Week 2

- Reciprocal lattice

Periodical functions

$$U(\mathbf{r}') = U(\mathbf{r}), \quad \mathbf{r}' = \mathbf{r} + u\,\mathbf{a} + v\,\mathbf{b} + w\,\mathbf{c}$$

$$U(\mathbf{r}) = \sum_{\mathbf{K}\in\mathbf{G}} U_{\mathbf{K}} \exp(i\,\mathbf{K}\cdot\mathbf{r})$$

$$\mathbf{K}\cdot\mathbf{a} = 2\pi h, \;\; \mathbf{K}\cdot\mathbf{b} = 2\pi k, \;\; \mathbf{K}\cdot\mathbf{c} = 2\pi l, \quad h, k, l \in Z$$

Reciprocal lattice

$$\mathbf{K} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*, \quad \mathbf{K} \in \mathbf{G}$$

$$\mathbf{a}^* = \frac{2\pi}{V}\mathbf{b}\times\mathbf{c}, \ \mathbf{b}^* = \frac{2\pi}{V}\mathbf{c}\times\mathbf{a}, \ \mathbf{c}^* = \frac{2\pi}{V}\mathbf{a}\times\mathbf{b}$$

$$V = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$$

General properties of reciprocal lattices

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

$\mathbf{K} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*, \quad \mathbf{K} \in \mathbf{G}$ Reciprocal lattice

- Reciprocal of sc is sc
- Reciprocal of hcp is hcp
- Reciprocal of fcc is bcc
- Reciprocal of bcc is fcc
- “Reciprocal” of the reciprocal is the initial lattice

Geometrical properties of reciprocal lattice

$$\mathbf{K} = \mathbf{K}_{h,k,l} = h\mathrm{a}^* + k\mathrm{b}^* + l\mathrm{c}^*$$

1. $\mathbf{K}_{h,k,l} \perp (h,k,l)$ plane of the original lattice

2. $|\mathbf{K}_{h,k,l}| = \dfrac{2\pi}{d_{h,k,l}}$, see next slide

$d_{h,k,l}$ is a distance between the planes (h,k,l)

Length of vectors in reciprocal lattice versus separation of planes in direct lattice

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

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

Consider set of planes with Miller indexes h,k,l. Their separation

d satisfiers: $d = a\cos\alpha = \mathbf{a}\cdot\mathbf{n} = \mathbf{b}\cdot\mathbf{n} = \mathbf{c}\cdot\mathbf{n} = \dfrac{\mathbf{a}\cdot\mathbf{K}}{|\mathbf{K}|} = ...,$

where $\mathbf{n}$ -is orthogonal unit vector.

$$d\,|\mathbf{K}| = \mathbf{a}\cdot\mathbf{K} = 2\pi\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = 2\pi, \qquad |\mathbf{K}_{h,k,k}| = \frac{2\pi}{d_{h,k,l}}$$

Brillouin zone

Brillouin zone is similar to the Wigner-Zeits cell of the original lattice