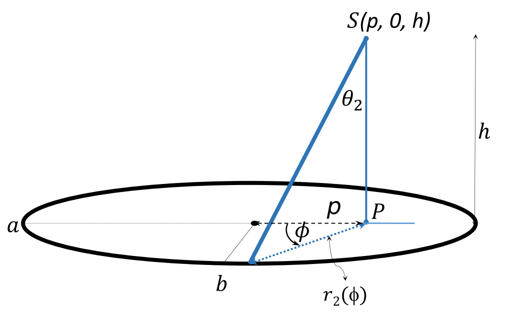
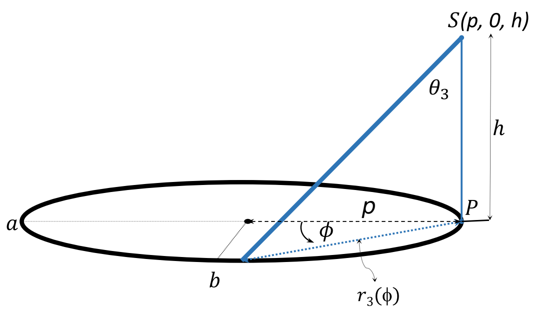
A.4 Prediction of sample–pinhole distance contrast

Abbas *et. al.*[27] demonstrate that analytic formulae for the solid angle subtended by an ellipse from an arbitrary point exist. To predict the detected intensity (for single scattering) as a function of the y position of a flat sample we can use a modification of these formulae, specifically those that consider the point source on the long axis of the ellipse. For a uniformly radiation point source the 'intensity' detected be a detector is proportional to the solid angle subtended by that detector from the point of radiation. A cosine distribution can easily be introduced: $\mathrm{d}\Omega \to \cos\theta\,\mathrm{d}\Omega$. Figure A.10 display the geometric definitions of the variables.

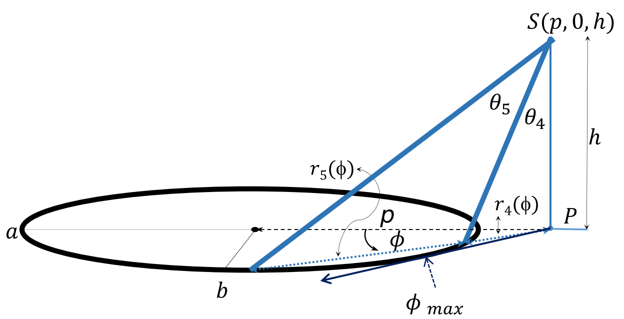
For the three cases that need to be considered there are a different set of formulae: equations A.39–A.41 are for $p < a$ with the point of interest being 'inside' the ellipse, figure A.10a; equations A.42–A.44 are for $p = a$, the point of interest being 'on' the ellipse, , figure A.10b; and equations A.45–A.50 are for $p > a$, the point of interest being outside the ellipse, figure A.10c. The position of the point of interest is specified by $(p, 0, h)$, in Cartesian coordinates, relative to an origin in the centre of the ellipse.



(a) $p < a$



(b) $p = a$



(c) $p > a$

Figure A.10: Definitions of the variables and constants for the three cases. The angles θ_i and the distances r_i are all functions of the azimuthal angle ϕ. The origin is taken to be at the centre of the ellipse with p the distance along the long axis of the ellipse and h the distance from the plane in which the ellipse lies. Figures adapted with permission from Abbas *et. al.*

Adapted from Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 771, M. Abbas *et. al.*, Analytical formulae to calculate the solid angle subtended at an arbitrarily positioned point source by an elliptical radiation detector, p. 2, Copyright (2017), 201, Copyright (2017), with permission from Elsevier.[27]

$$\Omega(p,0,h) = \int_0^{2\pi} \int_0^{\theta_2(\phi)} \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi \tag{A.39}$$

$$\theta_2(\phi) = \arctan\frac{r_2(\phi)}{h} \tag{A.40}$$

$$r_2(\phi) = \frac{-p\,b^2\cos\phi + a\,b\sqrt{b^2\cos^2\phi + (a^2-p^2)\sin^2\phi}}{a^2\sin^2\phi + b^2\cos^2\phi} \tag{A.41}$$

$$\Omega(a,0,h) = 2\int_0^{\frac{\pi}{2}} \int_0^{\theta_3(\phi)} \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi \tag{A.42}$$

$$\theta_3(\phi) = \arctan\frac{r_3(\phi)}{h} \tag{A.43}$$

$$r_3(\phi) = \frac{2\,a\,b^2\cos\phi}{a^2\sin^2\phi + b^2\cos^2\phi} \tag{A.44}$$

$$\Omega(p,0,h) = 2\int_0^{\phi_{\mathrm{nax}}} \int_{\theta_4(\phi)}^{\theta_5(\phi)} \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi \tag{A.45}$$

$$\theta_4(\phi) = \arctan\frac{r_4(\phi)}{h} \tag{A.46}$$

$$\theta_5(\phi) = \arctan\frac{r_4(\phi)+r_5(\phi)}{h} \tag{A.47}$$

$$\phi_{\mathrm{max}} = \arctan\sqrt{\frac{b^2}{p^2-a^2}} \tag{A.48}$$

$$r_4(\phi) = \frac{a^2\,p\sin^2\phi\sec\phi + a\,b\sqrt{b^2\cos^2\phi + (a^2-p^2)\sin^2\phi}}{a^2\sin^2\phi + b^2\cos^2\phi} - p\sec\phi \tag{A.49}$$

$$r_5(\phi) = \frac{2\,a\,b\sqrt{b^2\cos^2\phi + (a^2-p^2)\sin^2\phi}}{a^2\sin^2\phi + b^2\cos^2\phi} \tag{A.50}$$

To correctly calculate the detector intensity we need to modulate the equation for the solid angle by the cosine distribution. Hence the intensities as a function of p, h can be written as

$$I(p,h) = \begin{cases} \displaystyle\int_0^{2\pi} \int_0^{\theta_2(\phi)} \cos\theta\sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi & \text{for } p < a \\ \displaystyle 2\int_0^{\frac{\pi}{2}} \int_0^{\theta_3(\phi)} \cos\theta\sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi & \text{for } p = a \\ \displaystyle 2\int_0^{\phi_{\mathrm{max}}} \int_{\theta_4(\phi)}^{\theta_5(\phi)} \cos\theta\sin\theta \,\mathrm{d}\theta \,\mathrm{d}\phi & \text{for } p > a, \end{cases} \tag{A.51}$$

then performing the θ integral yields

$$I(p,h) = \begin{cases} \displaystyle\frac{\pi}{2} - \frac{1}{4}\int_0^{2\pi} \cos[2\,\theta_2(\phi)]\,\mathrm{d}\phi & \text{for } p < a \\ \displaystyle\frac{\pi}{4} - \frac{1}{2}\int_0^{\frac{\pi}{2}} \cos[2\,\theta_3(\phi)]\,\mathrm{d}\phi & \text{for } p = a \\ \displaystyle\frac{1}{2}\int_0^{\phi_{\mathrm{max}}} \{\cos[2\,\theta_4(\phi)] - \cos[2\,\theta_5(\phi)]\}\,\mathrm{d}\phi & \text{for } p > a, \end{cases} \tag{A.52}$$

and similarly for the solid angle without the cosine distribution

$$\Omega(p,h) = \begin{cases} 2\pi - \int_0^{2\pi} \cos[\theta_2(\phi)]\,\mathrm{d}\phi & \text{for } p < a \\ \pi - 2\int_0^{\frac{\pi}{2}} \cos[\theta_3(\phi)]\,\mathrm{d}\phi & \text{for } p = a \\ 2\int_0^{\phi_{\max}} \{\cos[\theta_4(\phi)] - \cos[\theta_5(\phi)]\}\,\mathrm{d}\phi & \text{for } p > a. \end{cases} \tag{A.53}$$

The integrals in equations A.52–A.53 can be solved numerically. A comparison of the result with and without the inclusion of the distribution allows us to compare the two effects. For the specific geometry of interest there is also a relation between p and h. We make h our independent variable

$$p = X + Y - h, \tag{A.54}$$

where we have defined X to be the distance from the main simulation origin (not the one defined for the above formulae) to the centre of the pinhole and Y to be the distance from the origin to the centre of the detector/ellipse.

Using the values for X, Y, a and b from the geometry of the microscope and a suitable range of h both the solid angle and intensity can be plotted. Figure D.11 shows the results.

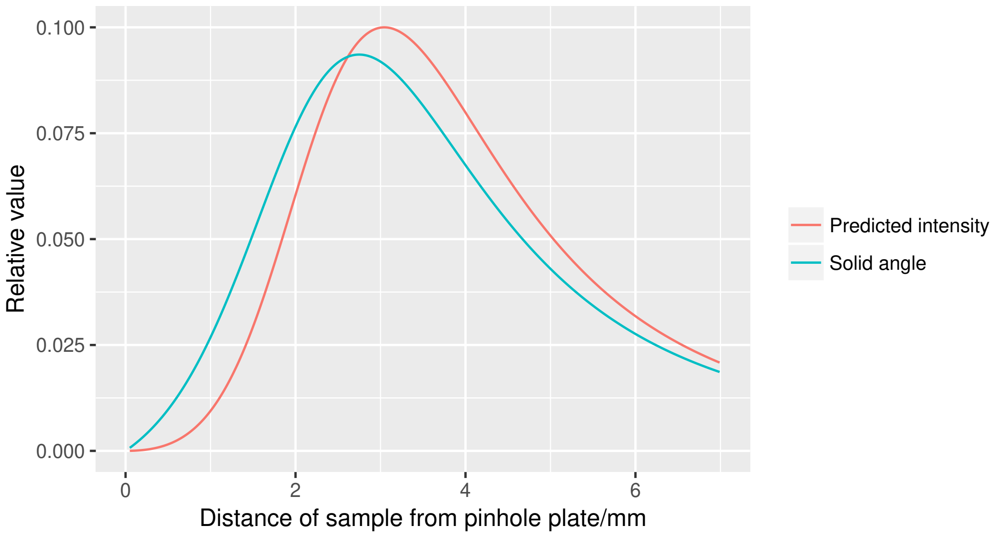


Figure A.11: Results of integration of the analytic formulae for the solid angle (measured in steradians) and the predicted intensity at the detector. The curves are normalised to have the same area beneath them. The difference made by the introduction of the cosine distribution is clear to see. The predicted intensity matches very well with that found from single scattering when the simulation is preformed, as in figure D.11.