Reciprocal lattice

The recip. lat. is important for
1) crystal diffraction
2) study of fncns with periodicity of Bravais lattic
3) momentum conservation in a crystal.

Definition

Consider a set of points constituting a Bravais lattice
For which k does the plane wave e^{ikr} have periodicity of the Br. L.?

The set of all wavevectors $\vec{K}$ that yeild plane waves with periodicity of a given Bravais lattice is known as its reciprocal lattice

$\vec{K}$ belongs to a recipr. lattice iff

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

$$e^{i\vec{K}\vec{R}} = 1$$

Recip. lattice is defined with resp. to a particular B.L.
Bravais lattice is called the direct lattice
(Even for lattice with a basis we use the underlying Br. la

The recip. lattice is also a Bravais lattice.
One can prove it by constructing it explicitely
$\vec{a}_1, \vec{a}_2, \vec{a}_3$ - primitive vectors

The recip. lattice is generated by

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

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

Clearly $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$

Any vector $\vec{k} = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3$

For Br. lat. $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$, n_i - integ

$$\vec{k} \cdot \vec{R} = 2\pi (k_1 n_1 + k_2 n_2 + k_3 n_3)$$

For $e^{i\vec{k}\vec{R}} = 1$ for $\forall R$ we should have all k_i's to be integer

The Reciproc. lat of the recip. lat is the original direct lattice: (use def above)

$$e^{i\vec{G}\cdot\vec{k}} = 1$$

Assume $\vec{G} = x_1 \vec{a}_1 + x_2 \vec{a}_2 + x_3 \vec{a}_3$

all x_i will have to be integer.

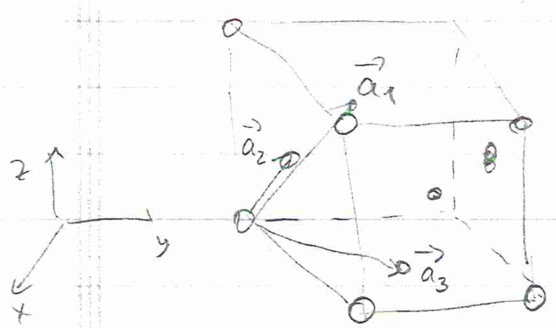
Examples.

1) The simple cubic Bravais lattice

$$\vec{a}_1 = a \cdot \hat{x} \qquad \vec{a}_2 = a \cdot \hat{y} \qquad \vec{a}_3 = a \cdot \hat{z}$$

$$\vec{b}_1 = \frac{2\pi}{a} \cdot \hat{x} \qquad \vec{b}_2 = \frac{2\pi}{a} \cdot \hat{y} \qquad \vec{b}_3 = \frac{2\pi}{a} \cdot \hat{z}$$

2) The FCC Bravais lattice



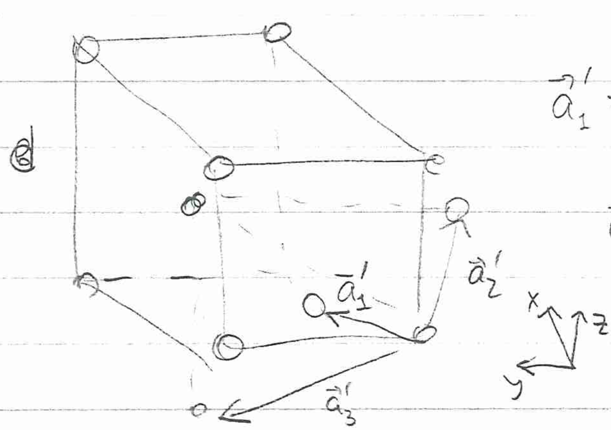
$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{x} + \hat{z})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$$

$$\left.\begin{aligned}
\vec{b}_1 &= \frac{4\pi}{a} \cdot \frac{1}{2} \cdot (\hat{y} + \hat{z} - \hat{x}) \\
\vec{b}_2 &= \frac{4\pi}{a} \cdot \frac{1}{2} (\hat{z} + \hat{x} - \hat{y}) \\
\vec{b}_3 &= \frac{4\pi}{a} \cdot \frac{1}{2} (\hat{x} + \hat{y} - \hat{z})
\end{aligned}\right\}$$

Primitive vectors of the BCC Br lat

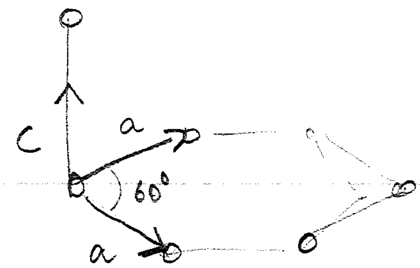


$$\vec{a}_1' = \frac{d}{2}(\hat{y} + \hat{z} - \hat{x})$$

$$\vec{a}_2' = \frac{d}{2}(\hat{x} + \hat{z} - \hat{y})$$

$$\vec{a}_3' = \frac{d}{2} \cdot (\hat{x} + \hat{y} - \hat{z})$$

The recip lattice of a simple hexagonal is simple hexagonal



The reciprocal lattice unit cell

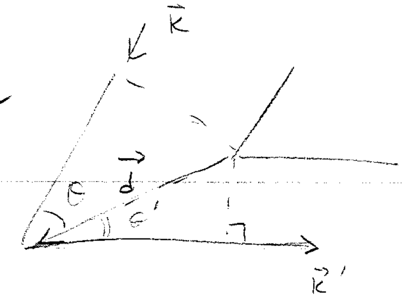
If v is the volume of the dir. lat prim cell, then $(2\pi)^3/v$.

The Wigner - Seitz primitive cell of the reciprocall lattice is known as the first Brillouin zone

X-ray difraction by a crystal

For certain sharply defined wavelengths and directions one finds intense peaks of scattered radiation

$\vec{k} = \frac{2\pi}{\lambda} \cdot \vec{n}$ - momentum of the incident photon



$\vec{k}' = \frac{2\pi}{\lambda} \vec{n}'$ - momentum of the reflected photon

$$d\cos\theta + d\cos\theta' = \vec{d}\,\vec{n} - \vec{d}\cdot\vec{n}' = m\lambda$$

$$\frac{2\pi}{\lambda} \cdot (\vec{d}\,\vec{n} - \vec{d}\,\vec{n}') = \frac{2\pi}{\lambda} \cdot m\lambda$$

$$\vec{d} \cdot \vec{k} - \vec{d} \cdot \vec{k}' = 2\pi m$$

$$\vec{R}\,(\vec{k} - \vec{k}') = 2\pi m$$

$$e^{i\vec{R}(\vec{k} - \vec{k}')} = 1$$

$\vec{k} - \vec{k}' \subset$ reciprocal lattice

Constructive inteference will occur provided that the change in wave vector $\vec{K} = \vec{k} - \vec{k}'$ is a vector of the reciprocal lattice

$$\vec{k} - \vec{k}' = \vec{K}$$

$$|\vec{k} - \vec{K}| \equiv |k'| = |k| \Rightarrow 2\vec{k} \cdot \vec{K} = \vec{K}^2 \Rightarrow k \cdot \hat{K} = \frac{1}{2} K$$

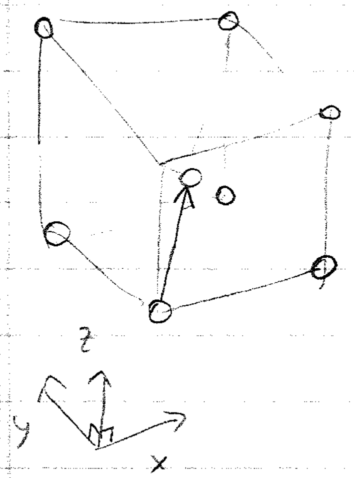
Diffraction by a monatomic lattice with a basis

Earlier we ~~dt~~ found the condition that rays scattered from each primitive cell should interfere constructively. If the cryst. structure has an n-atom basis with identical atoms (e.g. C in diamond) then the contents of the primitive cell may be further analyzed If the Bragg peak is associated with a change in wavevector $k'-k=K$, then the phase difference between the rays scattered at $\vec{d_i}$ and $\vec{d_j}$ will be $\vec{K}\cdot(\vec{d_i}-\vec{d_j})$ and the ~~amplitudes of the~~ net ray scattered by the entire primitive cell

$$S_{\vec{K}} = \sum_{j=1}^{n} e^{i\vec{K}\vec{d_j}} \quad \Big\} \text{ geometrical structure factor}$$

The intensity $\sim |S_K|^2$. It is not the only source of k dependence, but may play an important role

BCC ~~condise~~ considered as a simple cubic with a Basis



$\vec{d}_1 = 0 \qquad \vec{d}_2 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

A general $K = \frac{2\pi}{a}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z})$

$$S_K = 1 + e^{i\pi(n_1+n_2+n_3)} =$$

$$= 1 + (-)^{n_1+n_2+n_3} = \begin{cases} 2, & n_1+n_2+n_3 = \text{even} \\ 0, & n_1+n_2+n_3 = \text{odd} \end{cases}$$

Thus, those points in the simple cubic recip. lattice the sum of whose coord is odd will have no Bragg reflection. This converts a simple cubic lattice into the FCC lattice