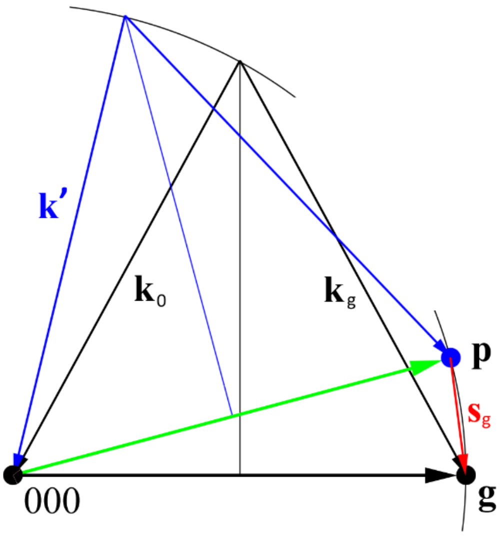
Technical note – calculation of deviation parameter s_g.



The above figure shows the Ewald sphere construction for an incident beam in the Bragg condition $\mathbf{k}_0$ and diffraction vector **g**. For an incident beam in a general orientation **k'**, the deviation parameter $\mathbf{s}_\mathbf{g}$ is given by the vector linking point **p** and **g**. The problem is to find the magnitude of $\mathbf{s}_\mathbf{g}$, given **k'** and **g**. There are three conditions that define point **p**.

1) The length of the vector **p** (green) has magnitude **g**, i.e.

$$p_1^2 + p_2^2 + p_3^2 = g^2 \tag{1}$$

2) The vector **k'** lies in the Bragg condition with relation to **p**, i.e.

$$\mathbf{k}'.\mathbf{p} = k'_1 p_1 + k'_2 p_2 + k'_3 p_3 = -\frac{g}{2} \tag{2}$$

3) The vectors **k'**, **p** and **g** are co-planar, i.e.

$$(\mathbf{k} \times \mathbf{g}).\mathbf{p} = 0 \tag{3}$$

The algebra can be simplified by choosing a reference frame in which the y-components of **k'**, **p** and **g** are zero and **g** lies along the x-axis, i.e. **g** = [g,0,0]. In this reference frame, $\mathbf{k}_0$ can be written as a vector **m** given by

$$\mathbf{m} = \left[\mathbf{k}_0.\hat{\mathbf{g}} \quad \mathbf{0} \quad \left(\boldsymbol{k}^2 - (\mathbf{k}_0.\hat{\mathbf{g}})^2\right)^{\frac{1}{2}}\right] = [m_1 \;\; 0 \;\; m_3] \tag{4}$$

where $\hat{\mathbf{g}}$ is a unit vector parallel to **g** and the vector **k'** can be written as a vector **n** given by

$$\mathbf{n} = \left[\mathbf{k}'.\hat{\mathbf{g}} \quad \mathbf{0} \quad \left(\boldsymbol{k}^2 - (\mathbf{k}'.\hat{\mathbf{g}})^2\right)^{\frac{1}{2}}\right] = [n_1 \;\; 0 \;\; n_3] \tag{5}$$

Thus, equations 1 and 2 become

$$p_1^2 + p_3^2 = g^2 \tag{6}$$

$$\mathbf{n}.\mathbf{p} = n_1 p_1 + n_3 p_3 = -\frac{g}{2} \tag{7}$$

i.e.

$$p_1 = -\frac{g}{2n_1} - \frac{n_3}{n_1} p_3 \tag{8}$$

Substituting into (6) gives

$$\left(\frac{g}{2} + n_3 p_3\right)^2 + n_1^2 p_3^2 = n_1^2 g^2 \tag{9}$$

Expanding

$$\frac{g^2}{4} + g n_3 p_3 + n_3^2 p_3^2 + n_1^2 p_3^2 = n_1^2 g^2 \tag{10}$$

Rearranging

$$p_3^2 (n_3^2 + n_1^2) + g n_3 p_3 + g^2 \left(\frac{1}{4} - n_1^2\right) = 0 \tag{11}$$

And since the vector **n** has magnitude *k* we have

$$k^2 p_3^2 + g n_3 p_3 + g^2 \left(\frac{1}{4} - n_1^2\right) = 0 \tag{12}$$

With the usual quadratic equation solution, i.e.

$$p_3 = \frac{g}{2k^2}\left(n_3 \pm \sqrt{n_3^2 - k^2(1 - 4n_1^2)}\right) \tag{13}$$

Equation (6) can then be used to obtain p_1. Finally, the magnitude of $\mathbf{s_g}$ is

$$s_g = ((g - p_1)^2 + p_3^2)^{1/2} \tag{14}$$

There are two regimes for the calculation plus a singularity.

a) when $\mathbf{k}'.\hat{\mathbf{g}} < 0$ the - solution in (13) is used.

c) when $\mathbf{k}'.\hat{\mathbf{g}} > 0$ the + solution in (13) is used.

When $\mathbf{k}'.\hat{\mathbf{g}} = 0$ equation (13) requires SQRT(ZERO), which can be avoided by using $s_g = g/2k$

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