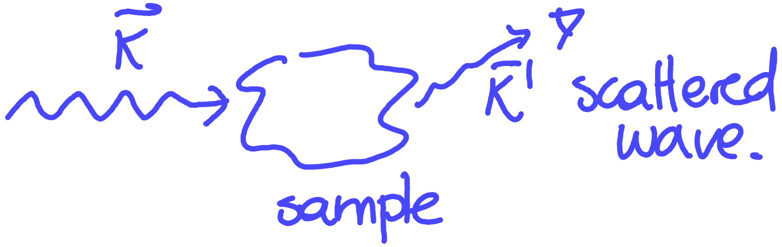
# Scattering

Lecture 2

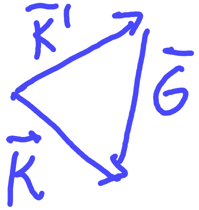
# Recap




Bragg Law: $2d\sin\theta = n\lambda$

Laue Condition: $\Delta\vec{K} = \vec{G}$ $\longrightarrow$ Elastic scattering

$$\Delta\vec{K} = \vec{K}' - \vec{K}$$

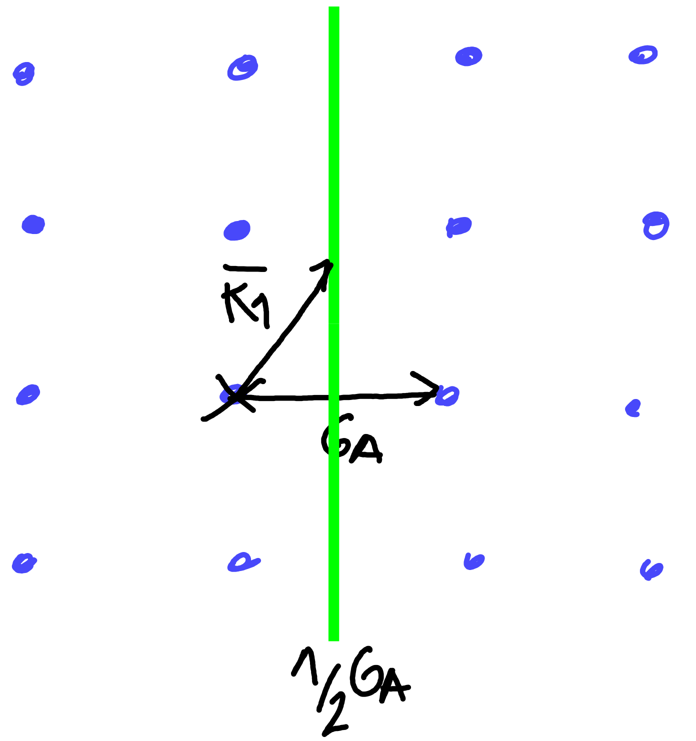



$$2\vec{K}\cdot\vec{G} = G^2$$

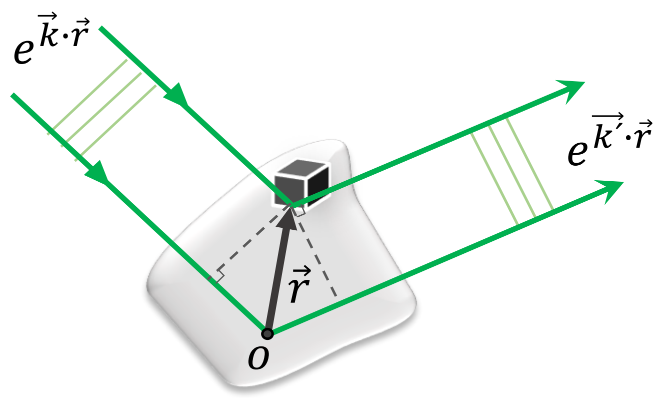
$$\vec{K}\cdot\left(\tfrac{1}{2}\vec{G}\right) = \left(\tfrac{1}{2}G\right)^2$$

Ex. $\vec{K}_1\cdot\left(\tfrac{1}{2}\vec{G}_A\right) = \left(\tfrac{1}{2}G_A\right)^2$

Special role of the Brillouin zone (border)!



# Structure Factor




Total Amplitude of the scattered wave in the direction $\vec{K}'$

$$F = \int_V dV\, n(\vec{r})\, e^{i\underbrace{(\vec{K}-\vec{K}')}_{=-\Delta\vec{K}}\cdot\vec{r}}$$

over sample volume

$$F = \sum_G \int dV\, n_G \exp\left(i(\vec{G}\cdot\Delta\vec{K})\cdot\vec{r}\right)$$

for $\Delta\vec{K} = \vec{G} \Rightarrow F = V n_{\bar{G}}$

(if $\Delta\vec{K} \neq \vec{G} \Rightarrow F$ is very small)

For a crystal of N cells,
and when $\Delta\vec{K} = \bar{G}$ is satisfied for a direction $\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$,

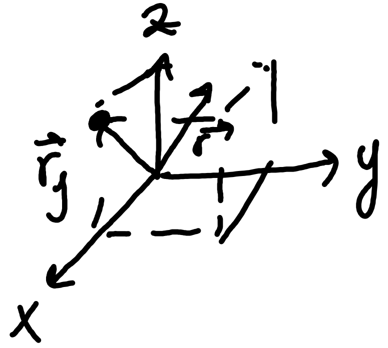
$$\boxed{F_G = N\underbrace{\int_{cell} n(\vec{r})\cdot e^{-i\vec{G}\cdot\vec{r}}\, d^3r}_{} \equiv N\cdot S_G}$$

$S_{\bar{G}} = S_{hkl}$ = Structure Factor

notice that $I_{hkl} \propto |S_{hkl}|^2$

# Atomic form factor

→ decompose $n(\vec{r})$ in atomic contributions within a cell :

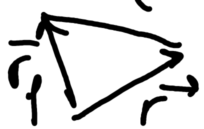



- $n_j(\vec{r}-\vec{r}_j)$
- electron density at $\vec{r}$ : $n(\vec{r}) = \sum_j^{s} n_j(\vec{r}-\vec{r}_j)$

atoms in the basis

$$S_{\vec{G}} = \int_{cell} n(\vec{r}) \cdot e^{-i\vec{G}\cdot\vec{r}} d^3r = \sum_j \int_{cell} n_j(\vec{r}-\vec{r}_j) e^{-i\vec{G}\vec{r}} d^3r$$

define $\rho = \vec{r} - \vec{r}_j$

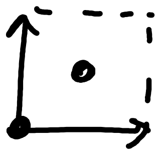



$$\boxed{S_G} = \sum_j \int_{cell} n_j(\rho) e^{-i\vec{G}\vec{\rho}} e^{-i\vec{G}\vec{r}_j} d^3\rho = \sum_j e^{-i\vec{G}\vec{r}_j} \underbrace{\int n_j(\vec{\rho}) e^{-i\vec{G}\vec{\rho}} d^3\rho}_{= f_j \,=\, \text{Atomic Form Factor}} = \boxed{\sum_j e^{-i\vec{G}\vec{r}_j} \cdot f_j}$$

structure Factor

if we consider point-like atoms: $n_j(\rho) = Z\delta(\vec{\rho}) \rightarrow f_j = Z$

position atoms of the basis within the (real) cell:



$\vec{r}_j = x_j\bar{a}_1 + y_j\bar{a}_2 + z_j\bar{a}_3$ $\qquad 0 \leq x_j, y_j, z_j \leq 1$

A reflexion $h, K, l$ $\longrightarrow$ correspond to $\vec{G} = h\bar{b}_1 + K\bar{b}_2 + l\bar{b}_3$

Atomic Form Factor

$$\boxed{S_{\bar{G}}} = S_{h,K,l} = \sum_j e^{-i\bar{G}\cdot\bar{r}_j}\cdot f_j = \boxed{\sum_j e^{-i2\pi(hx_j+Ky_j+lz_j)}\cdot f_j}$$

structure Factor

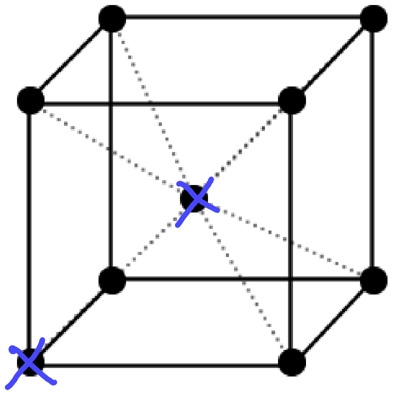
$\bar{b}_i\cdot\bar{a}_j = 2\pi\delta_{ij}$

$(\delta_{ij} = 0 \ \ i\neq j, \ \ \delta_{ij} = 1 \ \ i=j)$

it tells us with scattering peaks will be absent for a given Lattice!

see examples $\rightarrow$

# Structure factor for a monoatomic bcc



I (Body)

simple cubic cell
with a basis of 2 identical atoms @ $(0,0,0), \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$

$$\begin{array}{cccccc} \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ x_1 & y_1 & z_1 & x_2 & y_2 & z_2 \end{array}$$

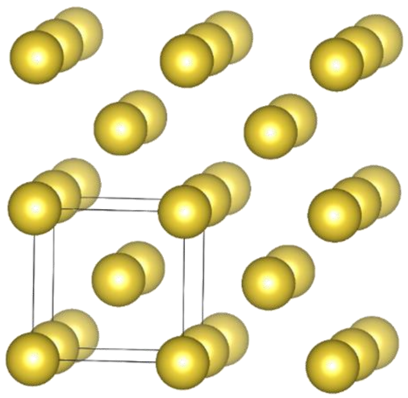
$$S_{hkl} = \sum_j e^{-i2\pi(hx_j + ky_j + lz_j)} \cdot f_j =$$

$$= f \cdot \left(e^{-i2\pi \cdot 0} + e^{-i\pi(h+k+l)}\right) =$$

$$= f \cdot \left(1 + (-1)^{(h+k+l)}\right)$$

For a BCC $\begin{cases} S_{hkl} = 0 & \text{when } h+k+l = \text{odd integer} \\ S_{hkl} = 2f & \text{" " = even integer} \end{cases}$

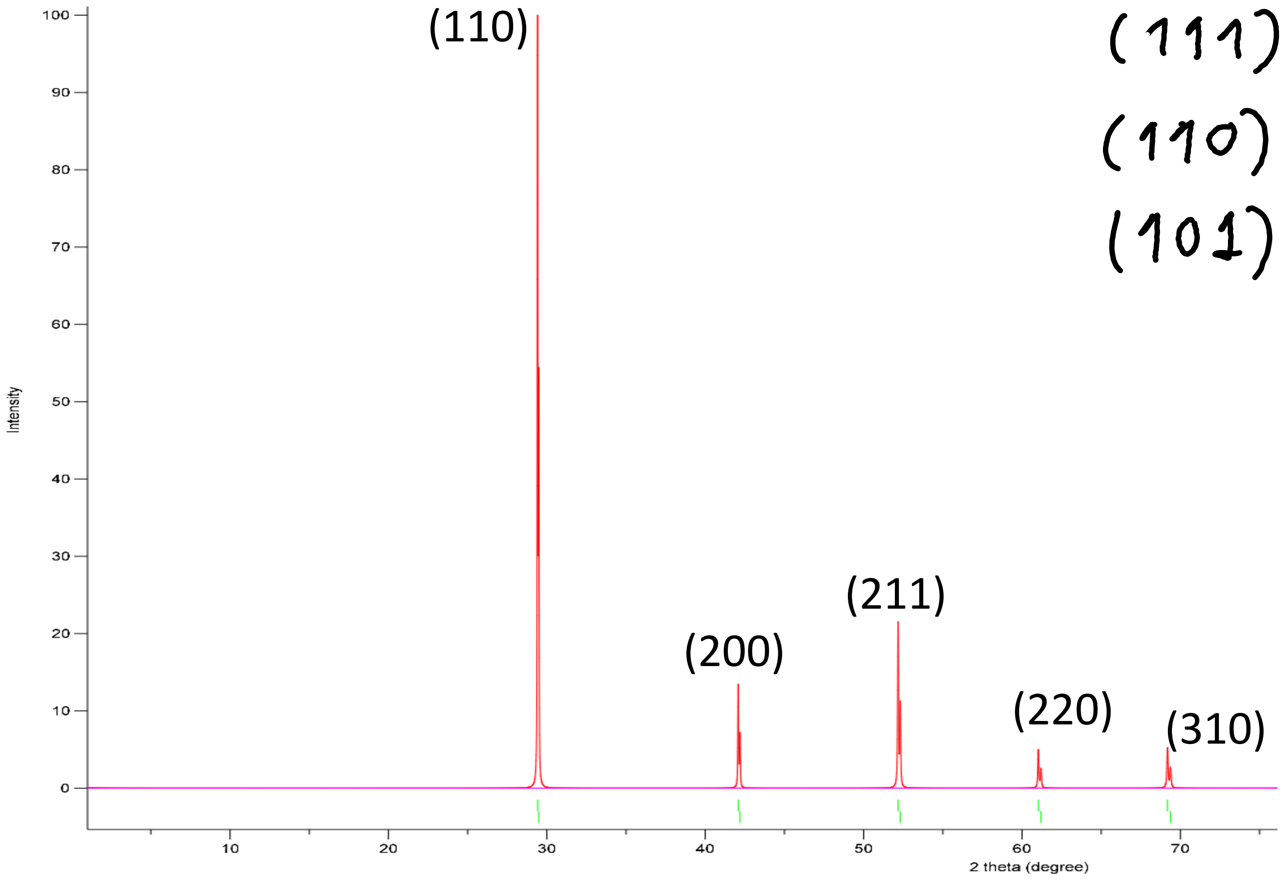
# Structure factor for Na



**Metallic Sodium**

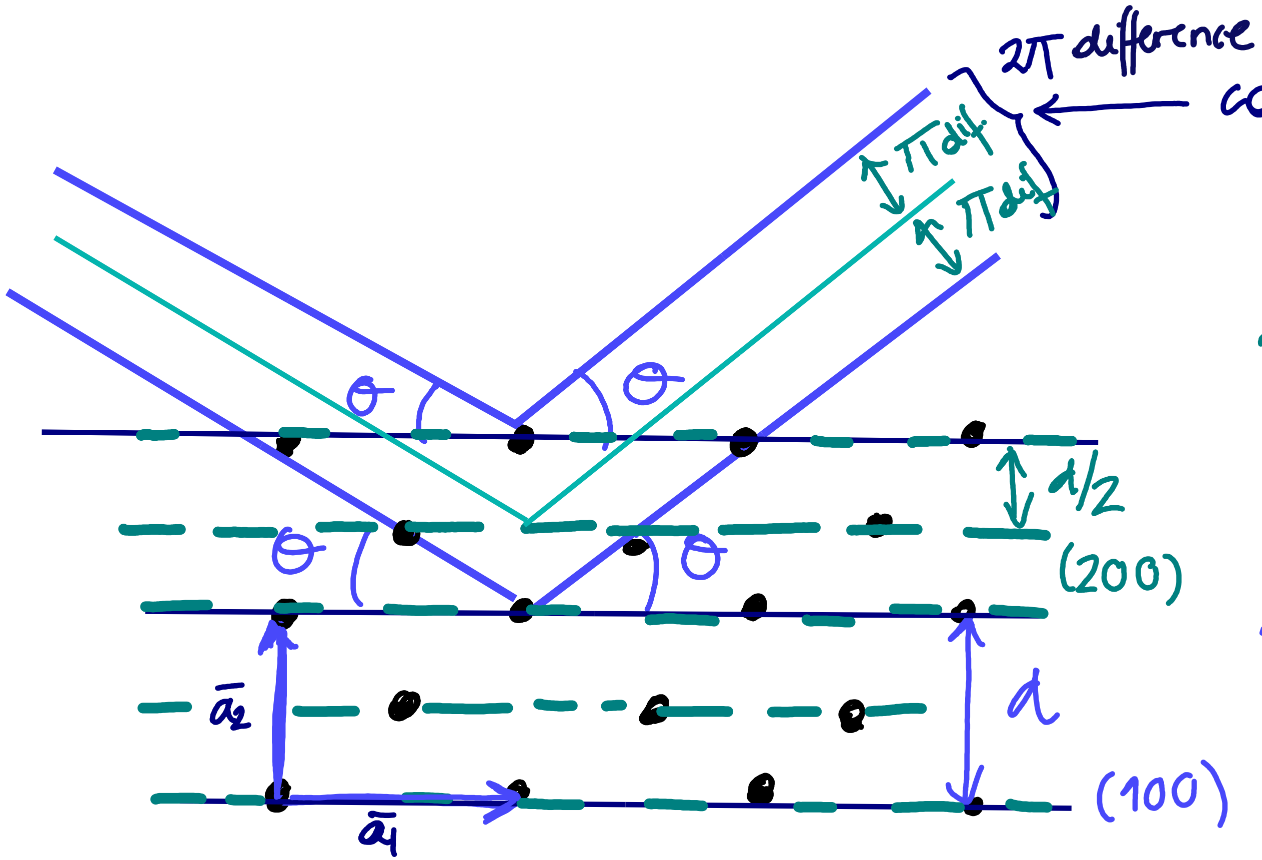
For a BCC $\begin{cases} S = 0 & h+K+l = \text{odd integer} \\ S = 2f & h+K+l = \text{even "} \end{cases}$

| | | |
|---|---|---|
| (100) | $h+K+l = 1$ | $\Rightarrow S_{100} = 0$ |
| (200) | " $= 2$ | $\Rightarrow S_{200} = 2f$ |
| (111) | " $= 3$ | $\Rightarrow S_{111} = 0$ |
| (110) | $= 2$ | $\Rightarrow S_{110} = 2f$ |
| (101) | $= 2$ | $\Rightarrow S_{101} = 2f$ |



# Geometric interpretation of the selection rules

we work with orthogonal axis cell instead of a more complex non orthogonal ⇒ some Miller indices do not correspond to families of planes



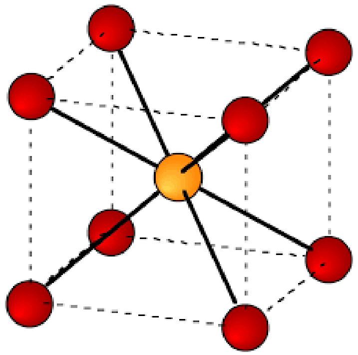

constructive interference expected for the simple cubic (100)

BCC : additional plane at $\frac{1}{2}a$

⇒ it causes destructive interference

⇒ (100) is absent in bcc

# Structure factor for CsCl



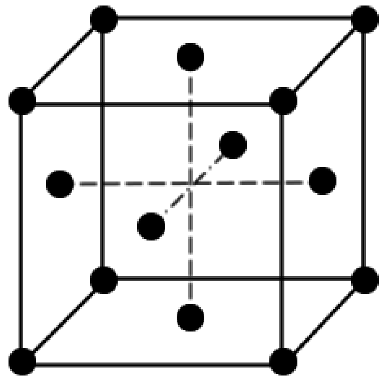
$$\text{simple cubic} + \begin{cases} Cs & [0,0,0] \\ Cl & [\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}] \end{cases}$$

$$S_{hkl} = \sum_j e^{-i2\pi(hx_j+ky_j+lz_j)} \cdot f_j =$$

$$= f_{Cs} + f_{Cl}\, e^{-i\pi(h+k+l)} =$$

$$= f_{Cs} + f_{Cl}\,(-1)^{h+k+l}$$

## Structure factor for a monoatomic fcc



F (Face)

$$\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$$

atoms basis

$$@\ \bar{r}_j = x_j\bar{a}_1 + y_j\bar{a}_2 + z_j\bar{a}_3$$

simple cubic with 4 atoms basis

$$\begin{array}{ccc} x_1 & y_1 & z_1 \\ (0, & 0, & 0) \end{array} , \quad \begin{array}{ccc} x_2 & y_2 & z_2 \\ (\tfrac{1}{2}, & \tfrac{1}{2}, & 0) \end{array}$$

$$(\tfrac{1}{2}, 0, \tfrac{1}{2}), \quad (0, \tfrac{1}{2}, \tfrac{1}{2})$$

$$S_{hkl} = \sum_j e^{-i2\pi(hx_j + ky_j + lz_j)} \cdot f_j$$

$$S_{hkl} = f \cdot \Big(1 + \underbrace{e^{-i\pi(h+k)}}_{\pm 1} + \underbrace{e^{-i\pi(h+l)}}_{\pm 1} + \underbrace{e^{-i\pi(k+l)}}_{\pm 1}\Big)$$

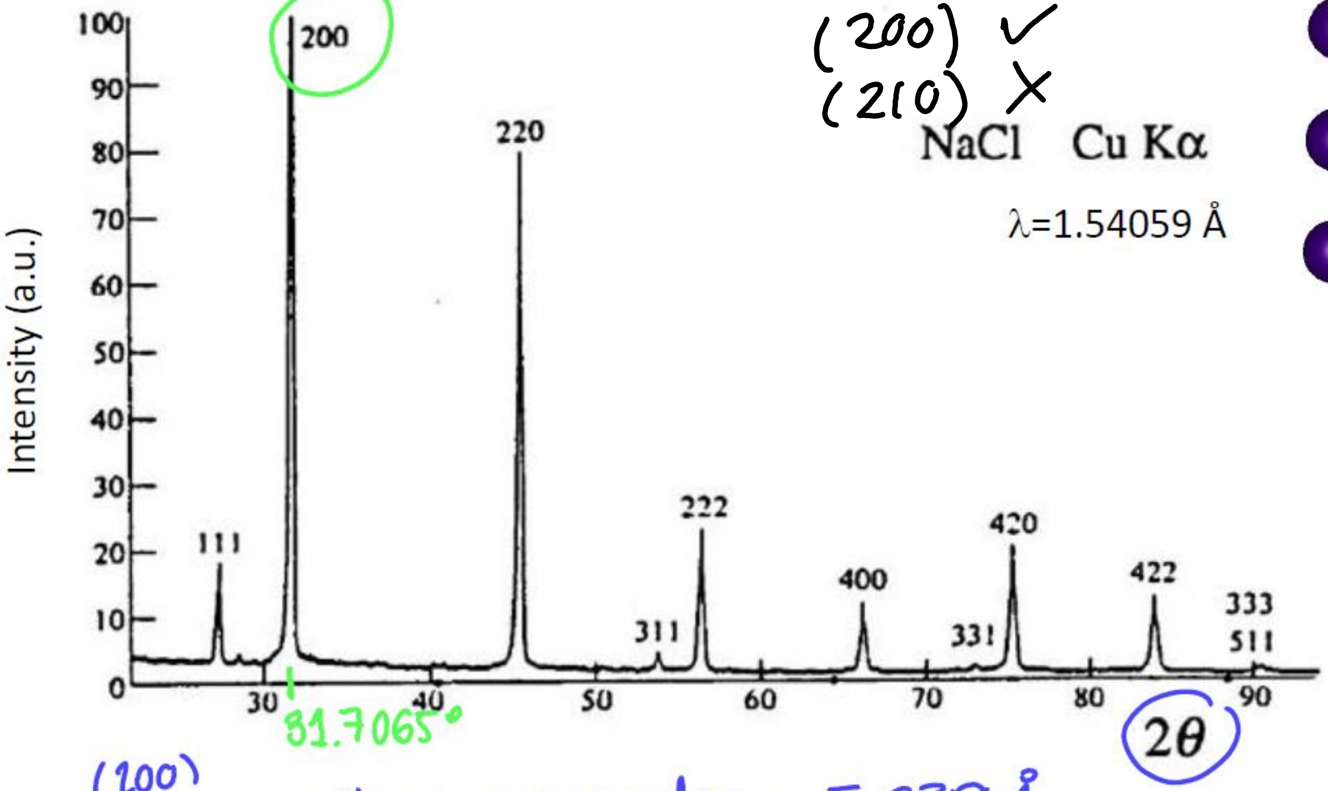
For FCC $\quad S_{hkl} \neq 0$ only if all $h, k, l$ are odd
all $hkl$ are even

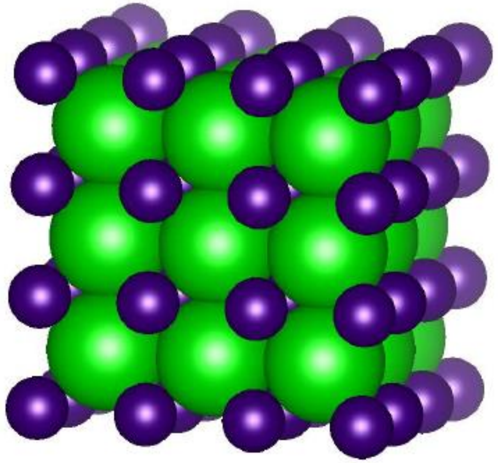
FCS $S_{hkl} \neq 0$ except if h, k, l are all odd or all even

## Previous class

Determine the lattice parameter for NaCl

(100) ✗
(110) ✗
(111) ✓
(200) ✓
(210) ✗



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

$$d = \frac{n\lambda}{2\sin\theta} \xrightarrow[n=2]{(200)} \text{lattice parameter} = 5.639\ \text{Å}$$

# Systematic absences of scattering

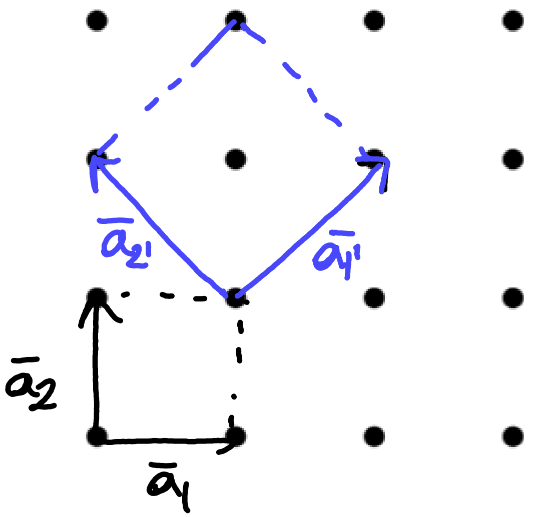
"Selection Rules" : which peaks <u>must</u> be absent for a given Lattice

(other peaks can vanish due to the details of the basis)

| Crystal structure | Condition for peak to occur |
|---|---|
| Simple cubic | All h, k, l allowed |
| bcc | $h + k + l$ must be even |
| fcc | $h, k, l$ must be all odd or all even |

$$S_{hkl} = S^{\text{Lattice}}_{(hkl)} \times S^{\text{Basis}}_{(hkl)} \longrightarrow \text{see exercices}$$

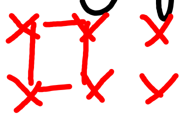
# Does the arbitrary choice of lattice vectors influence the reciprocal lattice and the diffraction pattern?



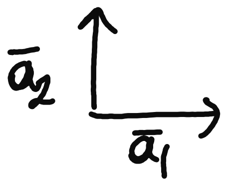

Real lattice: 2 ≠ sets of lattice vector chosen ($\bar{a}_1/\bar{a}_2$ ; $\bar{a}_1'/\bar{a}_2'$)

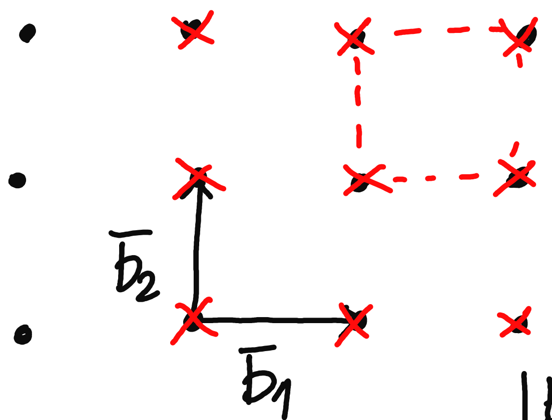
⇓

Same diffraction pattern independently of the choice



## Primitive Square




$S = f_0$ for all $hkl$

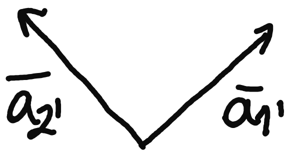
Real lattice

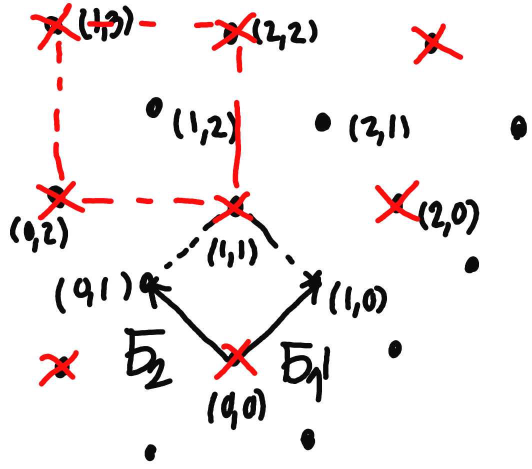
$|a_1| < |a_1'|$

Recipr. Latt.

$|b_1| > |b_1'|$

## Centered Square



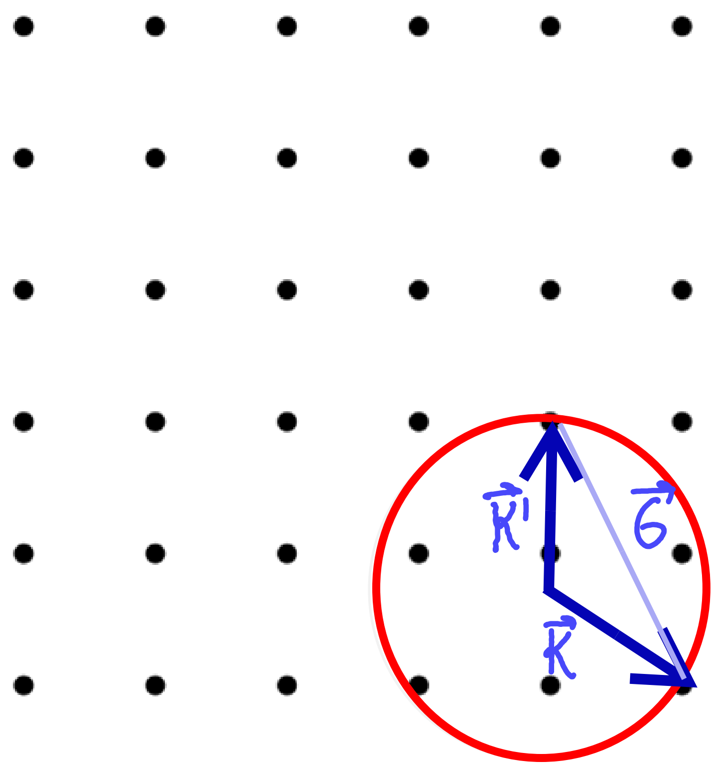

$S = 2f_0$ for $h+k+\ell$ = even

$S = 0$ for $h+k+\ell$ = odd

X diffraction max.

# Methods of Scattering experiments

Ewald construction for diffraction

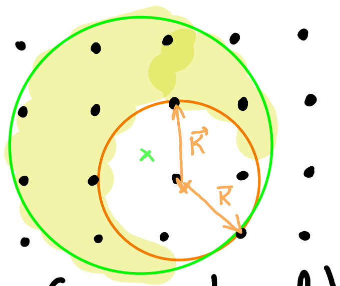



R.L.

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

Diffraction condition $\Delta\vec{K} = \vec{G}$

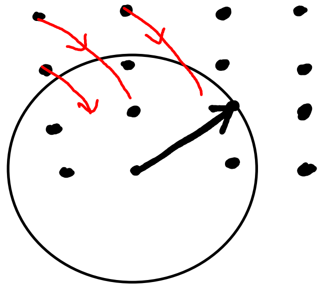
$\Rightarrow$ Probability to obtain a diffraction spot is low



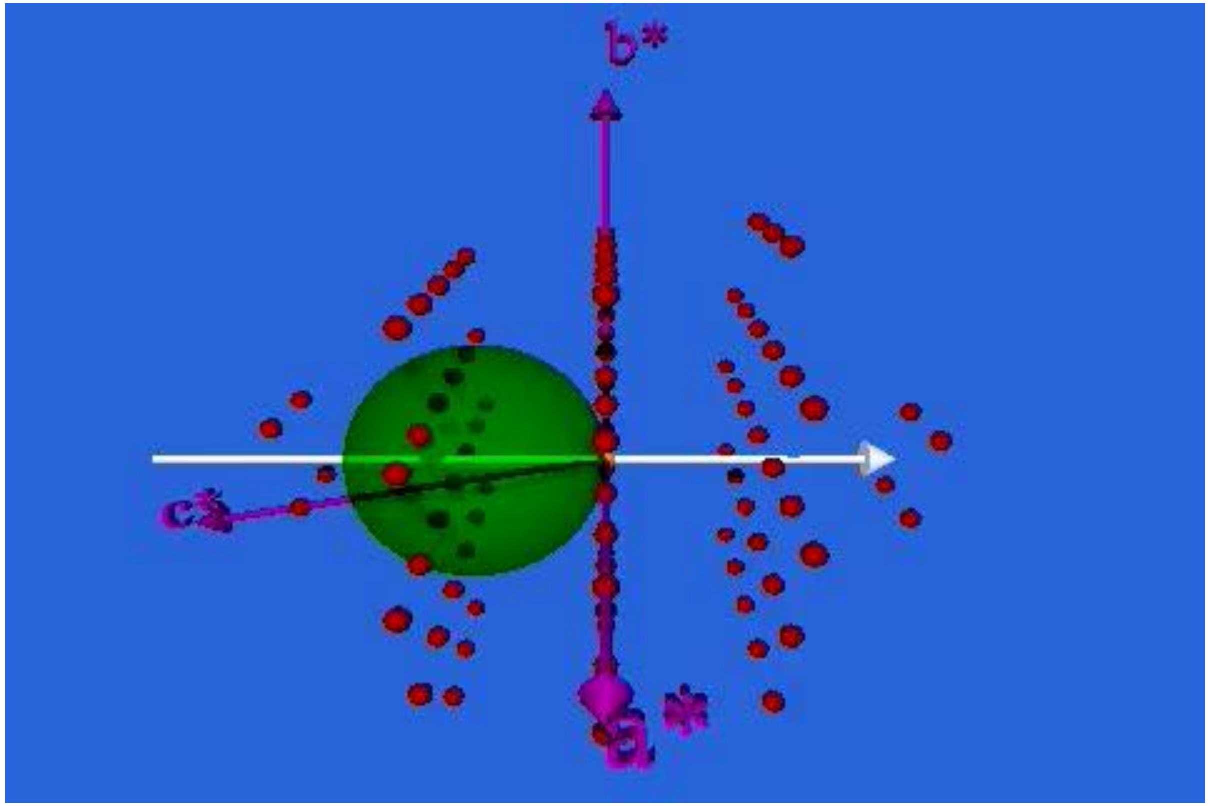
Methods

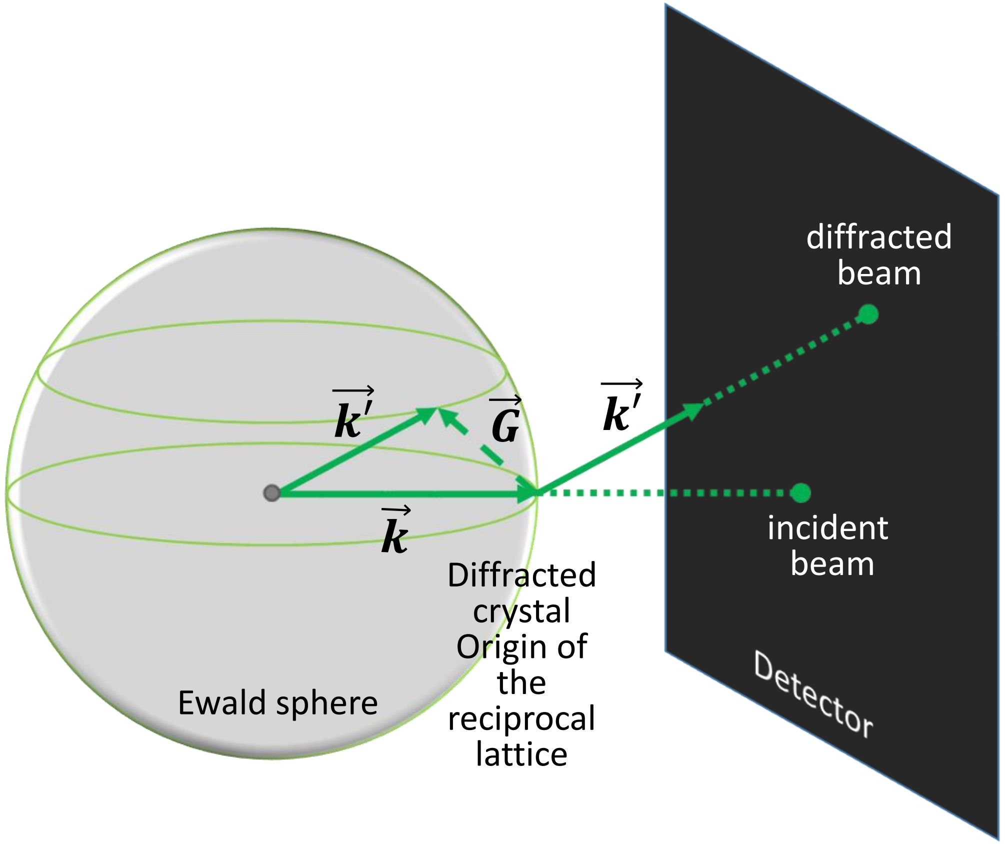
* Laue Method (range of $\lambda$ instead of a monochromatic incident wave)

* Rotating Crystal Method



# Ewald sphere

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