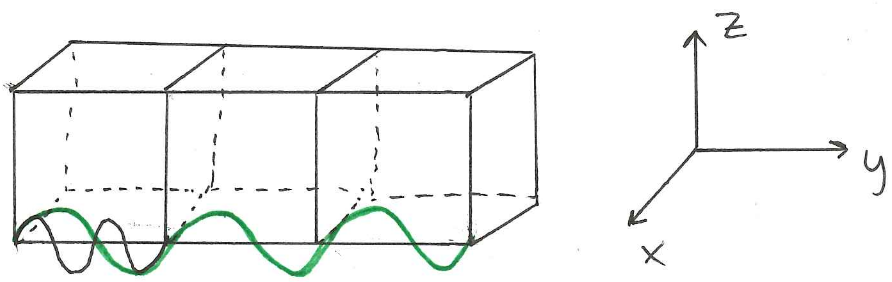
F3 ~~Ons~~ Tors LV1

Reellt (direkt) gitter
Reciprokt gitter

Definition: En samling vågvektorer, $\bar{G}$, av plana vågor, $\exp(i\bar{G}\bar{r})$ som har periodiciteter av Bravais-gittret

$$\exp(i\bar{G}\bar{r}) = \exp(i\bar{G}(\bar{r}+\bar{R})) \rightarrow \exp(i\bar{G}\bar{r}) = 1$$



$$\bar{R}_1 = a\hat{y}$$
$$\bar{R}_2 = 2a\hat{y}$$

$$\lambda = \frac{2\pi}{k}$$

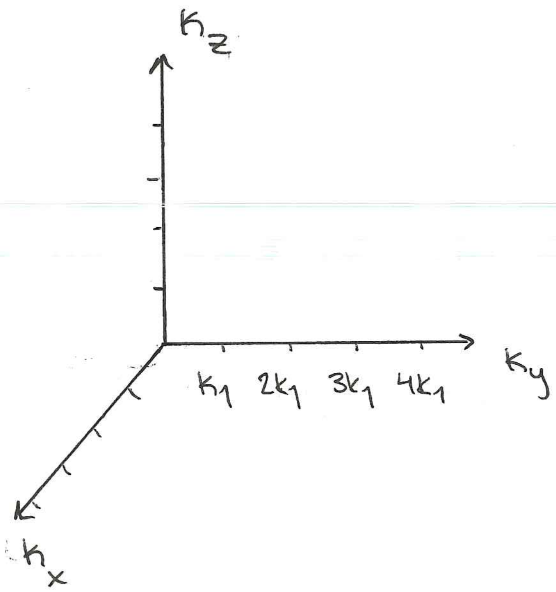
k = vågtal
$\bar{k}$ = vågvektor

$$\lambda_1 = a = \frac{2\pi}{k_1}$$
$$\lambda_2 = \frac{a}{2} = \frac{1}{2}\cdot\frac{2\pi}{k_1}$$
$$\lambda_3 = \frac{a}{3} = \frac{1}{3}\,\frac{2\pi}{k_1}$$

För y-riktningen har vi funnit en k-vektor, $\bar{k}_1$, som har periodicitet av Bravais-gittret

$$\boxed{k_1 = \frac{2\pi}{a}}$$

Reciprokt gitter



Reciproka gittervektorer $\bar{b}_1, \bar{b}_2, \bar{b}_3$

$$\begin{cases} \bar{G} = L_1\bar{b}_1 + L_2\bar{b}_2 + L_3\bar{b}_3 \\ L_i = 0, \pm 1, \pm 2, \dots \end{cases}$$

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

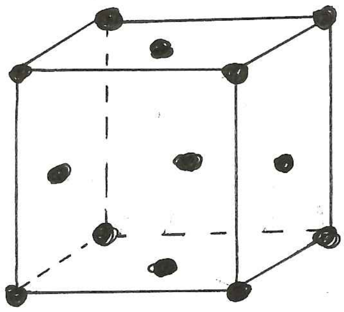
$$\bar{b}_2 = 2\pi \frac{\bar{a}_3 \times \bar{a}_1}{\bar{a}_1(\bar{a}_2 \times \bar{a}_3)}$$

$$\boxed{a_i b_j = 2\pi\,\delta_{ij}}$$

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

Ex.

Reciproka gittret för FCC?



$$\begin{cases} \bar{a}_1 = \frac{a}{2}(\hat{x} + \hat{z}) \\ \bar{a}_2 = \frac{a}{2}(\hat{x} + \hat{y}) \\ \bar{a}_3 = \frac{a}{2}(\hat{y} + \hat{z}) \end{cases}$$

$$b_1 = 2\pi \frac{\bar{a}_2 \times \bar{a}_3}{\bar{a}_1(\bar{a}_2 \times \bar{a}_3)}$$

$$\bar{a}_2 \times \bar{a}_3 = \begin{vmatrix} x & y & z \\ a/2 & a/2 & a/2 \\ 0 & 0 & 0 \end{vmatrix} = \frac{a^2}{4}\hat{x} - \frac{a^2}{4}\hat{y} + \frac{a^2}{4}\hat{z}$$

$$\bar{a}_1(\bar{a}_2 \times \bar{a}_3) = \frac{a}{2}(\hat{x}+\hat{z})\left(\frac{a^2}{4}\hat{x} + \frac{a^2}{4}\hat{y} + \frac{a^2}{4}\hat{z}\right)$$

$(\hat{x}\cdot\hat{x} = 1,\ \hat{x}\cdot\hat{y} = 0,\ \text{osv...})$

$$\rightarrow \hat{b}_1 = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z}) = \frac{2\pi}{a}[1\bar{1}1]$$

$$\bar{b}_2 = \frac{2\pi}{a}[11\bar{1}]$$

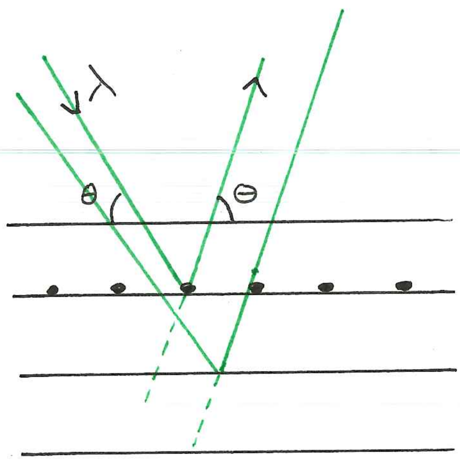
$$\bar{b}_3 = \frac{2\pi}{a}[\bar{1}11]$$

Dett reciproka gittret för ett FCC-gitter
är ett BCC-gitter!
(och tvärtom!)

Brillouin zonen: Den volym i k-rummet som avgränsas av de närmsta Brillouinzonplanerna kallas första Brillouinzonen.

Diffraktion

Bragg



Antar: Spekulär reflektion

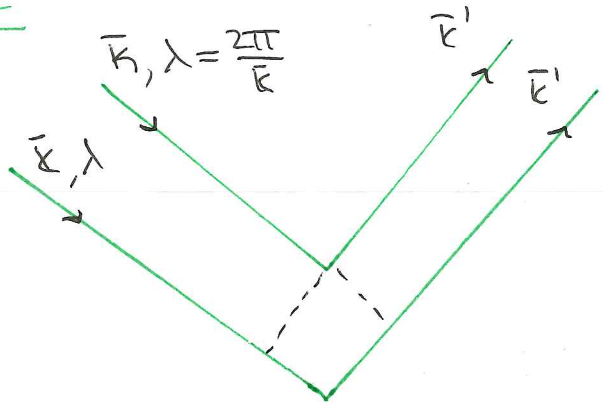
Elastisk

Ingen multipel spridning

Vågskillnad:

$$\boxed{2d\sin\theta = n\cdot\lambda}$$

Laue



Vågskillnad:

$$|\bar{d}|\cos\theta + |\bar{d}|\cos\theta' =$$

$$= \bar{d}\cdot\hat{n} + (-\bar{d}\cdot\hat{n}') = \bar{d}(\hat{n}-\hat{n}')$$

För konstruktiv interferens:

$$\bar{d}(\hat{n}-\hat{n}') = m\lambda, \quad m = 0, \pm 1, \pm 2, \ldots$$

$$\bar{d}\left(\frac{2\pi}{\lambda}\hat{n} - \frac{2\pi}{\lambda}\hat{n}'\right) = m\frac{2\pi}{\lambda}\lambda$$

$$\bar{d}(\bar{k}-\bar{k}') = m\cdot 2\pi$$

Om vi betraktar ett stort antal diffraktionspunkter i ett gitter måste $\bar{d}(\bar{k}-\bar{k}') = m \cdot 2\pi$ gälla för alla punkter

Alla avstånd mellan atomer, $\bar{d}$, är punkter i ett Bravais-gitter

$\rightarrow \bar{d} = \bar{R}$

$\rightarrow \bar{R}(\bar{k}-\bar{k}') = 2\pi m$

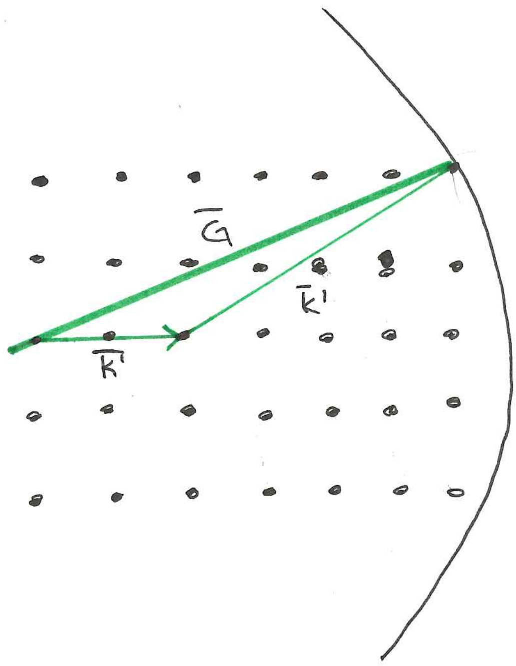
$$\exp(i\bar{R}(\bar{k}-\bar{k}')) = \exp(i \cdot 2\pi \cdot m) = 1$$

konstruktiv interferens då $\bar{G} = \bar{k}-\bar{k}'$

Ex. SC, 2D

λ, k'

(001)



Högst oklart....

Diff. villkor

$\bar{G} = \bar{k}-\bar{k}'$