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2. Scattering wave ampl.

$$A = \int_{\text{blob}} n(\mathbf{r}) \exp(-i\Delta\mathbf{k}.\mathbf{r}) d^3\mathbf{r}$$

The integral can be broken down to a sum of integrals for each atom

$$A = \sum_{\mathbf{r}_a} \int_{(\text{atom a})} n(\mathbf{r}) \exp(-i\Delta\mathbf{k}.(\mathbf{r}+\mathbf{r}_a)) d^3\mathbf{r}$$

$$= \sum_{\mathbf{R}_i} \sum_{\mathbf{r}_j} \int_{(\text{atom j})} n(\mathbf{r}) \exp\left(-i\Delta\mathbf{k}.\left(\mathbf{r}+\mathbf{R}_i+\mathbf{r}_j\right)\right) d^3\mathbf{r}$$

$$= \sum_{\mathbf{R}_i} \exp(-i\Delta\mathbf{k}.\mathbf{R}_i) \sum_{\mathbf{r}_j} \exp\left(-i\Delta\mathbf{k}.\mathbf{r}_j\right) \int_{(\text{atom j})} n(\mathbf{r}) \exp(-i\Delta\mathbf{k}.\mathbf{r}) d^3\mathbf{r}$$

$$= \sum_{\mathbf{R}_i} \exp(-i\Delta\mathbf{k}.\mathbf{R}_i) \sum_{\mathbf{r}_j} f_j \exp\left(-i\Delta\mathbf{k}.\mathbf{r}_j\right)$$

R_j – lattice vector (position of cell i)

$\mathbf{r}_j$ – position of atom j within cell I

$\mathbf{r}$ – position within electron cloud of atom j of cell i

For finite scattered amplitude both factors must be non zero

$$\sum_{\mathbf{R}_i} \exp(i\Delta\mathbf{k}.\mathbf{R}_i) \neq 0 \quad \Rightarrow \quad \Delta\mathbf{k}.\mathbf{R}_i = 2n\pi, \quad \Delta\mathbf{k} = h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^*$$

$$A \propto \sum_{\mathbf{r}_j} f_j \exp\left(i\Delta\mathbf{k}.\mathbf{r}_j\right) \propto \sum_{\mathbf{r}_j} f_j \exp\left(i\left(h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^*\right).\mathbf{r}_j\right)$$