degree)
model error
experimental error
30
35
40
45
50
55
60
65
angle 2θ (degree)


Angular error
$d = 2.2$ cm, $\beta = 33.6$ deg
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$\Delta_{2\theta}$ (degree)
model error
experimental error
30
35
40
45
50
55
60
65
angle 2θ (degree)


Angular error
$d = 1.1$ cm, $\beta = 33.9$ deg
$\Delta_{2\theta}$ (degree)
angle 2θ (degree)
model error
experimental error
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
30
35
40
45
50
55
60
65


Angular error
$d = 0.1$ cm, $\beta = 32.9$ deg
$\Delta_{2\theta}$ (degree)
angle 2θ (degree)
model error
experimental error
0.00
0.05
0.10
0.15
0.20
0.25
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