

we have 14 lattices for 3d
 " 5 lattices for 2d
 1 Lattice for 1d

how about in reciprocal lattice?

what is the purpose of moving into the reciprocal lattice?

it decreases the complexity of theoretical & practical analysis

electronic number density ($n(r)$) must be periodic $\rightarrow n(r) = n(r+R)$

$$\sum_{\mathbf{r}} n_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{r}} n_{\mathbf{r}} e^{i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})} \quad \leftarrow \text{fourier transform}$$

$$\sum_{\mathbf{r}} n_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{r}} n_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{R}}$$

So, $e^{i\mathbf{k}\cdot\mathbf{R}}$ must be equal to 1

$$\mathbf{R}\cdot\mathbf{R} = 2\pi \quad e^{i\mathbf{k}\cdot\mathbf{R}} = 1 \quad \begin{array}{l} \# \mathbf{R} \rightarrow \text{periodicity vector} \\ \# \mathbf{k} \rightarrow \text{Reciprocal lattice vector} \end{array}$$

$$\mathbf{R}_i \cdot \mathbf{R}_j = 2\pi \delta_{ij} \quad i, j = x, y, z \quad \delta_{ij} = 1 : i=j \mid 0 : \text{else}$$

When we move from real space to k (momentum) space, our differential equations turn into quadratic eqn which is easier to solve

let,

$$\mathbf{R} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

$$\text{and } \mathbf{k} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

where h, k, l are miller indices

reciprocal of the intersections

eg:

$$\mathbf{a} \cdot \mathbf{a}^* = 2\pi$$

since they are in the same direction,

$$a a^* = 2\pi$$

$$a^* = \frac{2\pi}{a}$$

So, reciprocal lattice \rightarrow

$$\mathbf{a} \cdot \mathbf{a}^* = 2\pi$$

for 3d

$$a a^* = 2\pi$$

$$b b^* = 2\pi$$

$$c c^* = 2\pi$$

but $b a^* = 0$

because of δ_{ij}

$$a^* = \frac{2\pi (b \times c)}{a \cdot (b \times c)}$$

$$b^* = \frac{2\pi (c \times a)}{b \cdot (c \times a)}$$

$$c^* = \frac{2\pi (a \times b)}{c \cdot (a \times b)}$$

Direct Lattice vector :

$$\mathbf{R} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

Reciprocal Lattice vector :

$$\mathbf{k} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

Reciprocal lattice is the fourier transform of the real lattice

note: set of reciprocal lattice vectors \mathbf{k} is also bravais lattice

since $b a^* = 0$

and $c a^* = 0$

So, a^* must be linear multiple of $(b \times c)$

i.e. \perp to both b and c

$$\text{So, } a^* = \lambda (b \times c)$$

$$a a^* = \lambda a \cdot (b \times c) = 2\pi$$

$$\lambda = \frac{2\pi}{a \cdot (b \times c)}$$

$$\text{So, } a^* = \frac{2\pi (b \times c)}{a \cdot (b \times c)}$$

2d

$$\mathbf{R} = u\mathbf{a} + v\mathbf{b}, \quad \mathbf{k} = m\mathbf{a}^* + n\mathbf{b}^*$$

$$a a^* = ?$$

$$\mathbf{R}_i \cdot \mathbf{k}_j = 2\pi \delta_{ij}$$

$$a a^* = 2\pi$$

$$b b^* = 2\pi$$

$$a b^* = 0$$

$b a^* = 0 \rightarrow a^* \perp b$
 and since $a a^* = 2\pi$,
 a and a^* must be parallel

$$\text{So, } a^* = \frac{2\pi}{a} \hat{a}$$

we can arrive here with the 3d also

$$\text{we had } a^* = \frac{2\pi (b \times c)}{a \cdot (b \times c)}$$

$$a^* = \frac{2\pi \hat{b}}{a \cdot \hat{b}} \quad \text{because 2d}$$

but direction remains

$$a^* = \frac{2\pi}{a} \hat{a}$$

$$b^* = \frac{2\pi}{b} \hat{b}$$

let \rightarrow

$$b^* = \frac{2\pi}{b} \quad \text{and} \quad a^* = \frac{2\pi}{a}$$

$$\hat{b}^*$$

$$\hat{a}^*$$

here b^* will be bigger than a^*

as compared to b, a ratio

because we took the reciprocal

$$\text{in } \rightarrow b^* = \frac{2\pi}{b}$$

Coordinate transformation

BCC

$$\begin{array}{l} \bar{a} = \frac{a}{2} (i+j-k) \\ \bar{b} = \frac{a}{2} (j+k-i) \\ \bar{c} = \frac{a}{2} (k+i-j) \end{array} \quad \left. \begin{array}{l} \\ \\ \end{array} \right\} \begin{array}{l} \text{Primitive unit} \\ \text{vector for BCC} \\ \text{crystal} \end{array}$$

$$\bar{a}^* = \frac{2\pi (\bar{b} \times \bar{c})}{\bar{a} \cdot (\bar{b} \times \bar{c})}$$

$$\bar{b} \times \bar{c} = \begin{vmatrix} i & j & k \\ -a/2 & a/2 & a/2 \\ a/2 & -a/2 & a/2 \end{vmatrix}$$

$$i \left(\frac{a^2}{4} + \frac{a^2}{4} \right) - j \left(-\frac{a^2}{2} - \frac{a^2}{2} \right) + k \left(\frac{a^2}{2} - \frac{a^2}{2} \right)$$

$$i \left(\frac{a^2}{2} \right) + j \left(\frac{a^2}{2} \right)$$

$$\bar{a}^* = \frac{2\pi \left(\frac{a^2}{2} (i+j) \right)}{\left(\frac{a}{2} (i+j) \right) \left(\frac{a^2}{2} (i+j) \right)}$$

$$\bar{a}^* = \frac{2\pi (a^2/2) (i+j)}{a^3/2}$$

$$\bar{a}^* = \frac{2\pi}{a} (\hat{i} + \hat{j})$$

$$\bar{b}^* = \frac{2\pi}{a} (\hat{j} + \hat{k})$$

$$\bar{c}^* = \frac{2\pi}{a} (\hat{k} + \hat{i})$$

Note: The Real space vector for FCC is:

$$\bar{a} = \frac{a}{2} (i+j)$$

$$\bar{b} = \frac{a}{2} (j+k)$$

$$\bar{c} = \frac{a}{2} (k+i)$$

we notice that the Reciprocal lattice of BCC is FCC and vice versa.

$$\text{Face centered cube} \xrightarrow[\text{Inverse Fourier transform}]{\text{Fourier transform}} \text{Body centered cube}$$

If we move into the Reciprocal space, the Weigner Seitz cell gives the first brillouin zone.

note: Weigner Seitz cell has square and hexagon structure

if we can find the energies in the brillouin zone, we can find the energy of holes in the, say, silicon structure

In the brillouin zone (FCC)

we have a square at

$$[001], [010], [100]$$

whereas we have a hexagon at $[111]$

Remember last question of the quiz

\hookrightarrow Work function

\hookrightarrow if it is diff for a particular material, then the min energy must be too

$E = \frac{\hbar^2 k^2}{2m} \Rightarrow$ quantum mechanics

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + V(x) \Psi(x) = E \Psi(x) \quad \leftarrow \text{time independent schrodinger's wave equation}$$

$$\text{let } \Psi(x) = A \sin(kx) + B \cos(kx)$$

$$\text{then } \frac{\partial^2 \Psi(x)}{\partial x^2} = -k^2 \Psi(x)$$

$$\text{So, } -\frac{\hbar^2 k^2}{2m} \Psi(x) + V(x) \Psi(x) = E \Psi(x)$$

for the ∞ potential well problem, $V(x)=0$

$$\text{So, } E = \frac{\hbar^2 k^2}{2m}$$

BRAGG'S LAW: $2d \sin \theta = n\lambda$

$2d \sin \theta$ (phase shift)

if $\lambda/2$ is similar to the wavelength of the incident beam then there is possibility of construct interference

$$d_{hkl}^{\text{cubic}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

a = lattice constant

h, k, l = miller indices

C-Si : Crystalline Si

PSi : Polycrystalline Si

XRD Pattern

intensity or

\sim peak height of structure in XRD pattern:

C-Si \gg Meso-Psi $>$ Micro-Psi $>$ Amorphous

\downarrow
 \sim no peak
 no diffraction

Defects in Crystalline Solids

Real crystals always some defects

controlling the defects is essential

pure Si crystalline wafer manufacturing = \$\$\$

defects

\hookrightarrow point

\hookrightarrow line

\hookrightarrow Schottky