

The Reciprocal Lattice - Chpt. 5

1.

Definition: K w/ periodicity of lattice:

$$e^{iK \cdot (r+R)} = e^{iK \cdot r}$$

$$\rightarrow \boxed{e^{iK \cdot R} = 1 \text{ for all } R \text{ in lattice}}$$

Explicit form:

$$\text{Let } \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3.$$

$$\rightarrow \vec{K} \cdot \vec{R} = n_1 \vec{K} \cdot \vec{a}_1 + n_2 \vec{K} \cdot \vec{a}_2 + n_3 \vec{K} \cdot \vec{a}_3 = 2\pi n$$

For this to be true for all n_1, n_2, n_3 integers,

$$\vec{K} \cdot \vec{a}_1 = 2\pi m_1 \quad (\text{necessary \& sufficient})$$

$$\vec{K} \cdot \vec{a}_2 = 2\pi m_2$$

$$\vec{K} \cdot \vec{a}_3 = 2\pi m_3,$$

$$\text{Let } \vec{b}_1 \cdot \vec{a}_1 = 2\pi$$

$$\vec{b}_1 \cdot \vec{a}_2 = 0$$

$$\vec{b}_1 \cdot \vec{a}_3 = 0, \dots$$

$$\text{or } \boxed{\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}}$$

$$\text{Write } \boxed{\vec{K} = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3}$$

$$\rightarrow \vec{K} \cdot \vec{a}_1 = 2\pi k_1$$

$$\vec{K} \cdot \vec{a}_2 = 2\pi k_2$$

$$\vec{K} \cdot \vec{a}_3 = 2\pi k_3$$

It is necessary & sufficient that k_1, k_2, k_3 be integers. The \vec{K} 's form a lattice called the reciprocal lattice.

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

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

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

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

Note: $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1) = \vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)$.

What is the reciprocal of the reciprocal lattice?

$$e^{i \vec{G} \cdot \vec{K}} = 1 \text{ for all } \vec{K}$$

$\vec{G} = \vec{R}$ satisfies this. Furthermore if $\vec{G} = \chi_1 \vec{a}_1 + \chi_2 \vec{a}_2 + \chi_3 \vec{a}_3$, then $\vec{K} \cdot \vec{G} = 2\pi(k_1 \chi_1 + k_2 \chi_2 + k_3 \chi_3)$. For this to be $2\pi m$ for all k_1, k_2, k_3 integers, the χ_1, χ_2, χ_3 must be integers. \rightarrow The reciprocal of the reciprocal lattice is the original lattice.

Examples:

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

Simple Cubic: $\vec{a}_1 = a \hat{x}$, $a_2 = a \hat{y}$, $a_3 = a \hat{z}$

$$b_1 = \frac{2\pi}{a} \hat{x}, \frac{2\pi}{a} \hat{y}, \frac{2\pi}{a} \hat{z}$$

Face Centered Cubic:

$$\vec{a}_1 = \frac{a}{2} (\hat{y} + \hat{z}) \quad \vec{b}_1 = \frac{4\pi}{a} (\hat{y} + \hat{z} - \hat{x})$$

$$\vec{a}_2 = \frac{a}{2} (\hat{z} + \hat{x}) \quad \vec{b}_2 = \frac{4\pi}{a} (\hat{z} + \hat{x} - \hat{y})$$

$$\vec{a}_3 = \frac{a}{2} (\hat{x} + \hat{y}) \quad \vec{b}_3 = \frac{4\pi}{a} (\hat{x} + \hat{y} - \hat{z})$$

Body Centered Cubic:

$$\vec{a}_1 = \frac{a}{2} (\hat{y} + \hat{z} - \hat{x}) \quad \vec{b}_1 = \frac{4\pi}{a} (\hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{a}{2} (\hat{z} + \hat{x} - \hat{y}) \quad \vec{b}_2 = \frac{4\pi}{a} (\hat{z} + \hat{x})$$

$$\vec{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z}) \quad \vec{b}_3 = \frac{4\pi}{a} (\hat{x} + \hat{y})$$

Volume unit cell = $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = v$.

Volume reciprocal unit cell = $\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{v}$.

Wigner-Seitz primitive cell for the reciprocal lattice = 1st Brillouin zone.

Lattice Planes

Plane containing at least 3 non-collinear Bravais lattice points.

Family of lattice planes = equally spaced lattice plane which contain all points in the lattice.

Let \hat{n} be perpendicular to the planes and let d be the separation between planes.

$$\rightarrow \hat{n} \cdot \vec{R} = md \text{ for } \vec{R} \text{ in lattice} \\ \text{and } m \text{ an integer}$$

$$\rightarrow \frac{2\pi\hat{n}}{d} \cdot \vec{R} = 2\pi m \text{ for all } \vec{R}$$

$$\rightarrow \frac{2\pi\hat{n}}{d} \text{ is a reciprocal lattice vector.}$$

Furthermore if \vec{K} is a reciprocal lattice vector, then $\vec{K} \cdot \vec{R} = 2\pi m$ for all \vec{R} . Let \vec{K}_0 be the smallest vector in given direction.

$$\vec{K}_0 \cdot \vec{R} = 0, \pm 2\pi m_0, \pm 4\pi m_0, \dots$$

for the different lattice planes. If $m_0 \neq 1$, then K_0/m_0 is also a reciprocal lattice vector and smaller. $\rightarrow m_0 = 1$. Adjacent lattice planes are separated by $d \rightarrow$

$$|K_0|d = 2\pi \text{ or } |K_0| = 2\pi/d.$$

The reciprocal lattice vectors have the form $m\left(\frac{2\pi}{d}\hat{n}\right)$.

Miller Indices:

For a given family of lattice plane let the shortest perpendicular lattice vector be

$$h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3.$$

h, k, l are the Miller indices.

Depends on basis.

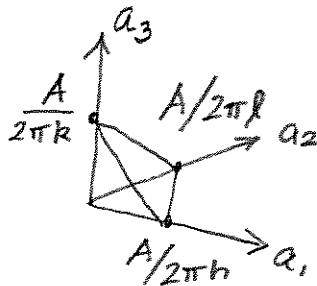
Convention FCC & BCC use SC lattice w/ basis.

Geometric interpretation:

$$\vec{K} \cdot \vec{a}_1 = 2\pi h$$

$$\vec{K} \cdot \vec{a}_2 = 2\pi k$$

$$\vec{K} \cdot \vec{a}_3 = 2\pi l$$



$$\vec{K} \cdot (\chi_1 \vec{a}_1 + \chi_2 \vec{a}_2 + \chi_3 \vec{a}_3) = A \text{ for a given plane}$$

$$= 2\pi h \chi_1 + 2\pi k \chi_2 + 2\pi l \chi_3.$$

→ Intercepts are $\frac{A}{2\pi h}, \frac{A}{2\pi k}, \frac{A}{2\pi l}$.

Conventions:

Equivalent lattice planes $(100), (010), (001) = \{100\}$.

If not doing planes, but simply lattice points, then $n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ denoted as $[n_1 n_2 n_3]$.