Quadrant II – Transcript and Related Materials

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Unit-1: Crystal Structure

Module Name: Reciprocal Lattice

Module No: 08

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Notes

Concept of Reciprocal Lattice Vectors:

The electronic number density ***n(r)*** in the crystal is a periodic function in space:

$$n(r) = n(r+T)$$

where $T = n_1 a_1 + n_2 a_2 + n_3 a_3$ is the direct translation vector. So, ***n(r)*** can be expressed as a (spatial) Fourier series expansion.

For a one-dimensional model crystal, the ***n(x)*** can be represented as

$$n(x) = \sum_p n_p \, e^{i2\pi px/a}$$ where the ***p*'s** are integers.

The Fourier coefficient of the number density can be written as:

$$n_p = \frac{1}{a}\int_0^a dx\, n(x) e^{-i2\pi px/a}$$

In 3-Dimensions, the Fourier coefficient of the number density has the form

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \rightarrow n_{\mathbf{G}} = \frac{1}{V_c}\int_0^a dV n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} \quad \ldots(1)$$

The vectors ***G's*** are called **Reciprocal Lattice Vectors.**

Since, the electronic density ***n(r)*** is required to be invariant (periodic) under lattice translations:

$$n(r) = n(r + T) \quad \ldots(2)$$

$$n(r+T) = \sum_G n_G e^{iG\bullet(r+T)} = \sum_G n_G e^{iG\bullet r} e^{iG\bullet T}$$

$$= n(r)e^{iG\bullet T} = n(r) \quad \ldots(3)$$

Eq. (3) holds true , only if $\boxed{e^{iG\bullet T} = 1}$ …(4)

Only the set of Reciprocal lattice Vectors *G* that satisfy both Eq.(1) and Eq.(4) leads to an electronic number density n(r) that is invariant under lattice translations.

The set of *G'*s that meet this requirement are of the form

$$\boxed{G = v_1 b_1 + v_2 b_2 + v_3 b_3}$$

where v_1, v_2 and v_3 are integers. The $\boldsymbol{b_i}$'s are vectors which defined as:

$$\boxed{b_1 = \frac{2\pi}{V} a_2 \times a_3, \;\; b_2 = \frac{2\pi}{V} a_3 \times a_1, \; b_3 = \frac{2\pi}{V} a_1 \times a_2}$$

and $V = a_1 \cdot (a_2 \times a_3)$ is the volume of the unit cell.

Note that: $b_i \cdot a_j = 2\pi\delta_{ij}$, and $\delta_{ij} = \begin{matrix} 1 \; if \; i = j \\ 0 \; if \; i \neq j \end{matrix}$

The $\boldsymbol{a_j}$'s are the fundamental lattice vectors for the real crystal structure.

- ✓ A Set of Reciprocal Lattice Vectors G forms a Bravais Lattice.
- ✓ An X-Ray diffraction pattern of the lattice can be interpreted as a map of the reciprocal lattice of the crystal.
- ✓ The set of Reciprocal Lattice Vectors G determine the possible X-ray reflections.

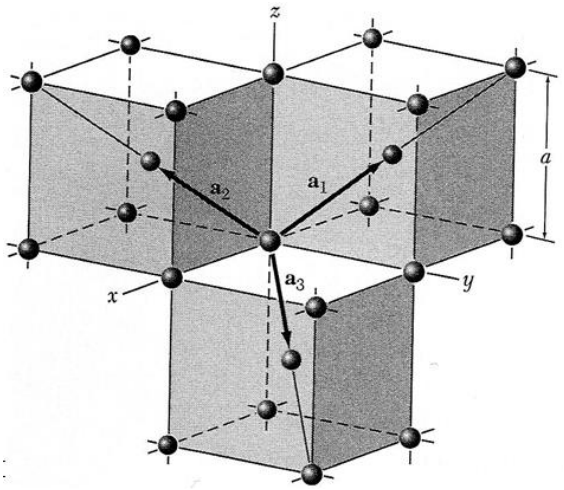
Reciprocal lattice of simple cubic lattice:

$$a_1 = a\,\hat{x},\ a_2 = a\,\hat{y}\ \text{and}$$
$$a_3 = a\,\hat{z}$$
$$V = a_1 \cdot (a_2 \times a_3) = a^3$$
$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} = \frac{2\pi\,\hat{x}}{a}$$
$$b_2 = \frac{2\pi\,\hat{y}}{a}\ \text{and}\ b_3 = \frac{2\pi\,\hat{z}}{a}$$

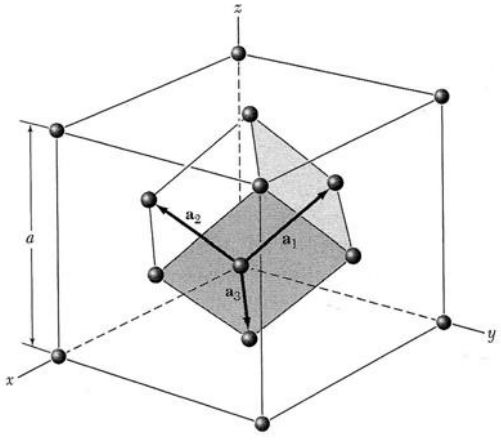
Reciprocal lattice of simple cubic is also a simple cubic with lattice constant $2\pi/a$.

Reciprocal lattice of body centered cubic lattice:

$$a_1 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$$
$$a_2 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$
$$a_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$
$$V = a_1 \cdot (a_2 \times a_3) = \frac{1}{2}a^3$$



$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} = \frac{2\pi}{a}(\hat{y} + \hat{z})$$
$$b_2 = \frac{2\pi}{a}(\hat{x} + \hat{z})\ \text{and}$$
$$b_3 = \frac{2\pi}{a}(\hat{x} + \hat{y})$$



But these are the primitive vectors of face centered cubic lattice. **Reciprocal of a bcc lattice is a fcc lattice.**

Note that: the reciprocal lattice of a fcc lattice is a bcc lattice.

	Direct Lattice	Reciprocal Lattice	Volume
SC	$\begin{cases} \mathbf{a}_1 = a\mathbf{x} \\ \mathbf{a}_2 = a\mathbf{y} \\ \mathbf{a}_3 = a\mathbf{z} \end{cases}$	$\begin{cases} \mathbf{b}_1 = (2\pi/a)\mathbf{x} \\ \mathbf{b}_2 = (2\pi/a)\mathbf{y} \\ \mathbf{b}_3 = (2\pi/a)\mathbf{z} \end{cases}$	$(2\pi/a)^3$
FCC	$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}) \\ \mathbf{a}_2 = \frac{1}{2}a(\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{z}+\mathbf{x}) \end{cases}$	$\begin{cases} \mathbf{b}_1 = \frac{2\pi}{a}(-\mathbf{x}+\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}-\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y}-\mathbf{z}) \end{cases}$	$2(2\pi/a)^3$
BCC	$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}-\mathbf{z}) \\ \mathbf{a}_2 = \frac{1}{2}a(-\mathbf{x}+\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{x}-\mathbf{y}+\mathbf{z}) \end{cases}$	$\begin{cases} \mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y}) \end{cases}$	$4(2\pi/a)^3$