Structural Chemistry Methods Workshop

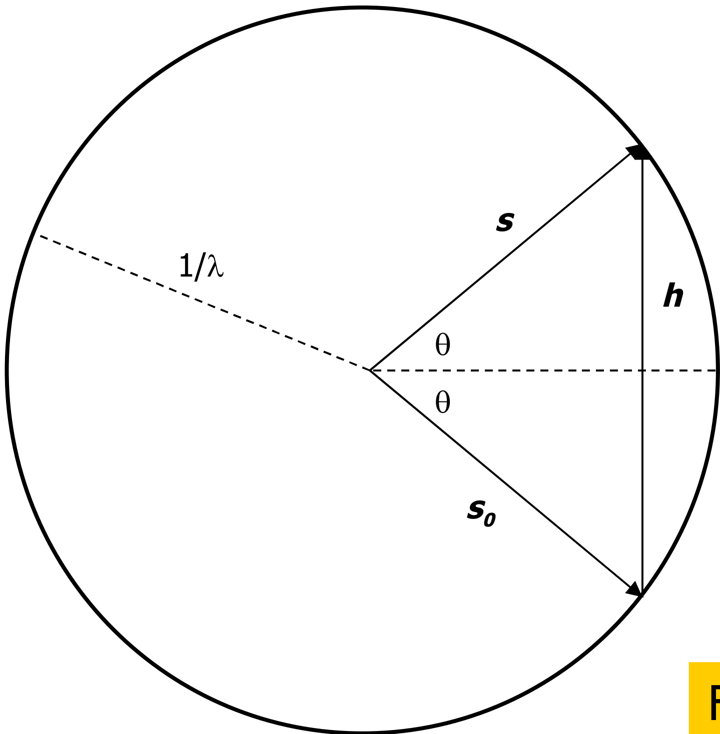
Crystallography V:

Ewald Sphere, Structure Factor Equation

The Ewald Sphere

s_0 vector of incident beam

s vector of diffracted beam



$n\,\lambda = 2\,d\,\sin\theta$

$n/d = |\boldsymbol{h}| = 1/\lambda\ 2\sin\theta$

h is the diffraction vector, with

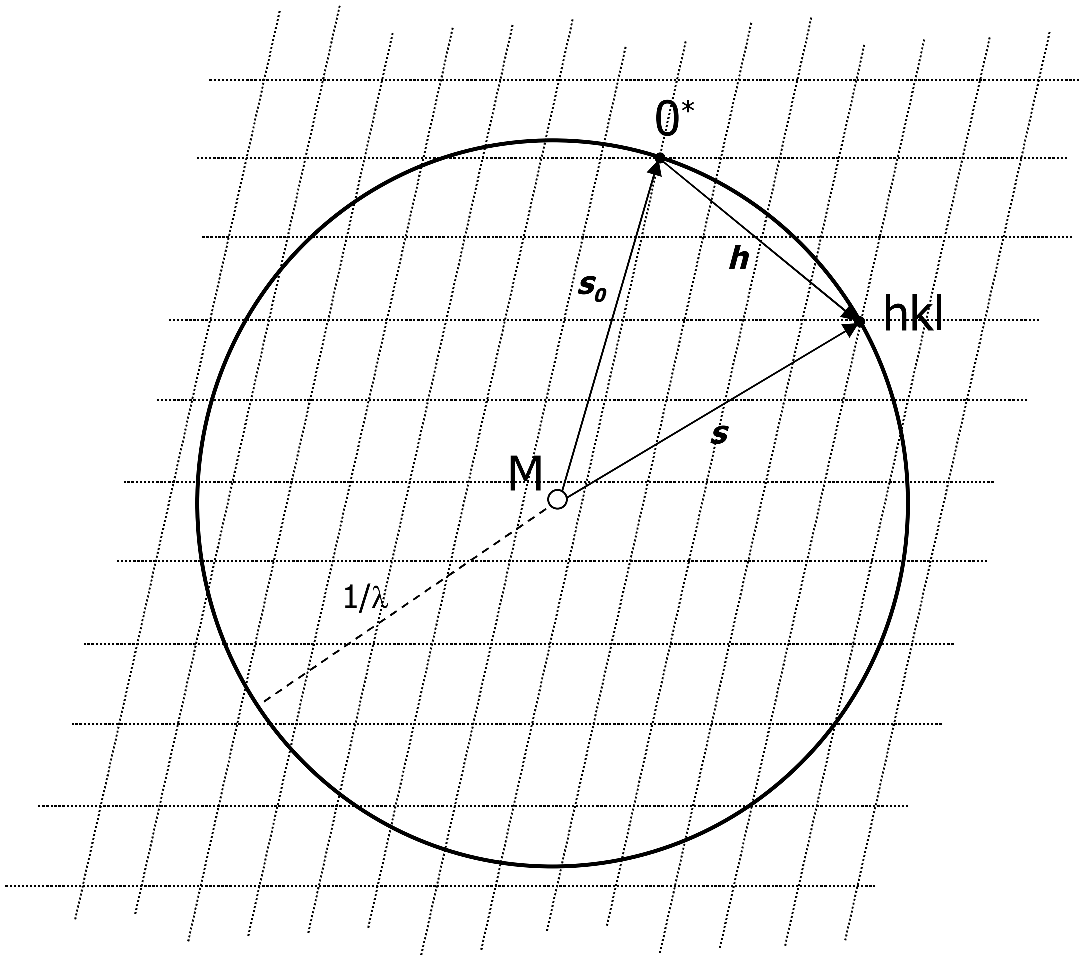
$\boldsymbol{h} = \boldsymbol{s} - \boldsymbol{s}_0$

h is perpendicular to the diffracting set of planes (hkl)

$|\boldsymbol{h}| = 1/d_{hkl}$

For a given incoming beam $\boldsymbol{s}_0$, the endpoints of all vectors ***s*** and ***h*** are on the surface of a sphere. The sphere has the radius $1/\lambda$.

The Ewald Construction

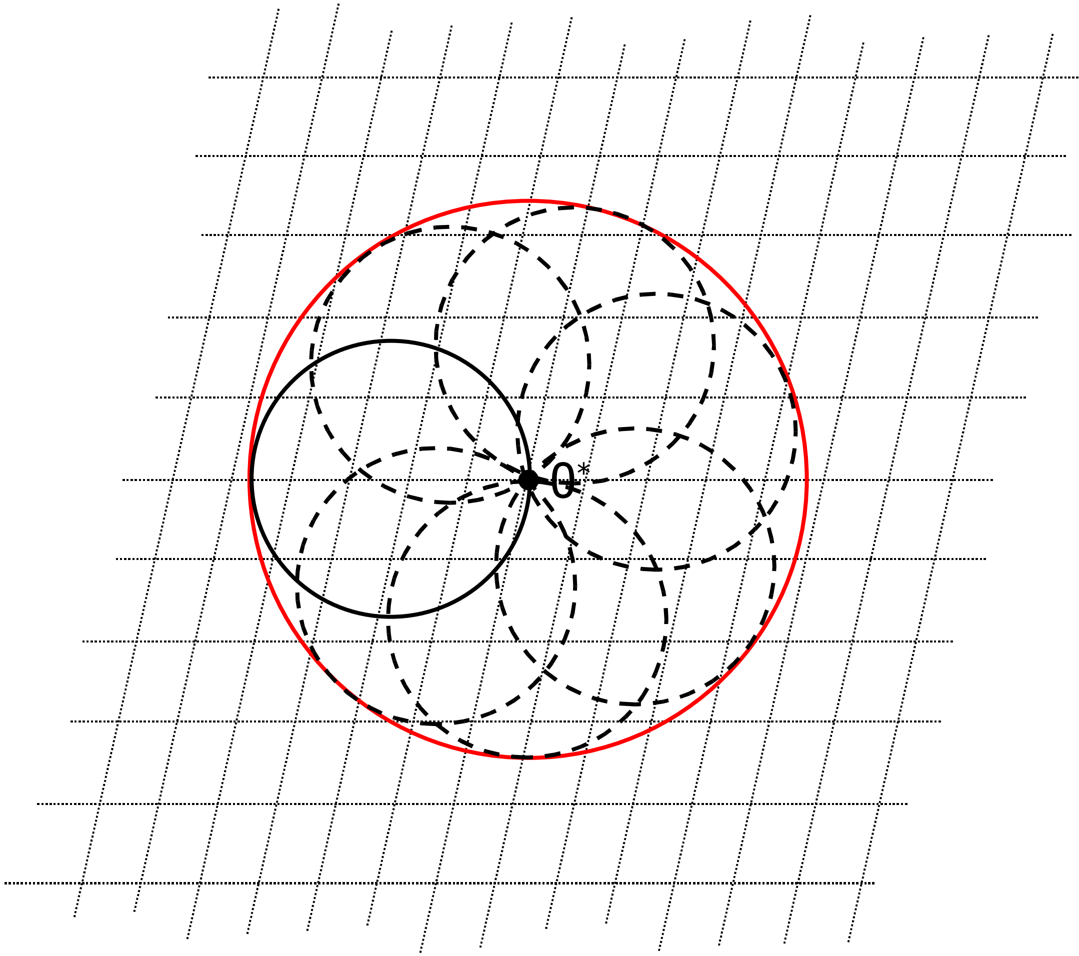


The conditions for Bragg's law are met, when the origin (endpoint of $\boldsymbol{s_0}$) and another point of the reciprocal lattice (endpoint of ***h***) come to lie on the surface of a sphere with radius $1/\lambda$.

Reflection only happens under special conditions. With fixed wavelength λ, the reciprocal lattice (and thus the crystal!) needs to be moved, in order to achieve reflection at different sets of planes (hkl).

Alternatively, if the crystal is invariant, one needs to use X-rays with different wavelengths. In this case, multiple spheres with varying radii describe the situation.

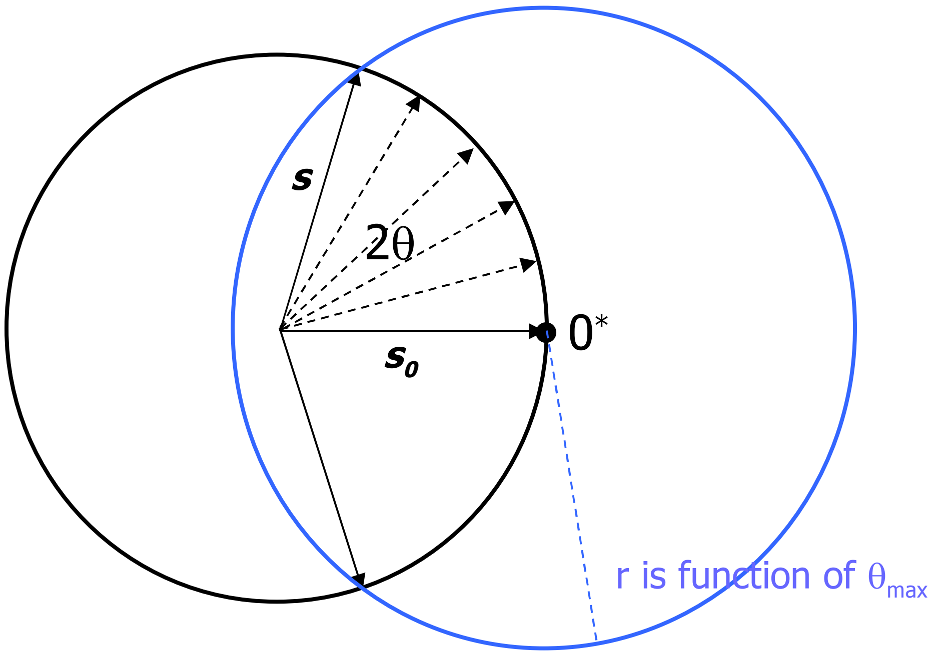
The Ewald Construction



If we rotate the crystal, the Ewald sphere will enclose different portions of space. But the origin is always a point on the surface!

At fixed wavelength, only reflections can be observed that lie within a limiting sphere with radius $2/\lambda$.

The Ewald Construction



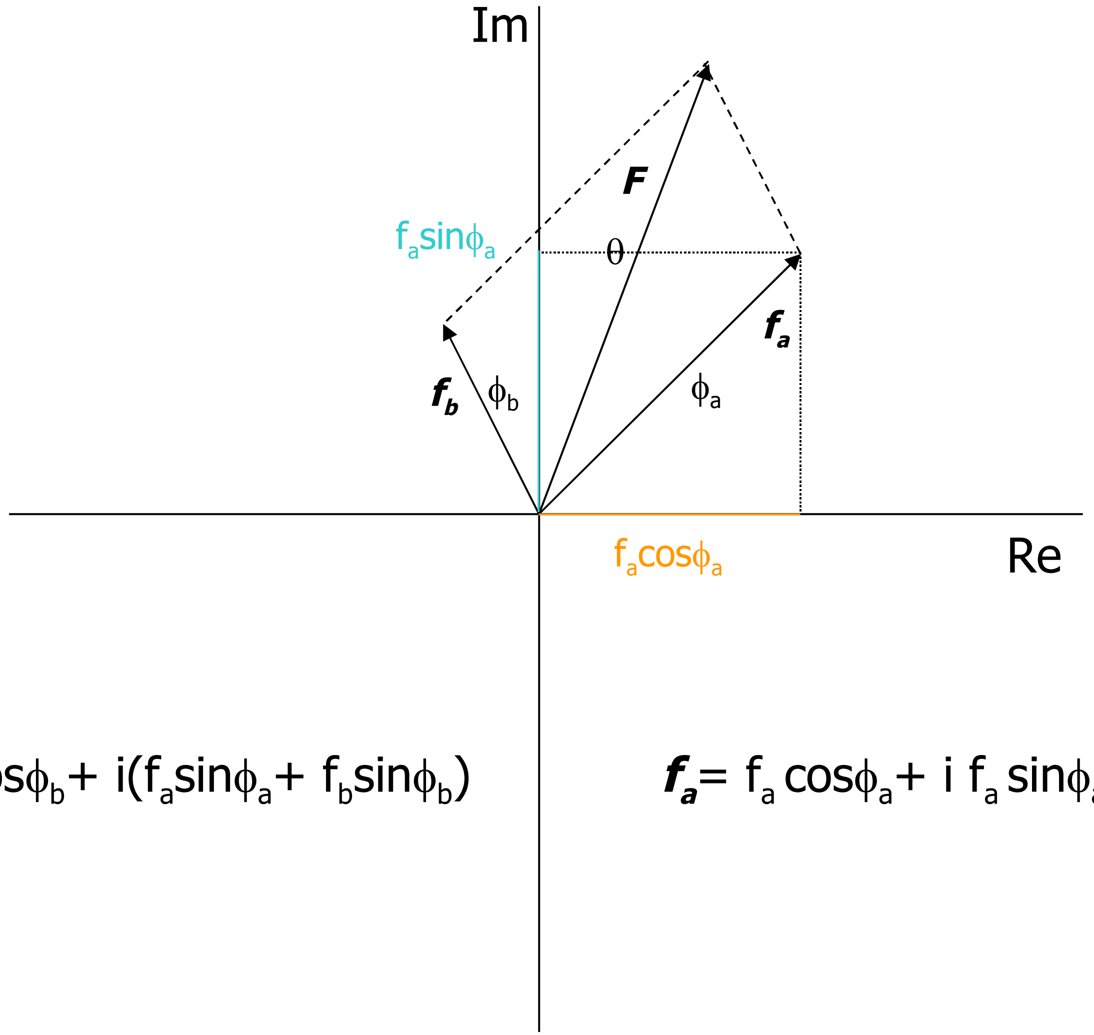
Sphere of reflections with θ_{max}.

$n\lambda = 2d\sin\theta$

θ_{max} corresponds to $d_{min.}$

The sphere describes the highest resolution of the data set.

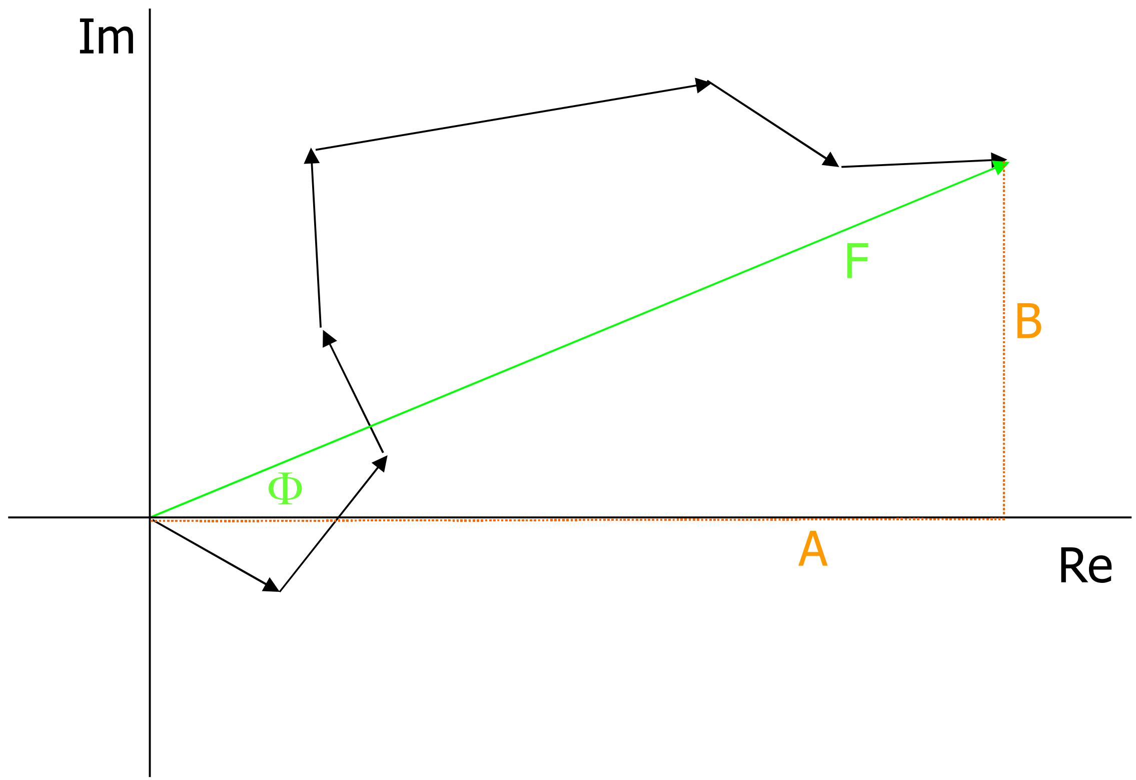
Superposition of two diffracted beams



$$\boldsymbol{F} = f_a\cos\phi_a + f_b\cos\phi_b + i(f_a\sin\phi_a + f_b\sin\phi_b)$$

$$\boldsymbol{f_a} = f_a\cos\phi_a + i\, f_a\sin\phi_a$$

Superposition of diffracted beams



$\boldsymbol{F} = \Sigma f_j \cos\phi_j + i\, \Sigma f_j \sin\phi_j$

$A = \Sigma f_j \cos\phi_j$, $B = \Sigma f_j \sin\phi_j$

$\boldsymbol{F} = \Sigma f_j e^{2\pi i \phi_j}$

$\Phi = \tan^{-1} B/A$

$|\boldsymbol{F}| = F = \mathrm{sqrt}(A^2 + B^2)$

The Structure Factor Equation

The phase difference against the incident X-ray beam is the projection of the vector $\boldsymbol{r}$ describing the position of the localisation of the scatterer onto the diffraction vector $\boldsymbol{h}$.

$\Delta = \boldsymbol{rh}$

$$\phi = 2\pi\, \boldsymbol{rh}$$

$$\phi = 2\pi\, (x\boldsymbol{a}+y\boldsymbol{b}+z\boldsymbol{c})(h\boldsymbol{a}^*+k\boldsymbol{b}^*+l\boldsymbol{c}^*)$$

$$\phi = 2\pi\, (hx+ky+lz)$$

$$\boldsymbol{F}_{hkl} = \Sigma f_j \cos 2\pi\, (hx+ky+lz) + i\, \Sigma f_j \sin 2\pi\, (hx+ky+lz)$$

Structure Factor: F

Atomic Form Factor: f

$$\boldsymbol{F} = F\, (\cos\Phi + i \sin\Phi) = F\, e^{i\Phi}$$

The link between intensity and the structure factor

In X-ray experiments, we cannot measure the structure factors F. The observable is the intensity I.

$$I = \boldsymbol{FF^*} = F * e^{2\pi i\Phi} * F * e^{-2\pi i\Phi} = F^2$$

The structure factor equation provides a link between the atoms and their spatial location (x, y, z) within a unit cell, and the reflections hkl.

Useful references and links

Interactive tutorial on reciprocal space and Ewald sphere:
http://www.doitpoms.ac.uk/tlplib/reciprocal_lattice/index.php

Impressum

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