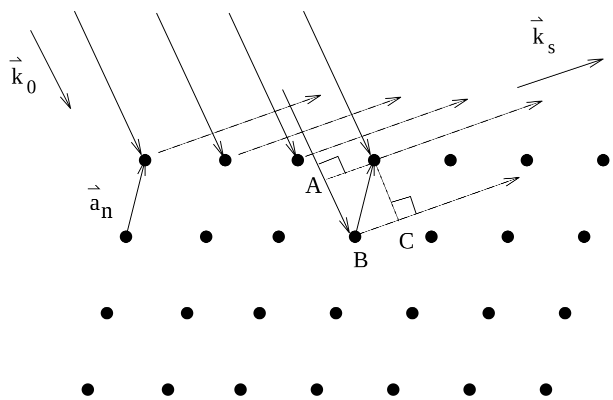
Physics 0551 Lecture #5

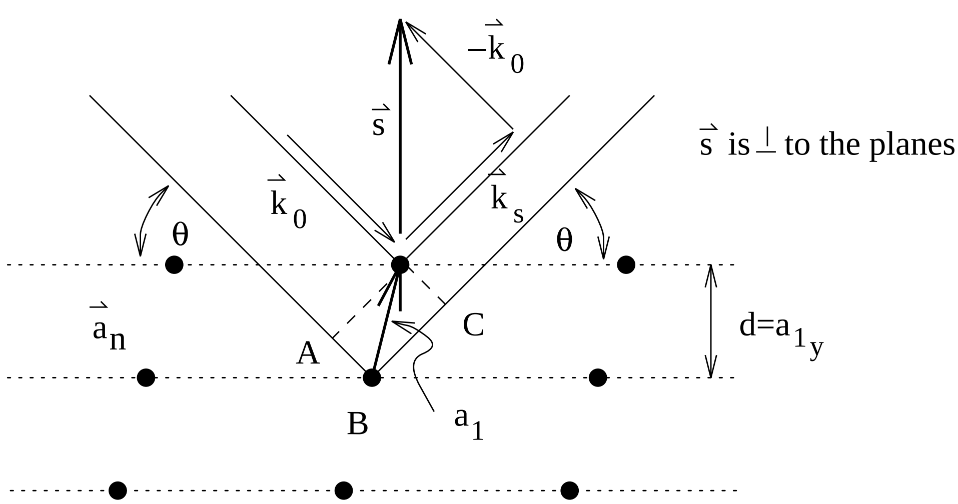
Title: "Intuitive" construction of the *reciprocal lattice*

Equivalence of Bragg's Law and Laue condition: Assume waves are incident on a lattice as shown



$| \overline{AB} | = -\vec{a}_n \cdot \hat{k}_0$
$| \overline{BC} | = +\vec{a}_n \cdot \hat{k}_s$

Constructive interference (Bragg condition)
when $|AB| + |BC|$=nλ $|k| = \frac{2\pi}{\lambda}$ = momentum of wave
$\vec{a}_n \cdot (\hat{k}_s - \hat{k}_0)$ = nλ = n$\frac{2\pi}{|k|}$
$\vec{a}_n \cdot (\vec{k}_s - \vec{k}_0) = 2\pi$n
$\boxed{\vec{a}_n \cdot \vec{s} = 2\pi\text{n}}$
Choose a symmetrical configuration so that $\vec{s}$ is $\perp$ to the planes or $\vec{s} \parallel$ to perpendicular. Example: (specular reflection for constructive interference of atoms within a plane.)



$|AB| = -\vec{a}_1 \cdot \hat{k}_0 \qquad \hat{k}_0 = \cos\theta\ \hat{x}$ - $\sin\theta\ \hat{y}$

$|BC| = +\vec{a}_1 \cdot \hat{k}_s \qquad \hat{k}_s = \cos\theta\ \hat{x} + \sin\theta\ \hat{y}$

$|AB| + |BC| = \mathrm{n}\lambda$

$|AB| = -\cos\theta a_{1_x} + \sin\theta a_{1_y}$

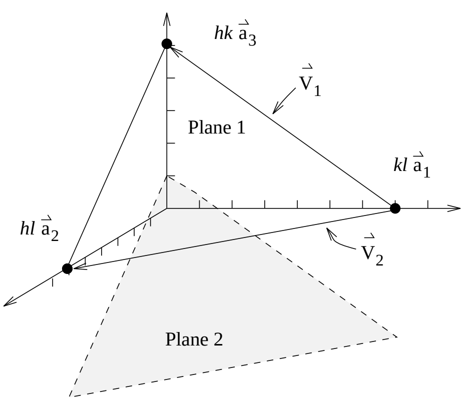
$|BC| = +\cos\theta a_{1_x} + \sin\theta a_{1_y}$

$|AB| + |BC| = 2\ \sin\theta\ \mathrm{a}_{1y} = \mathrm{n}\lambda$

$$\boxed{2\sin\theta\ \mathrm{d} = \mathrm{n}\lambda \qquad \text{Bragg's Law}}$$

Constructive interference occurs when above condition is satisfied. Now to show that the reciprocal lattice is the "natural" representation from the crystal planes! This lattice identifies all constructive interference conditions of the real-space lattice.

Note that the spacing of atoms within a particular plane is of no consequence, only the distance d and that $\vec{s}$ is perpendicular to the planes!



Assume $(hk\ell)$ is the set of planes we are interested in studying $hk\ell\left[\frac{1}{h}\vec{a}_1, \frac{1}{k}\vec{a}_2, \frac{1}{\ell}\vec{a}_3\right]$ or $[k\ell\vec{a}_1, h\ell\vec{a}_2, hk\vec{a}_3]$ are the Bravais lattice points.

These two planes which define our plane are parallel, but the dotted plane is the closest plane to the origin (by construction)! The planes passing through [0,1,0] and [1,0,0] are not (by construction)!

So $\vec{P}$ is perpendicular to plane 1

$\vec{P}$ is also $\perp$ to plane 2

and $\vec{a}_3 \cdot \hat{P}$ = distance between nearest planes. (Another plane intercepts the origin).

$$\hat{P} = \vec{P}/|\vec{P}|$$

The Laue conditions for coherent scattering

$\vec{G} \cdot \vec{a}_1 = 2\pi \mathrm{n}_1 \quad \mathrm{n}_1,\mathrm{n}_2,\mathrm{n}_3$ are integers

$\vec{G} \cdot \vec{a}_2 = 2\pi \mathrm{n}_2 \quad \vec{G}$ is the diffraction vector

$\vec{G} \cdot \vec{a}_3 = 2\pi \mathrm{n}_3$

Bragg condition $\mathrm{n}\lambda = 2\mathrm{d}\sin\theta$ states that $\vec{G}$ must be $\perp$ to the planes hence $\vec{G}||\vec{P}$!

$k\ell\vec{a}_1 + \vec{V}_1 = h\ell\vec{a}_2$ and $k\ell\vec{a}_1 + \vec{V}_2 = hk\vec{a}_3$

where $\vec{V}_1$ and $\vec{V}_2$ are vectors in plane 1.

Thus $\vec{V}_1 \times \vec{V}_2$ is a vector $\perp$ to the planes of interest!

$\vec{V}_1 = h\ell k\ (\frac{1}{k}\vec{a}_2 - \frac{1}{h}\vec{a}_1)$ $\qquad\qquad$ $\vec{V}_2 = h\ell k\ (\frac{1}{\ell}\vec{a}_3 - \frac{1}{k}\vec{a}_1)$

So

$$\vec{P} = \vec{V}_1 \times \vec{V}_2 = h^2k^2\ell^2\ (\tfrac{1}{k}\vec{a}_2 - \tfrac{1}{h}\vec{a}_1)\ \times(\tfrac{1}{\ell}\vec{a}_3 - \tfrac{1}{h}\vec{a}_1)$$

$$\boxed{\vec{P} = h^2k^2\ell^2[\tfrac{1}{h\ell}(\vec{a}_3 \times \vec{a}_1) + \tfrac{1}{k\ell}(\vec{a}_2 \times \vec{a}_3) + \tfrac{1}{hk}(\vec{a}_1 \times \vec{a}_2)]}$$

Now $\hat{P} = \vec{P}/|\vec{P}|$

and $\vec{G} = |\vec{G}|\hat{G} = |\vec{G}|\hat{P}$

and $\vec{G} \cdot \vec{a}_3 = 2\pi \mathrm{n}_3$

$|\vec{G}|\hat{G} \cdot \vec{a}_3 = 2\pi \mathrm{n}_3$

$$|\vec{G}| = \frac{2\pi n_3}{\hat{G}\cdot\vec{a}_3}$$

$$\vec{G} = \frac{2\pi n_3}{\hat{G}\cdot\vec{a}_3}\hat{P}$$

$$\vec{G} = \frac{2\pi n_3}{\hat{G}\cdot\vec{a}_3}\ \frac{\vec{P}}{|\vec{P}|} \qquad (\hat{G} = \hat{P})$$

$$\boxed{\vec{G} = \frac{2\pi n_3}{\vec{P}\cdot\vec{a}_3}\frac{\vec{P}}{|P|} = \frac{2\pi n_3}{\vec{P}\cdot\vec{a}_3}\quad \vec{P}}$$

$$\vec{P} \cdot \vec{a}_3 = h^2k^2\ell^2[\tfrac{1}{h\ell}\ (\mathrm{a}_3 \times a_1) + \tfrac{1}{k\ell}\ \ (\vec{a}_2 \times \vec{a}_3) + \tfrac{1}{hk}(\vec{a}_1 \times \vec{a}_2)]\ \cdot\vec{a}_3$$

$$= \mathrm{h}^2k^2\ell^2\tfrac{1}{hk}(\vec{a}_1 \times \vec{a}_2)\ \cdot\vec{a}_3 \qquad (\text{Note: } \vec{a}\cdot(\vec{b}\times\vec{c}) = (\vec{a}\times\vec{b})\cdot c)$$

$$\boxed{\vec{G} = \frac{2\pi n_3 hk}{\vec{a}_1\cdot(\vec{a}_2\cdot\times\vec{a}_3)}[\tfrac{1}{h\ell}\ (\vec{a}_3 \times \vec{a}_1) + \tfrac{1}{k\ell}(\vec{a}_2 \times \vec{a}_3) + \tfrac{1}{hk}(\vec{a}_1 \times \vec{a}_2)]}$$

If $\mathrm{n}_3 = \ell$ then

$$\boxed{\vec{G} = \frac{2\pi}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}[k(\vec{a}_3 \times \vec{a}_1) + h(\vec{a}_2 \times \vec{a}_3) + \ell(\vec{a}_1 \times \vec{a}_2)]}$$

where $\vec{G} = \mathrm{h}\vec{a}_1^* + \mathrm{k}\vec{a}_2^* + \ell\vec{a}_3^*$ $\qquad$!

$\mathrm{a}_1^* = \frac{2\pi}{V_c}(\vec{a}_2 \times \vec{a}_3)$ $\qquad$ $\mathrm{V}_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

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

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

Properties of the reciprocal lattice

$\vec{a}_1{}^* \cdot \vec{a}_1 = \vec{a}_2{}^* \cdot \vec{a}_2 = \vec{a}_3{}^* \cdot \vec{a}_3 = 2\pi$

$\vec{a}_k \cdot \vec{a}_\ell^* = 0$ if $k \neq \ell$

$\vec{G}_{hk\ell} = ha_1^* + ka_2^* + \ell a_3^*$

$\vec{G}_{hk\ell} \perp (hk\ell)$ planes

$\frac{\lambda|\vec{G}_{hk\ell}|}{4\pi} = \sin\theta$