The Reciprocal Lattice - Chpt. 5

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:

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,

$$\vec{K}\cdot\vec{a}_1 = 2\pi m_1 \qquad \text{(necessary \& sufficient)}$$
$$\vec{K}\cdot\vec{a}_2 = 2\pi m_2$$
$$\vec{K}\cdot\vec{a}_3 = 2\pi m_3.$$

Let
$$\vec{b}_1\cdot\vec{a}_1 = 2\pi$$
$$\vec{b}_1\cdot\vec{a}_2 = 0 \qquad \text{or} \qquad \boxed{\vec{b}_i\cdot\vec{a}_j = 2\pi\delta_{ij}}$$
$$\vec{b}_1\cdot a_3 = 0, \ldots$$

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.

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

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

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

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

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

<u>What is the reciprocal of the reciprocal lattice?</u>

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

$\vec{G} = \vec{R}$ satisfies this. Furthermore if $\vec{G} = x_1 \vec{a}_1 + x_2 \vec{a}_2 + x_3 \vec{a}_3$, then $\vec{K} \cdot \vec{G} = 2\pi (k_1 x_1 + k_2 x_2 + k_3 x_3)$. For this to be $2\pi m$ for all k_1, k_2, k_3 integers, the x_1, x_2, x_3 must be integers. $\rightarrow$ The reciprocal of the reciprocal lattice is the <u>original lattice</u>.

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:

$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}) \qquad \vec{b}_1 = \frac{4\pi}{a}\frac{1}{2}(\hat{y}+\hat{z}-\hat{x})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}) \qquad \vec{b}_2 = \frac{4\pi}{a}\frac{1}{2}(\hat{z}+\hat{x}-\hat{y})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}) \qquad \vec{b}_3 = \frac{4\pi}{a}\frac{1}{2}(\hat{x}+\hat{y}-\hat{z})$$

Body Centered Cubic:

$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}-\hat{x}) \qquad \vec{b}_1 = \frac{4\pi}{a}\frac{1}{2}(\hat{y}+\hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}-\hat{y}) \qquad \vec{b}_2 = \frac{4\pi}{a}\frac{1}{2}(\hat{z}+\hat{x})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z}) \qquad \vec{b}_3 = \frac{4\pi}{a}\frac{1}{2}(\hat{x}+\hat{y})$$

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 primitative 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.

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

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

$\rightarrow \quad \frac{2\pi\hat{n}}{d}$ 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.

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

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 $d \rightarrow$

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

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

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

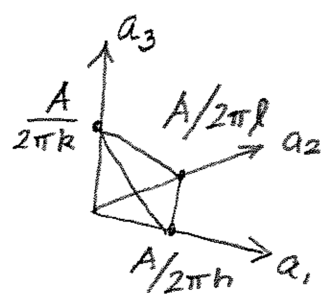
h, k, ℓ are the Miller indicies.

Depends on basis.

Convention FCC & BCC use SC lattice w/ basis.

Geometric interpretation:

$$\vec{K}\cdot\vec{a}_1 = 2\pi h$$
$$\vec{K}\cdot\vec{a}_2 = 2\pi k$$
$$\vec{K}\cdot\vec{a}_3 = 2\pi \ell$$



$\vec{K}\cdot(x_1\vec{a}_1 + x_2\vec{a}_2 + x_3\vec{a}_3) = A$ for a given plane

$= 2\pi h x_1 + 2\pi k x_2 + 2\pi \ell x_3 .$

$\rightarrow$ Intercepts are $\frac{A}{2\pi h}, \frac{A}{2\pi \ell}, \frac{A}{2\pi k}$.

Conventions:

Equivalent lattice planes $(1\,0\,0), (0\,1\,0), (0\,0\,1) = \{1\,0\,0\}$.

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 $[n_1 n_2 n_3]$.