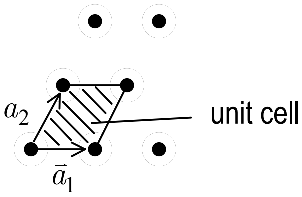
Scattering from a lattice



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:

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

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

in-phase addition guaranteed if $\vec{Q}\cdot\vec{R} = 2\pi \times$ integer .
Construct special set of wave vector transfers for which this is the case.

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

$$\vec{a}_1{*} = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)} = \frac{2\pi}{v}\left(\vec{a}_2 \times \vec{a}_3\right)$$ v = volume of unit cell

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

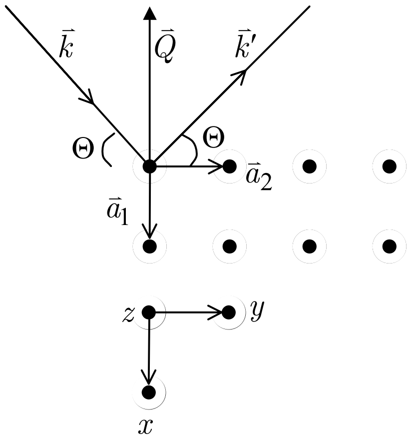
$$\vec{a}_3{*} = \frac{2\pi}{v}\left(\vec{a}_1 \times \vec{a}_2\right)$$

$$\vec{K}\cdot\vec{R} = 2\pi\left(hn_1 + kn_2 + l\,n_3\right) = 2\pi \times \text{ integer}$$

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

$$\boxed{\vec{Q} = \vec{K}}$$ (Bragg condition)

Example: cubic crystal



$$\vec{a}_1 = a\hat{x}$$
$$\vec{a}_2 = a\hat{y}$$
$$\vec{a}_3 = a\hat{z}$$
$$\vec{a}_1{}^* = \frac{2\pi}{a}\frac{\hat{y}\times\hat{z}}{\hat{x}\cdot(\hat{y}\times\hat{z})} = \frac{2\pi}{a}\hat{x}$$

etc.

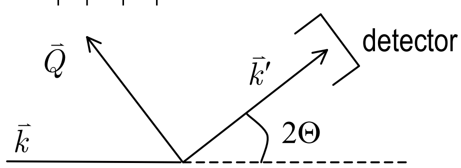
$$\vec{K} = \frac{2\pi}{a}\left(h\hat{x} + k\hat{y} + l\hat{z}\right)$$
$$\vec{Q} = \vec{k}' - \vec{k} = \frac{4\pi}{\lambda}\sin\Theta\,\hat{x} = \frac{2\pi}{a}h\hat{x}$$
$$\Rightarrow 2a\sin\Theta = h\lambda$$

h = integer

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) $|\vec{Q}| = |\vec{K}|$



detector must be set at correct angle 2Θ with respect to incident beam

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

(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.