The <u>Reciprocal Lattice</u> of a Bravais lattice.

The set of wave vectors $\{\vec{K}\}$ that specify the periodicity of a Bravais lattice of sites $\{\vec{R}\}$.

Will be usefull in discussing X-ray scattering off ions and electron eigenstates in ionic potential.

Suppose we have a function $U(\vec{r})$ that is periodic on the Bravais lattice, ie we have

$$U(\vec{r}+\vec{R}) = U(\vec{r})$$

for all $\vec{R}$ in the Bravais lattice. You may think of the ionic potential the electron sees as a physical example. Taking the Fourier transform

$$U(\vec{r}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, U(\vec{k})$$

the above condition becomes

$$U(\vec{r}+\vec{R}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot(\vec{r}+\vec{R})}\, U(\vec{k})$$

$$= \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, U(\vec{k}) = U(\vec{r})$$

If this is to be true, then the only values of $\vec{k}$ for which $U(\vec{k}) \neq 0$ must be the set of $\{\vec{K}\}$ such that $e^{i\vec{K}\cdot\vec{R}} = 1$ for all

$\vec{R}$ in the Bravais lattice. This defines the ~~recipro~~ reciprocal lattice $\{\vec{K}\}$.

Alternatively, the set of wave vectors $\{\vec{K}\}$ that yield plane waves with the periodicity of the Bravais lattice is called the reciprocal lattice

$$e^{i\vec{K}\cdot(\vec{r}+\vec{R})} = e^{i\vec{K}\cdot\vec{r}} \quad \text{for all } \vec{R} \text{ in B.L.}$$

plane wave is invariant under translation by $\{\vec{R}\}$.

$$\Rightarrow \boxed{e^{i\vec{K}\cdot\vec{R}} = 1 \quad \text{for all } \{\vec{R}\} \text{ in B.L.}}$$

The reciprocal lattice is itself a Bravais lattice

If $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are the primitive vectors of a B.L., then

$$\left.\begin{aligned} \vec{b}_1 &\equiv 2\pi \frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \\ \vec{b}_2 &\equiv 2\pi \frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \\ \vec{b}_3 &\equiv 2\pi \frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \end{aligned}\right\} \text{are primitive vectors for the reciprocal lattice}$$

~~proof~~

Note that $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$ and that $\vec{b}_i$'s are not all in the same plane since the $\vec{a}_i$'s are not.

$\Rightarrow$ $\{\vec{b}_i\}$ can be taken as a set of basis vectors for $\vec{k}$-space, ie we can write any wave-vector $\vec{k}$ as a linear combination

$$\vec{k} = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3 \qquad (k_i \text{ not necessarily integers})$$

then for any $\vec{R}$ in the B.L.

$$\vec{k} \cdot \vec{R} = (k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3)(n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3)$$

$$= 2\pi (n_1 k_1 + n_2 k_2 + n_3 k_3)$$

If $\vec{k}$ is in the reciprocal lattice, we must have

$e^{i\vec{k}\cdot\vec{R}} = 1$ for all $\vec{R}$

$\Rightarrow$ $n_1 k_1 + n_2 k_2 + n_3 k_3 =$ integer for all integers n_1, n_2, n_3

$\Rightarrow$ k_1, k_2, k_3 must be integer

$\Rightarrow$ reciprocal lattice vectors $\vec{K}$ must be of the form

$\vec{K} = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3$ with k_1, k_2, k_3 integer

The reciprocal of the reciprocal lattice is the original Bravais lattice - in this context the original B-L is called the "direct" lattice.

<u>proof</u>

If $\{\vec{G}\}$ are vectors of the reciprocal to the reciprocal lattice, then $e^{i\vec{G}\cdot\vec{K}} = 1$ for all $\vec{K}$ in R.L.

But $\{\vec{R}\}$ satisfies this ~~definition~~ condition by the definition of $\{\vec{K}\}$. So clearly $\{\vec{R}\}$ is a subset of $\{\vec{G}\}$. Now suppose there was some $\vec{G} \in \{\vec{G}\}$ but $\vec{G} \notin \{\vec{R}\}$. Then $\vec{G} = x_1\vec{a}_1 + x_2\vec{a}_2 + x_3\vec{a}_3$ where at least one of the x_i is not integer. But then we would have $e^{i\vec{G}\cdot\vec{K}} = \prod_j e^{i2\pi x_j k_j} \neq 1$, so there can't be any such $\vec{G}$. $\Rightarrow \{\vec{G}\} = \{\vec{R}\}$.

Examples

1) <u>simple cubic</u> $\begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_3 = a\hat{z} \end{cases}$

$$\Rightarrow \begin{cases} \vec{b}_1 = \frac{2\pi}{a}\hat{x} \\ \vec{b}_2 = \frac{2\pi}{a}\hat{y} \\ \vec{b}_3 = \frac{2\pi}{a}\hat{z} \end{cases}$$

so R.L. is also <u>single cubic</u> with side of length $\frac{2\pi}{a}$

2) <u>fcc</u> $\begin{cases} \vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}) \\ \vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}) \\ \vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}) \end{cases}$

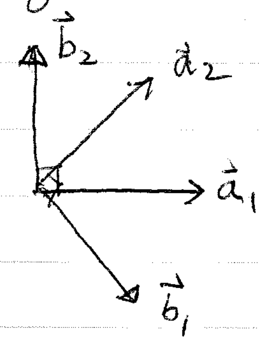
construct the $\vec{b}_i$ to get $\begin{cases} \vec{b}_1 = \frac{2\pi}{a}(\hat{y}-\hat{x}+\hat{z}) \\ \vec{b}_2 = \frac{2\pi}{a}(\hat{z}-\hat{y}+\hat{x}) \\ \vec{b}_3 = \frac{2\pi}{a}(\hat{x}-\hat{z}+\hat{y}) \end{cases}$

these $\vec{b}_i$ are just the primitive vectors of ~~an~~ <u>bcc</u> lattice with side of the cubic unit cell equal to $\frac{4\pi}{a}$

3) <u>bcc</u> since the reciprocal of the reciprocal lattice is the direct lattice, we conclude from (2) that the reciprocal of the bcc lattice is an <u>fcc</u> lattice. If the bcc direct lattice has a unit cubic cell of length a, then the reciprocal fcc lattice has unit cubic cell of length $\frac{4\pi}{a}$

4) The reciprocal of the simple hexagonal Bravais lattice with lattice constants a and c is also a simple hexagonal lattice with lattice constants $|\vec{b}_1| = |\vec{b}_2| = \frac{4\pi}{\sqrt{3}a}$ and $|\vec{b}_3| = \frac{2\pi}{c}$

The directions of $\vec{b}_1$ and $\vec{b}_2$ are rotated with respect to $\vec{a}_1$ and $\vec{a}_2$



angle between $\vec{a}_1$ and $\vec{a}_2$ is 60°

angle between $\vec{b}_1$ and $\vec{b}_2$ is 120°

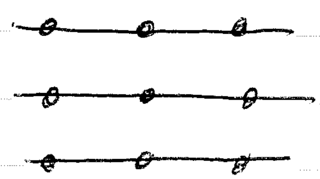
If v is the volume of the primitive cell of the direct lattice, then $(2\pi)^3/v$ is the volume of the primitive cell of the reciprocal lattice.

The Wigner-Seitz primitive cell for the reciprocal lattice is known as the First Brillouin Zone (later we will see the 2^{nd} and higher Brillouin Zones)

The 1^{st} Brillouin Zone of an fcc direct lattice is the Wigner-Seitz cell of a bcc reciprocal lattice and vice versa.

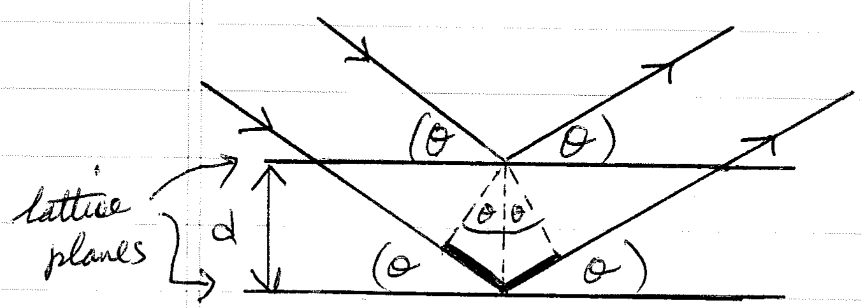
X-ray diffraction

Bragg formulation



"lattice planes" – set of parallel planes containing the points of the lattice

Imagine a set of lattice planes as if they are reflecting surfaces. An incoming light wave will get reflected by the successive planes. There will be a peak in the reflected wave amplitude when the reflections from all the planes add with <u>constructive</u> interference.



incoming light wave of wavelength λ gets specularly reflected ($\theta_{out} = \theta_{in}$). There will be constructive interference between reflected waves from top plane and the one underneath it when the difference in optical path length is an integral number of wavelengths λ. If the planes have separation d, and the incident angle is θ, then the optical path length difference (heavy lines in the figure) is:

$$\boxed{2d\sin\theta = n\lambda}$$ condition for Bragg scattering