Scattering from a lattice

For simplicity: one type of atom, one atom /unit cell.
"primitive" vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$

Location of any atom in crystal described by linear combination of primitive vectors:

$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

"form factor" of entire crystal:

$$F_{\text{crystal}}(\vec{Q}) = \sum_{\vec{R}} f(\vec{Q}) e^{i\vec{Q} \cdot \vec{R}} \sim 1 \text{ for arbitrary phase factors}$$

$$\frac{d\sigma}{d\Omega} = |F_{\text{crystal}}(\vec{Q})|^2 \sim N \text{ if all contributions add in phase}$$

In-phase addition guaranteed if $\vec{Q} \cdot \vec{R} = 2\pi \times \text{integer}$.

Construct special set of wave vector transfers for which this is the case.

$\vec{K} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$  \hspace{1cm} "reciprocal lattice vectors"

$\vec{a}_1^* = \frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{v} (\vec{a}_2 \times \vec{a}_3) \hspace{1cm} v = \text{volume of unit cell}$

$\vec{a}_2^* = \frac{2\pi}{v} (\vec{a}_1 \times \vec{a}_3)$

$\vec{a}_3^* = \frac{2\pi}{v} (\vec{a}_1 \times \vec{a}_2)$

$\vec{K} \cdot \vec{R} = 2\pi (hn_1 + kn_2 + ln_3) = 2\pi \times \text{integer}$

Condition for in-phase scattering from all atoms in crystal lattice:

$\vec{Q} = \vec{K}$  \hspace{1cm} (Bragg condition)
Example: cubic crystal

\[ \vec{Q} = \vec{k'} - \vec{k} = \frac{4\pi}{\lambda} \sin \Theta \hat{x} = \frac{2\pi}{a} h \hat{x} \]
\[ \Rightarrow 2a \sin \Theta = h \lambda \]

familiar form of Bragg's law

Scattered intensity is distributed in "Bragg peaks" with \( \vec{Q} = \vec{K} \). Background between Bragg peaks due to inelastic scattering, air scattering etc. Very small compared to peak intensity. \( \vec{Q} = \vec{K} \) contains two conditions:

1. \( |\vec{Q}| = |\vec{K}| \)

\[ \vec{Q} \]
\[ \vec{k'} \]
\[ \vec{k} \]
\[ 2\Theta \]

\[ |\vec{k}| = |\vec{k'}| = k \quad \Rightarrow \quad \sin \Theta = \frac{|\vec{K}|}{2k} \]

2. \( \vec{Q} \parallel \vec{K} \)

- For given \( \vec{k}, \vec{k'} \), crystal must have correct orientation.
  - Automatically satisfied for powder (collection of many small crystallites with random orientation).
  - X-ray powder diffraction is the most common method for identifying crystal structures of materials.
- For given orientation, X-rays must have correct wave length to be Bragg-scattered \( \Rightarrow \) can use single crystal as X-ray monochromator.