Bragg's condition, Laue conditions, Brillouin zone

as a result of the interatomic force balance in solids

July 1, 2021

Laue conditions

- The laue condition describes how waves scatter in the lattice:
  $$\Delta\vec{k} = \vec{G}$$
  or
  $$\vec{d} \cdot \Delta\vec{k} = 2\pi m$$
  where $\vec{G}$ is a reciprocal lattice vector and $\vec{d}$ is a lattice vector of the form $\vec{d} = p\vec{a} + q\vec{b} + r\vec{c}$

Laue conditions derivation

- The incoming and the outcoming:

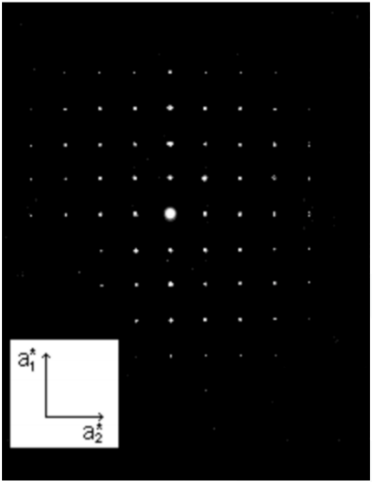
$$f_{\text{in}}(t,\vec{x}) = A_{\text{in}} \cos\left(\omega t - \vec{k}_{\text{in}} \cdot \vec{x}\right)$$
$$f_{\text{out}}(t,\vec{x}) = A_{\text{out}} \cos\left(\omega t - \vec{k}_{\text{out}} \cdot \vec{x}\right)$$

- In order to represent scattered waves, they have to meet at some point in the lattice. This meant that they have to be in sync:
$\Rightarrow \cos\left(\omega t - \vec{k}_{\text{in}} \cdot \vec{x}\right) = \cos\left(\omega t - \vec{k}_{\text{out}} \cdot \vec{x}\right) \iff \Delta\vec{k}\cdot\vec{x} = \left(\vec{k}_{\text{out}} - \vec{k}_{\text{in}}\right)\cdot\vec{x} = 2\pi n$
- if $\Delta\vec{k} = \vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$ the conditions is satisfied by definition.
To understand better the result we need to introduce the reciprocal lattice

Reciprocal lattice

- A periodic function $f(\vec{r})$ on a lattice can be written as a Fourier series
$$f(\vec{r}) = \sum_m f_m e^{i\vec{G}_m \cdot \vec{r}}$$
where $\vec{G}_m$ is such that
$$\vec{G}_m \cdot \vec{R}_n = 2\pi N$$
- The set of vectors $\vec{G}_m$ form the reciprocal space.
- Intuitively speaking in the space we work with spacial coordinates, in the reciprocal space we work with wavevectors.
- The reciprocal space is convenient because we can describes functions by simply referring to wavevectors, that is frequencies or wavelengths.

- The diffraction pattern is not a direct representation of the crystal lattice
- The diffraction pattern is a representation of the reciprocal lattice



Reciprocal lattice

- We can define a base in the reciprocal lattice. For example in 3D the first vector is given by
$$\vec{b}_1 = \frac{2\pi}{V}\vec{a}_2 \times \vec{a}_3$$
so that the first base vector in the reciprocal space is orthogonal to the second and third in the lattice. The same holds for $\vec{b}_2, \vec{b}_3$ by permutation.

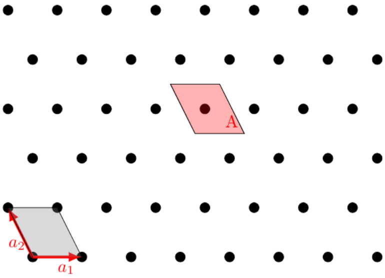


Figure 6: hexagonal lattice

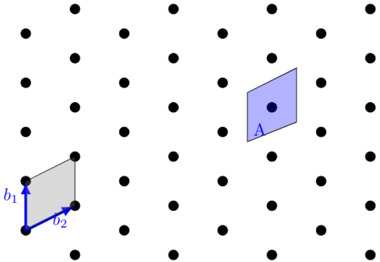


Figure 7: Reciprocal lattice

Figure 1: Lattice and reciprocal lattice basis

Ewald sphere

- Laue conditions implies two facts
  - elastic process $\longrightarrow$ $|\vec{k}_i| = |\vec{k}_2|$
  - $\vec{k}_i - \vec{k}_f$ must be a reciprocal lattice vector
- $\Longrightarrow$ $\vec{k}_i$ and $\vec{k}_f$ must lie on a sphere of the same radius
- The arrows must point on two points of the reciprocal lattice
- The difference of two reciprocal lattice vector is still a reciprocal lattice vector
- $\Longrightarrow$ Laue conditions satisfied

Ewald sphere

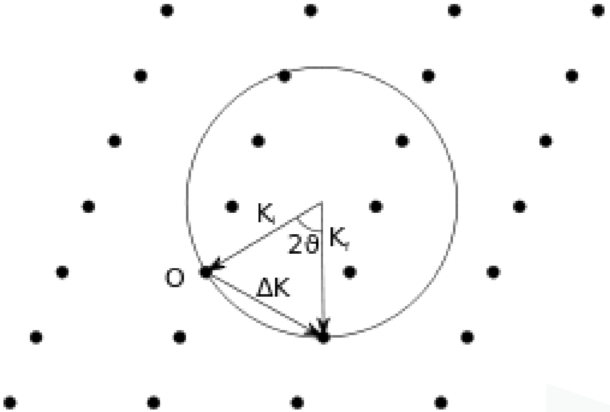


Figure 2: Ewald construction

Bragg's law

- Braggs's law is a particular case of the Laue conditions

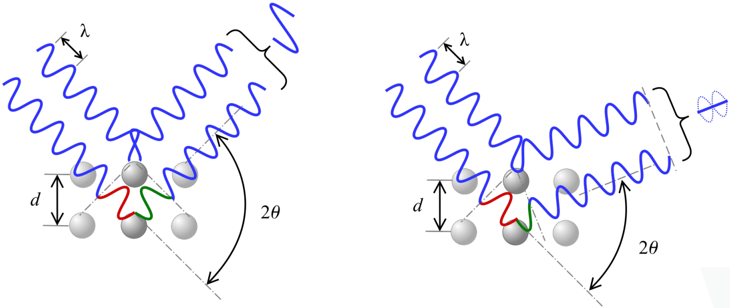


Figure 3: Bragg's law

- Bragg's law gives the the relation between the wavelength and the angle of the incoming radiation and the interatomic distance in a crystal in order to have constructive interference.

$$n\lambda = 2d \sin\theta$$

Bragg's construction (heuristical derivation)

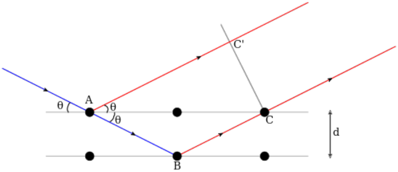


Figure 4: Geometrical derivation of the Bragg's law

$$\text{Path difference} \qquad (AB + BC) - (AC')$$
$$\text{Condition} \qquad n\lambda = (AB + BC) - (AC')$$
$$AB = BC = \frac{d}{\sin\theta} \text{ and } AC = \frac{2d}{\tan\theta}$$
$$AC' = AC \cdot \cos\theta = \frac{2d}{\tan\theta}\cos\theta = \left(\frac{2d}{\sin\theta}\cos\theta\right)\cos\theta = \frac{2d}{\sin\theta}\cos^2\theta$$
$$n\lambda = \frac{2d}{\sin\theta} - \frac{2d}{\sin\theta}\cos^2\theta = \frac{2d}{\sin\theta}\left(1 - \cos^2\theta\right) = \frac{2d}{\sin\theta}\sin^2\theta = 2d\sin\theta$$

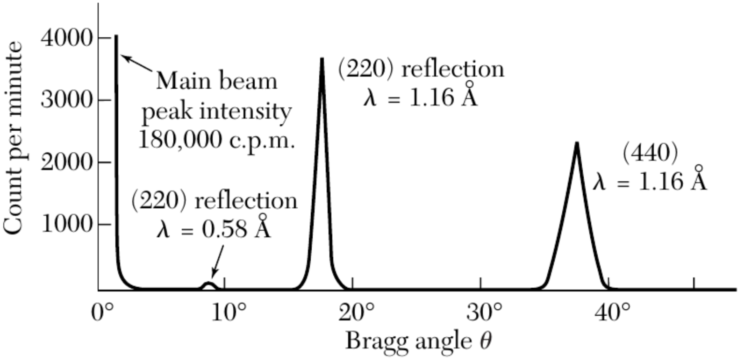


Figure 5: Bragg's condition

Bragg's planes

- Bragg's law can be rewritten as
$$\mathrm{k} \cdot \left(\frac{1}{2}\mathrm{G}\right) = \left(\frac{1}{2}G\right)^2$$
- This means that constructive interference occurs for those vectors whose projection along $\frac{1}{2}\mathrm{G}$ is equal to $\left(\frac{1}{2}G\right)^2$. This equation identifies a plane, the Bragg's plane.
  The intersection of the Bragg's planes form the edge of the Brillouin zone.

Brilluoin zone