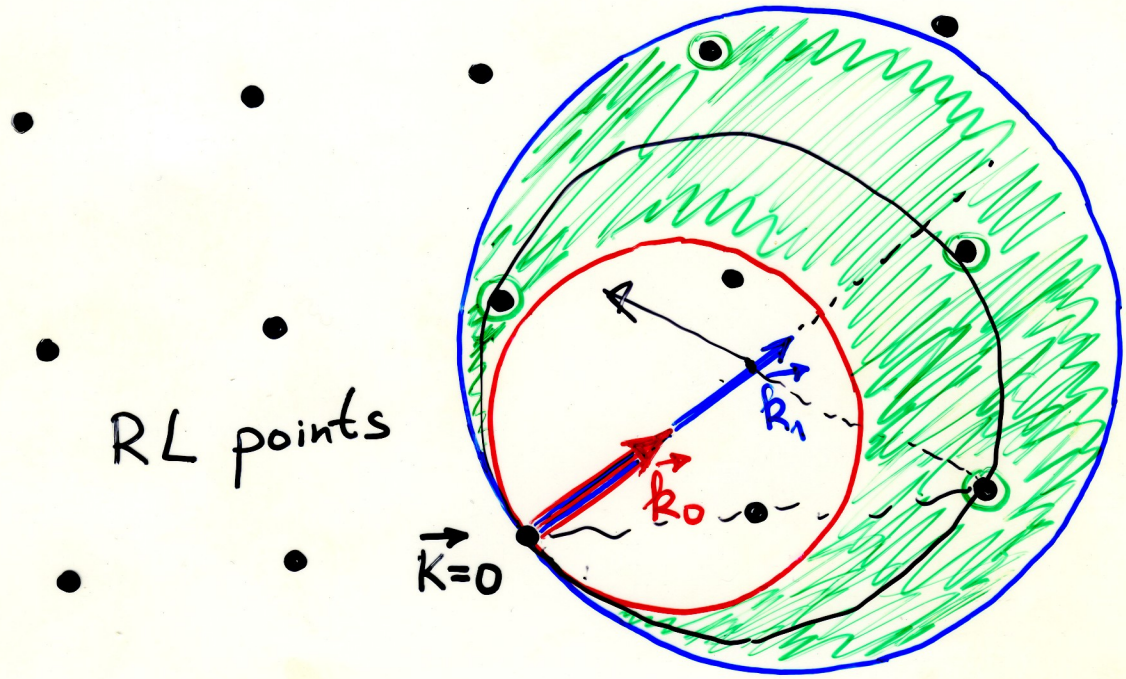
The Laue Method

- direction of incidence $\vec{k}/|\vec{k}|$ fixed
- $|\vec{k}|$ in some finite interval: $k_0 < |\vec{k}| < k_1$ (non-monochromatic X-rays)
- one crystal

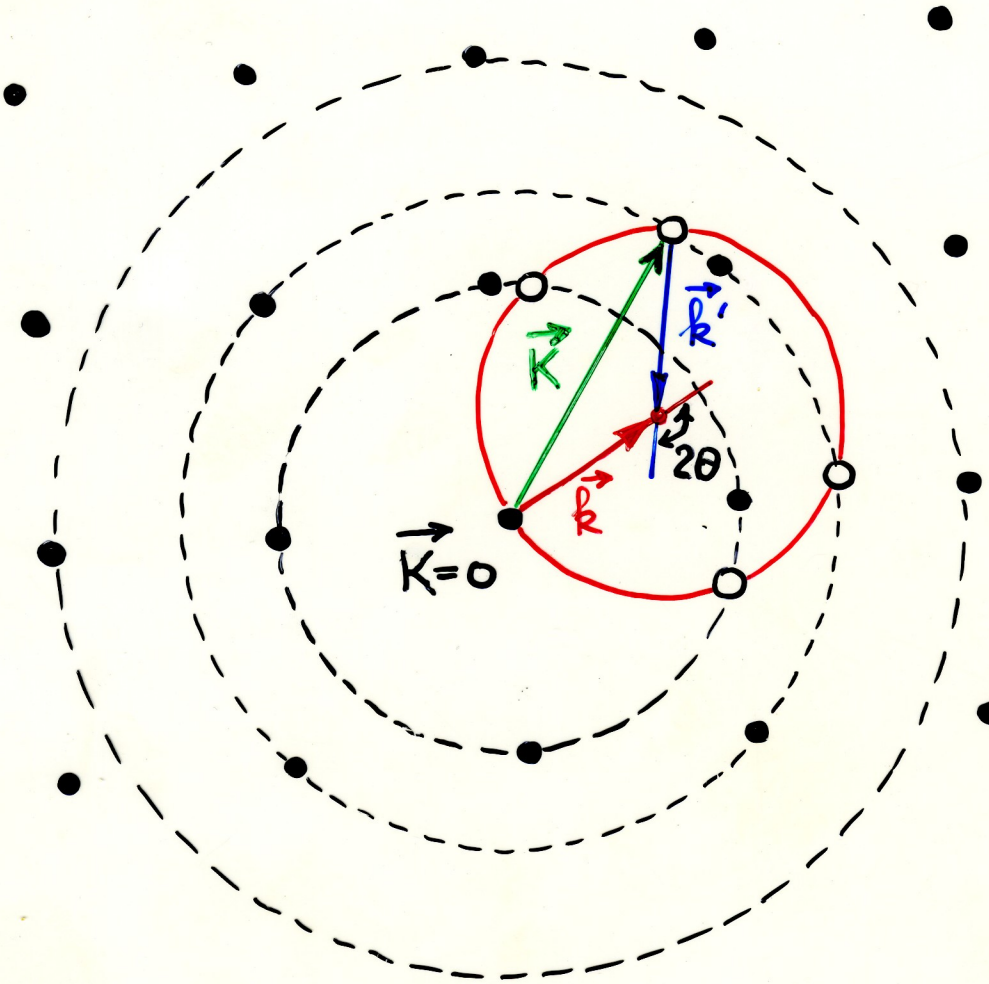


All reciprocal lattice points within the shaded area (here 4 ⊙) give Bragg peaks

Rotating Crystal Method

- incident $\vec{k}$ fixed
- one crystal

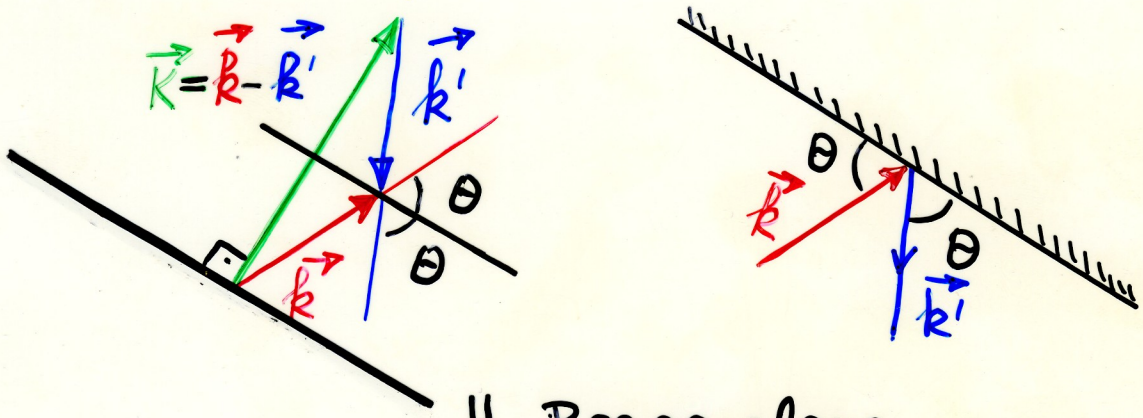
RL rotates



Laue

$\vec{K}=\vec{k}-\vec{k}' \in RL$

several (here 4) Bragg peaks. One is shown



|| Bragg plane

The Powder or DeBye-Scherer Method

- polycrystalline sample or powder used
- incident $\vec{k}$ fixed (monochromatic X-rays)

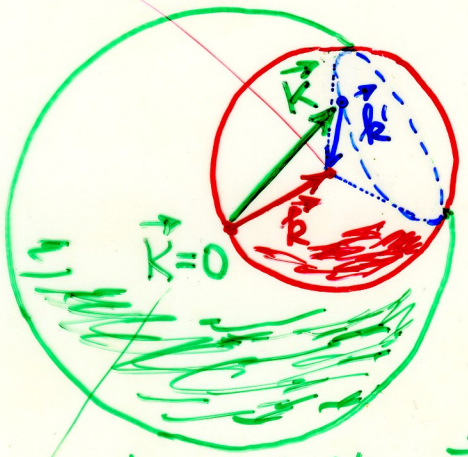
equivalent to a rotating crystal method;
+ axis of rotation is varied over all possible orientations

⇒ RL rotates thru all possible angles about the origin $\vec{K}=0$

⇒ each $\vec{K}$ generates a sphere of radius $|\vec{k}|$

but the Ewald sphere is fixed!

center of the Ewald sphere

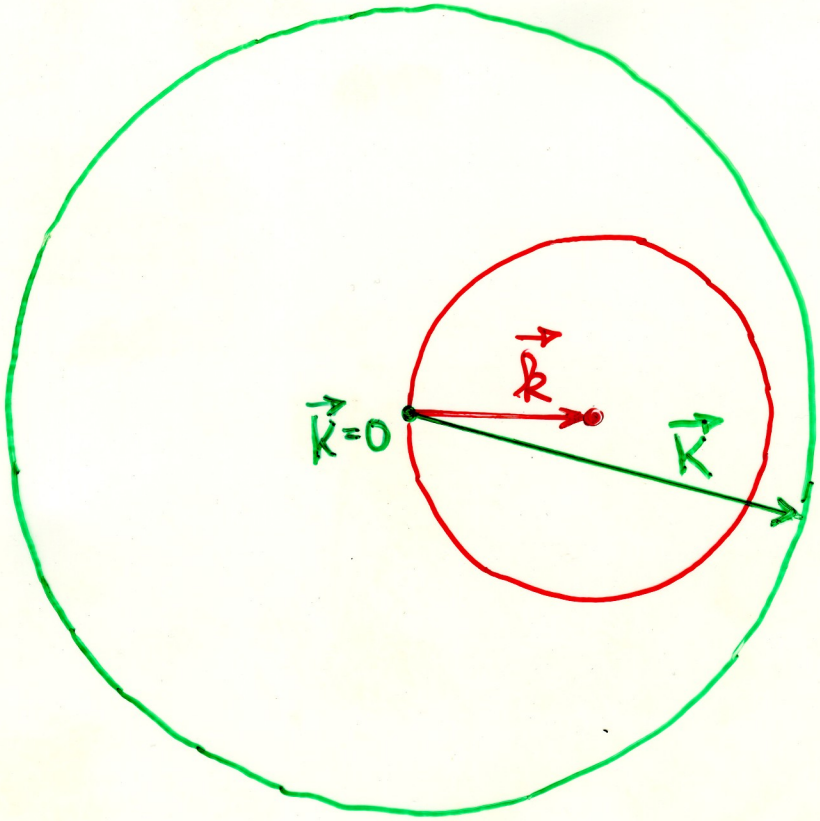


A cone of radiation is formed

center of the $\vec{k}$-sphere
one point on the surface of the Ewald sphere

$\vec{K}$- and $\vec{k}$- spheres intercept: $|\vec{K}| \leq 2|\vec{k}|$
(circle ⬭)

Cross-section of $\vec{K}$- and Ewald spheres



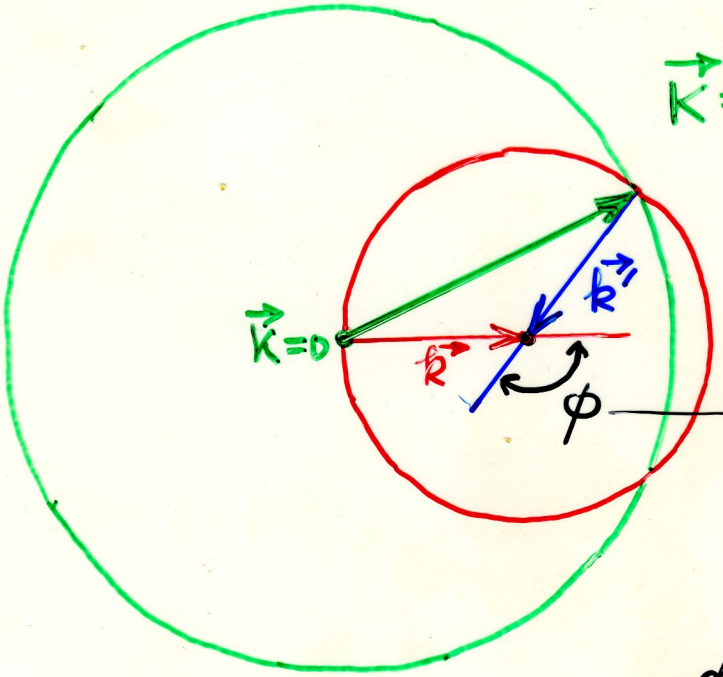
$|\vec{K}| > 2|\vec{k}|$

No Bragg peaks

$|\vec{K}| \leq 2|\vec{k}|$

Laue is satisfied:

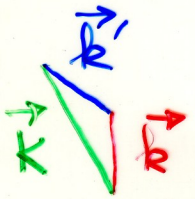
$\vec{K} = \vec{k} - \vec{k}' \in RL$



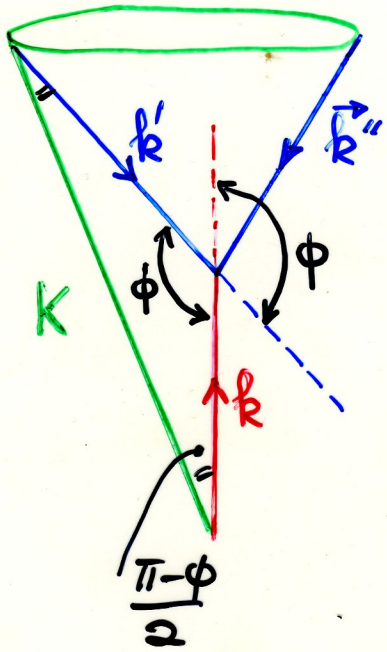
angle between incident and scattered radiation

$\phi = \hat{\vec{k}, \vec{k}'}$

$|\vec{k}'| = |\vec{k}|$



isosceles

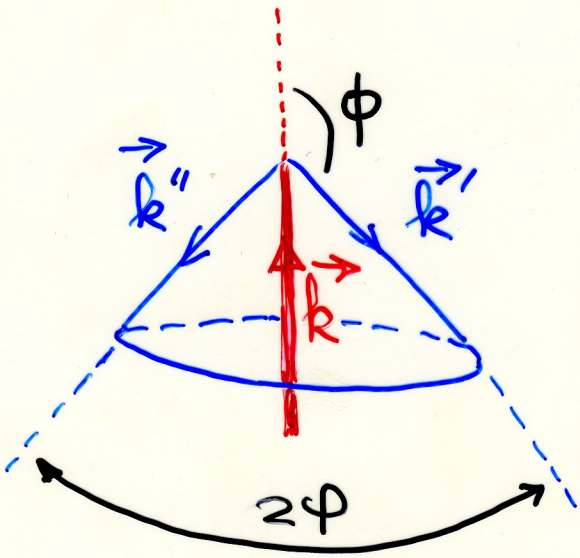


$k \cdot \cos\frac{\pi-\phi}{2} = \frac{1}{2}K$

$k \cdot \sin\frac{\phi}{2} = \frac{1}{2}K$

$$\sin\frac{\phi}{2} = \frac{K}{2k} \leq 1 \quad \checkmark$$

The cone of radiation



$\varphi = \pi - \phi$

As $k \to \frac{K}{2}$
(gets smaller)

$\phi \to \pi$

$\varphi \to 0$

Backscattering

Monatomic lattice with a Basis.

Laue condition for constructive interference:

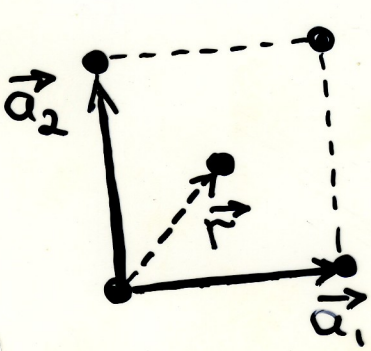
$$\vec{R}\cdot(\vec{k}-\vec{k}') = 2\pi m \quad \text{or} \quad e^{i(\vec{k}'-\vec{k})\cdot\vec{R}} = 1$$

($\vec{k}$: incident, $\vec{k}'$: scattered)

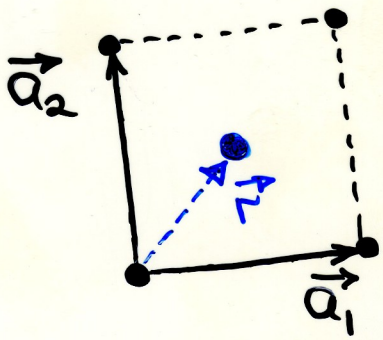
for all BL vectors $\vec{R} = \sum_{i=1}^{3} n_i \vec{a}_i$.

This is for just one (atom / ion) scatterer per unit cell.

How must the Laue condition be modified for a lattice with a Basis?



(Real space)



I. Monatomic (identical scatterers)

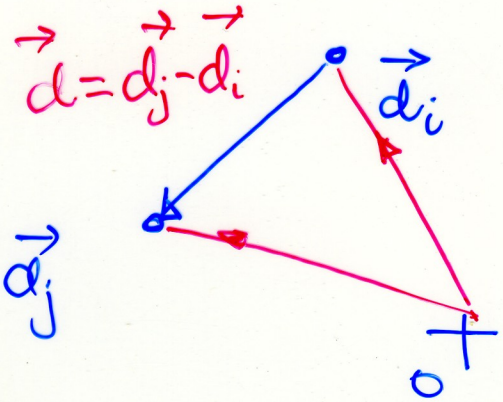
II. Not identical scatterers

$$S_{\vec{K}} = \sum_{j=1}^{n} e^{i\vec{K}\cdot\vec{d}_j}$$ **Geometric Structure Factor**

Several atoms (≡ scatterers) in a primitive cell. at positions

$\vec{d}_1, \vec{d}_2, \ldots : \{\vec{d}_j\}$ $j = 1, \ldots, n$

rays scattered by the atoms interfere. **Path difference?**



$\vec{d} \cdot (\vec{k} - \vec{k}')$

Bragg peak occurs for $\vec{k} - \vec{k}' = \vec{K}$

Path difference = $\vec{d} \cdot \vec{K}$

Phase difference:

$$e^{i\vec{K}\cdot\vec{d}} = e^{i\vec{K}\cdot(\vec{d}_j - \vec{d}_i)}$$

Thus the phases of the rays scattered by atoms at $\vec{d}_1, \ldots \vec{d}_n$ are in the ratios $e^{i\vec{K}\cdot\vec{d}_1}, e^{i\vec{K}\cdot\vec{d}_2}, \ldots$

BCC as Simple Cubic with a Basis

① a two-point basis: $\vec{d}_1 = 0 \quad \vec{d}_2 = \frac{1}{2}a(\hat{x}+\hat{y}+\hat{z})$

② Structure factor

$$S_{\vec{K}} = 1 + \exp\left(i\vec{K}\cdot\frac{1}{2}a(\hat{x}+\hat{y}+\hat{z})\right)$$

③ RL vectors (for Simple Cubic!) $\vec{b}_i = \frac{2\pi}{a}\cdot\hat{x}_i$

$$\vec{K} = \frac{2\pi}{a}\left(n_1\hat{x} + n_2\hat{y} + n_3\hat{z}\right)$$

we get $S_{\vec{K}} = 1 + \exp\left(i\pi(n_1+n_2+n_3)\right)$

or $S_{\vec{K}} = 1 + (-1)^{n_1+n_2+n_3}$

$$S_{\vec{K}} = \begin{cases} 2, & n_1+n_2+n_3 = 2p \quad [\text{even}] \\ 0, & n_1+n_2+n_3 = 2p+1 \quad [\text{odd}] \end{cases}$$

Scattering by RL vectors $(\vec{k}'-\vec{k}=\vec{K})$

with $\sum_{i=1}^{3} n_i = 2p$ gives the doubled contribution,

with $\sum_{i=1}^{3} n_i = 2p+1$ vanishes.

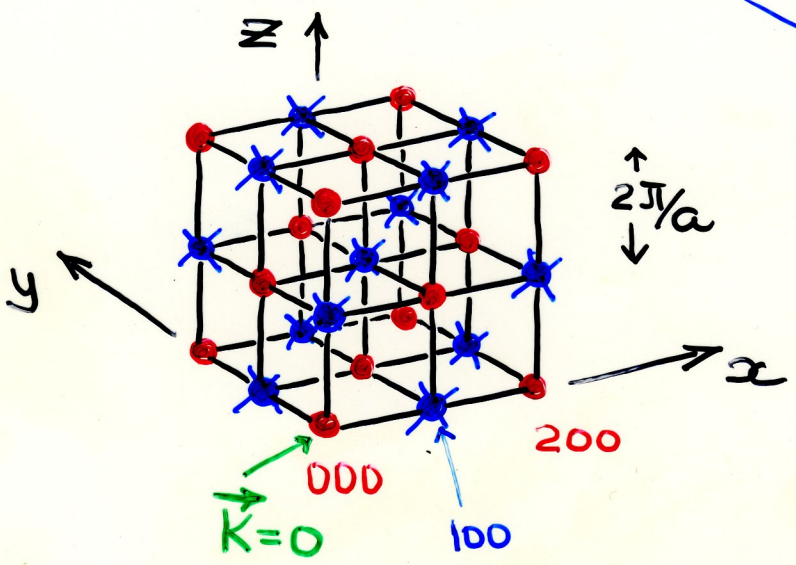
How to interprete?

Reciprocal lattice: simple cubic.

Count $n_1+n_2+n_3$ — even, odd

even
• $S_K=2$

odd
× $S_K=0$



Only "even" (red) points give contribution.

They form FCC lattice,

which is a reciprocal lattice for Bcc.

Period of FCC $= \frac{4\pi}{a}$,

as it should be.

Monatomic Diamond Lattice

① BL lattice is FCC with a two-point basis: $\vec{d}_1 = 0 \quad \vec{d}_2 = \frac{1}{4}a(\hat{x}+\hat{y}+\hat{z})$

② RL is BCC with primitive vectors

$$\vec{b}_1 = \frac{4\pi}{a}\cdot\frac{1}{2}(\hat{y}+\hat{z}-\hat{x})$$

$$\vec{b}_2 = \frac{4\pi}{a}\cdot\frac{1}{2}(\hat{z}+\hat{x}-\hat{y})$$

$$\vec{b}_3 = \frac{4\pi}{a}\cdot\frac{1}{2}(\hat{x}+\hat{y}-\hat{z})$$

③ Structure factor

$$S_{\vec{K}} = \sum_{j=1,2} \exp\left\{ i\,\vec{K}\cdot\vec{d}_j \right\}, \quad \vec{K} = \sum_{i=1}^{3} n_i \vec{b}_i$$

Calculations yield

$$S_{\vec{K}} = 1 + \exp\left\{ i\frac{\pi}{2}\cdot[n_1+n_2+n_3] \right\} = 1+(i)^{n_1+n_2+n_3}$$

$$S_{\vec{K}} = \begin{cases} 2, & n_1+n_2+n_3 = 2\cdot 2p \\ 1+i\cdot(-1)^p, & n_1+n_2+n_3 = 2p+1 \\ \phi, & n_1+n_2+n_3 = 2\cdot(2p+1) \end{cases} \qquad p = 0, \pm 1, \pm 2, \pm 3, \ldots$$

Geometric interpretation?

Polyatomic crystals

How to account for different scatterers in a unit cell?

$\Downarrow$

atomic form factors, $f_j(\vec{K})$

$f_j(\vec{K})$ is determined by the electron internal structure of the atom (ion...) of sort j:

The total structure factor

$$S_{\vec{K}} = \sum_j f_j(\vec{K}) \exp(i\vec{K}\cdot\vec{d}_j)$$

$$f_j(\vec{K}) = -\frac{1}{e}\int d^3r\, e^{i\vec{K}\cdot\vec{r}}\, \rho_j(\vec{r})$$

$\rho_j(\vec{r})$: electron density in real space

Example: Diamond → zincblende (GaAs,...) and $S_{\vec{K}}$ does not vanish