Bragg's Law

$$n\lambda = 2d_{\text{unit cell}} \sin(\theta)$$

$$\lambda = 2d_{h,k,l} \sin(\theta_{h,k,l})$$

smallest $d_{h,k,l}$ is resolution

$$\frac{1}{d_{h,k,l}} = \frac{2 \sin(\theta_{h,k,l})}{\lambda} \quad \textbf{so} \quad \frac{\sin(\theta_{h,k,l})}{\lambda}$$ **is a measure of resolution**

Scalar value of amplitude equals the square root of the intensity (energy) of the wave.

$$|F_{hk\ell}| = (I_{hk\ell})^{1/2} \qquad I_{hk\ell} = |F_{hk\ell}|^2$$

"Intensity" has been corrected for polariztion and other consequences of data collection method.

A diffracted ray is the sum of contributions from all atoms.

$$\vec{F} = |F_{hk\ell}| \cdot e^{i\phi_{hk\ell}} = \sum_{n}^{N} O_n \cdot f_{n,\theta} \cdot e^{-B_n (\sin\theta / \lambda)^2} \cdot e^{i\,2\pi(\,hx_n + ky_n + \ell z_n\,)}$$

A diffracted ray is the sum of contributions from all electron density.

$$|F_{hk\ell}| \cdot e^{i\phi_{hk\ell}} = \frac{\text{Volume}}{\left(\begin{smallmatrix}\text{of repeat-}\\ \text{ing unit}\end{smallmatrix}\right)} \sum_{x}\sum_{y}\sum_{z} \rho_{xyz} \cdot e^{i\,2\pi(\,hx + ky + \ell z\,)}$$

Electron density is the Fourier transform of all diffracted rays.

$$\rho_{xyz} = (\text{Vol})^{-1} \sum_{h}^{-\infty\rightarrow\infty}\sum_{k}^{\infty}\sum_{\ell}^{\infty} m_{hk\ell} \cdot |F_{hk\ell}| \cdot e^{i\phi_{hk\ell}} \cdot e^{-i\,2\pi(\,hx + ky + \ell z\,)}$$

Patterson map is the Fourier transform of the intensities.

$$P_{xyz} = (\text{Vol})^{-2} \sum_{h}^{-\infty\rightarrow\infty}\sum_{k}^{\infty}\sum_{\ell}^{\infty} |F_{hk\ell}|^2 \cdot e^{-i\,2\pi(\,hx + ky + \ell z\,)}$$

product of all electron densities separated by the x,y,z vector distance
same shape and dimension unit cell

Residuals, R-values, assess agreement between datasets. (here model vs experimental)

$$R_{cryst} = \frac{\sum \big|\, |F_{obs}| - |F_{calc}| \,\big|}{\sum |F_{obs}|}$$

R_{free} calculated from otherwise unused 5%

λ	:	wavelength of radiation
d	:	interplanar spacing, the effective distance associated with a particular diffracted ray
$\theta_{hk\ell}$	:	angle of incident beam to the *h, k, ℓ* Bragg plane
h, k, ℓ	:	integer index numbers of a particular Bragg Plane, a diffracted ray, a "reflection", index of a point of the reciprocal lattice "reciprocal space"
$\|F_{hk\ell}\|$	:	amplitude of the $hk\ell^{th}$ diffracted ray
$\phi_{hk\ell}$	:	the phase of the $hk\ell^{th}$ diffracted ray
B	:	B-factor (historically the Temperature Factor, but dominated by other uncertainties)
$f_{n,\theta_{hk\ell}}$	:	individual atomic scattering factor of the n^{th} atom as a function of $\theta_{hk\ell}$
x_n, y_n, z_n	:	coordinates of the n^{th} atom
$m_{hk\ell}$	:	figure of merit for phase of the $hk\ell^{th}$ diffracted ray
N	:	total number of atoms in the repeating unit of the crystal
O_n	:	occupancy of the n^{th} atom.
Vol	:	volume of the repeating unit, the unit cell
ρ_{xyz}	:	electron density at coordinates x, y, z in the crystal "real space"
P_{xyz}	:	Patterson function value at coordinates x,y,z : vector distances-between atom positions