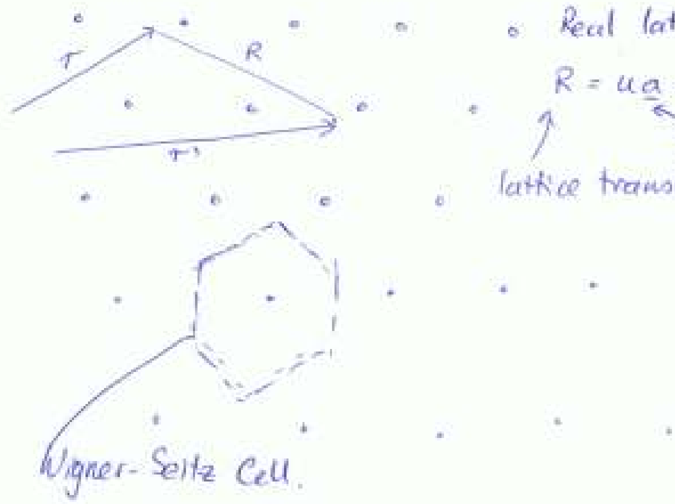
Lecture 1 Summary



Real lattice (Bravais)

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

primitive lattice vectors

lattice translation vector

3D Lattices

Simple Cubic ... Face Centred Cubic ... Body Centred Cubic

and hexagonal close packed!

Reciprocal Space - describes periodic structures.

Set of imaginary points constructed such that

(i) direction from one point to another coincides with the direction normal to the real space plane

(ii) the seperation of these pts is equal to the reciprocal of the real interplanar distance.

We define reciprocal lattice such that

$$\boxed{\exp i\underline{G}.\underline{R} = 1} \quad \text{where } \underline{G} = ha^* + kb^* + lc^*$$

Miller indicies

Each pt (h,k,l) in reciprocal lattice corresponds to a set of lattice planes in real space.

$\underline{a}^*, \underline{b}^*, \underline{c}^*$ are the primitive lattice vectors of the reciprocal lattice

$$\underline{a}^* = \frac{2\pi\, \underline{b} \times \underline{c}}{\underline{a}\cdot\underline{b}\times\underline{c}} \qquad \underline{b}^* = \frac{2\pi\, \underline{c} \times \underline{a}}{\underline{a}\cdot\underline{b}\times\underline{c}} \qquad \text{etc}$$

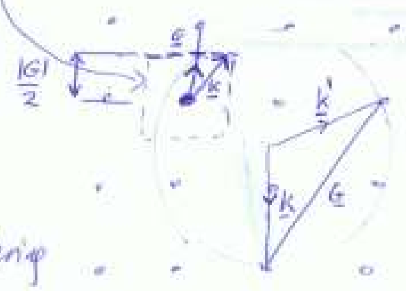
$$\rightarrow e^{i\underline{G}\cdot\underline{r}} = e^{i\underline{G}\cdot\underline{r}}\, e^{i\underline{G}\cdot\underline{R}} = e^{i\underline{G}(\underline{r}+\underline{R})}$$

ie. the vectors of the reciprocal lattice can be viewed as wave vectors with periodicity of the Bravais lattice.

Bragg Diffraction and Brillouin Zones

The Wigner-Seitz Cell of reciprocal space, containg one lattice pt at its centre : FIRST BRILLOUIN ZONE

The Bragg diffraction condition is met at its boundaries.



$$\underline{k}' = \underline{k} + \underline{G}$$

allowed scattering vectors

Assume elastic scattering ie $\underline{k}' = \underline{k}$ $\rightarrow$ $2\underline{k}\cdot\underline{G} = -G^2$

$$\rightarrow \boxed{2\underline{k}\cdot\underline{G} = G^2}$$

$\div 4$

$$\underline{k}\cdot\tfrac{1}{2}\underline{G} = \left(\tfrac{1}{2}G\right)^2$$

ie the Bragg diffraction condition will be met by any vector from the origin to the plane that bisects $\underline{G}$

$$= n\lambda = 2d\sin\theta$$

$\frac{2\pi}{k}$ $\qquad$ $\frac{2\pi}{|G|}$