

The equations: (Good-Parts version: segue into a trick...)

The wave equation depends on a model of the structure (i.e. atomic coordinates) --- but that is the result of the process, the whole problem is that we don't know any of the coordinates in the beginning! We really want to run that equation backwards and calculate the model from the diffracted waves. The trick is to cast the equation into the form of a Fourier Transform equation which can be reformulated backwards.

So, take this equation:

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

$$\vec{F} = |F_{hkl}| \cdot e^{i\phi_{hkl}} = \sum_n O_n \cdot f_{n,\theta_{hkl}} \cdot e^{-B_n (\sin\theta_{hkl}/\lambda)^2} \cdot e^{i 2\pi(hx_n + ky_n + lz_n)}$$

And recast it in terms of continuous density instead of individual atoms:

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

$$|F_{hkl}| \cdot e^{i\phi_{hkl}} = \left(\begin{array}{c} \text{Volume} \\ \text{of} \\ \text{unit cell} \end{array} \right) \sum_x \sum_y \sum_z \rho_{xyz} \cdot e^{i 2\pi(hx + ky + lz)}$$

And now we can work it backwards: the **Trick**

Electron density is the Fourier transform of all diffracted waves.

$$\rho_{xyz} = (\text{Vol})^{-1} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} m_{hkl} \cdot |F_{hkl}| \cdot e^{i\phi_{hkl}} \cdot e^{-i 2\pi(hx + ky + lz)}$$

Amplitude = (Amplitude-factors) • (Phase-factors)
(electron density has no phase) here the x,y,z is the point in the unit cell where we are calculating the density, if we do this for the whole unit cell, then we'll see everything that is possible to see.

So, can we do it? What is known about the factors on the right side of the equation?

m_{hkl} is the figure of merit for phases, we'll get that when we figure out the phases.

$|F_{hkl}|$ is the amplitude of the hkl^{th} diffracted wave, $|F_{hkl}| = (I_{hkl})^{1/2}$ and I_{hkl} is the Intensity of the diffracted wave, which we can measure!

$e^{-i 2\pi(hx + ky + lz)}$ is easy: we know h,k,l for each wave and the x,y,z of the point being calculated.
 $e^{i\phi_{hkl}}$ is the hooker, we do NOT know ϕ_{hkl} the phase for the hkl^{th} diffracted wave.

So now we have to do some work -- find ways to recover the phase of each diffracted wave that was lost when we measured just the intensity.