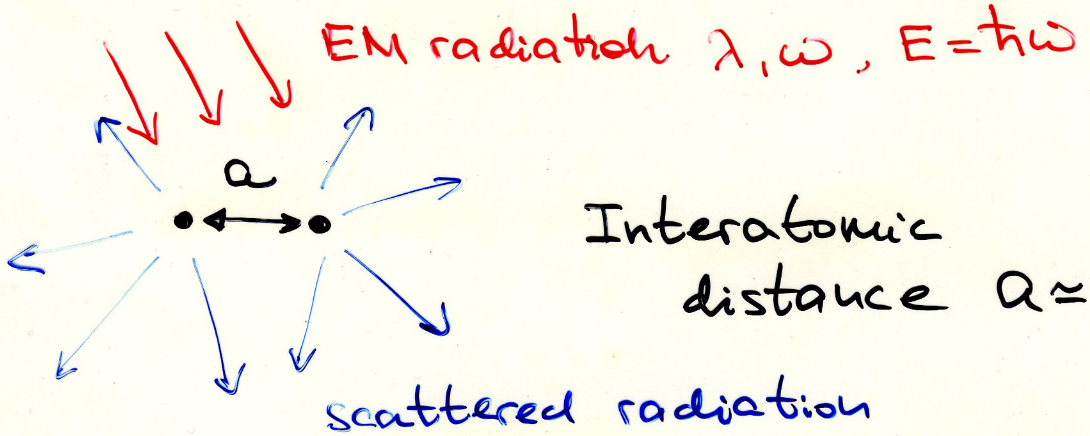
X-ray diffraction $\Longleftrightarrow$ Crystal structures



Interatomic distance $a \simeq 1\,\mathring{A} = 10^{-8}\,cm$

To resolve structures $\sim a$ $\quad \lambda \lesssim a$

Frequency $\nu = \frac{1}{T} = \frac{c}{\lambda} \simeq \frac{3\times 10^{10}\,cm/sec}{10^{-8}\,cm} = 3\times 10^{18}\,Hz$

Energy $h\nu = 6.62\times 10^{-27}\,erg\cdot sec \cdot 3\times 10^{18}\,sec^{-1}$

$h\nu \approx 2\times 10^{-8}\,erg \simeq 1.2\times 10^{4}\,eV$

$1\,erg = 6.2\times 10^{11}\,eV$ $\qquad$ X-rays

X-rays discovered by Röntgen 1895

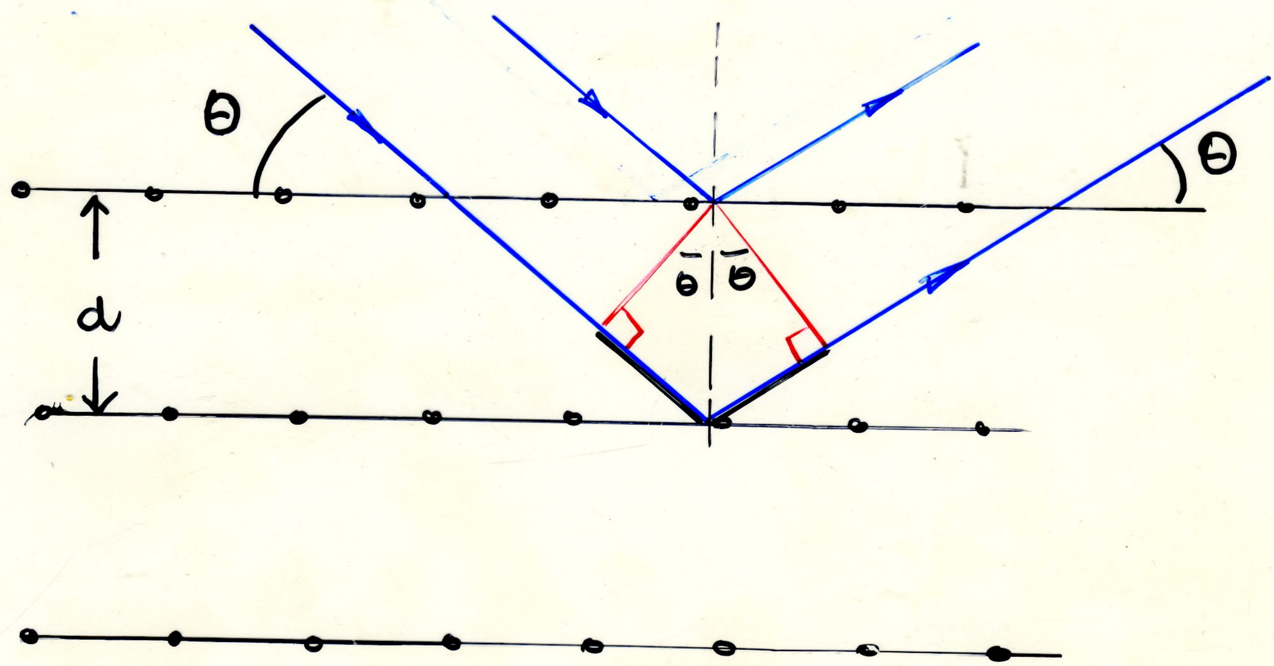
Used for studying periodic crystal structures W.H. Bragg & W.L. Bragg 1913

Bragg formulation

- crystal as a set of parallel equidistant planes
- X-rays are specularly reflected by (atoms, ions in) each plane
- reflections from different planes interfere

To have sharp peaks in reflection:

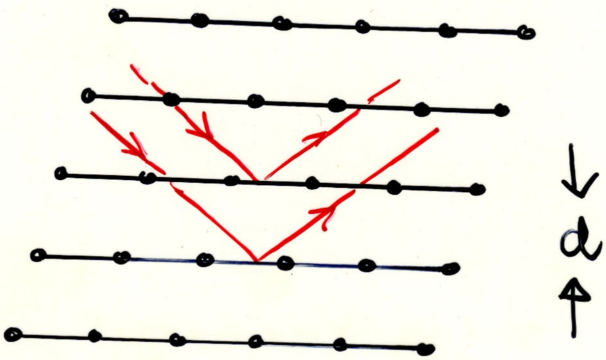
constructive interference in certain directions



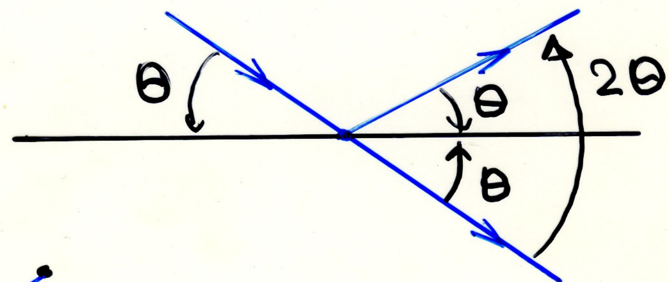
$$2d \sin\Theta = n\lambda$$ Bragg condition

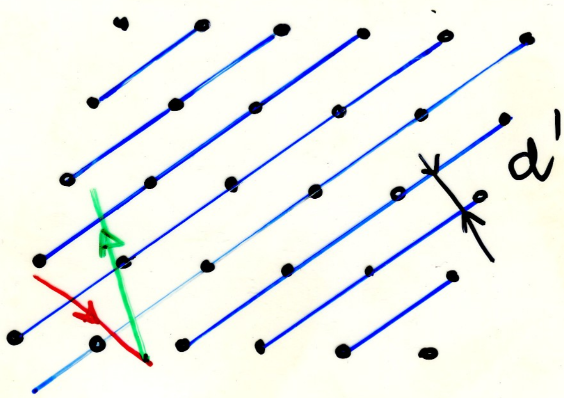
① integer $n = 1, 2, \ldots$ (called order of reflection)

②



Specular reflection





Other choice of crystal planes may produce another reflections for the same incident angle and fixed λ

③ "White" radiation (non-monochromatic)

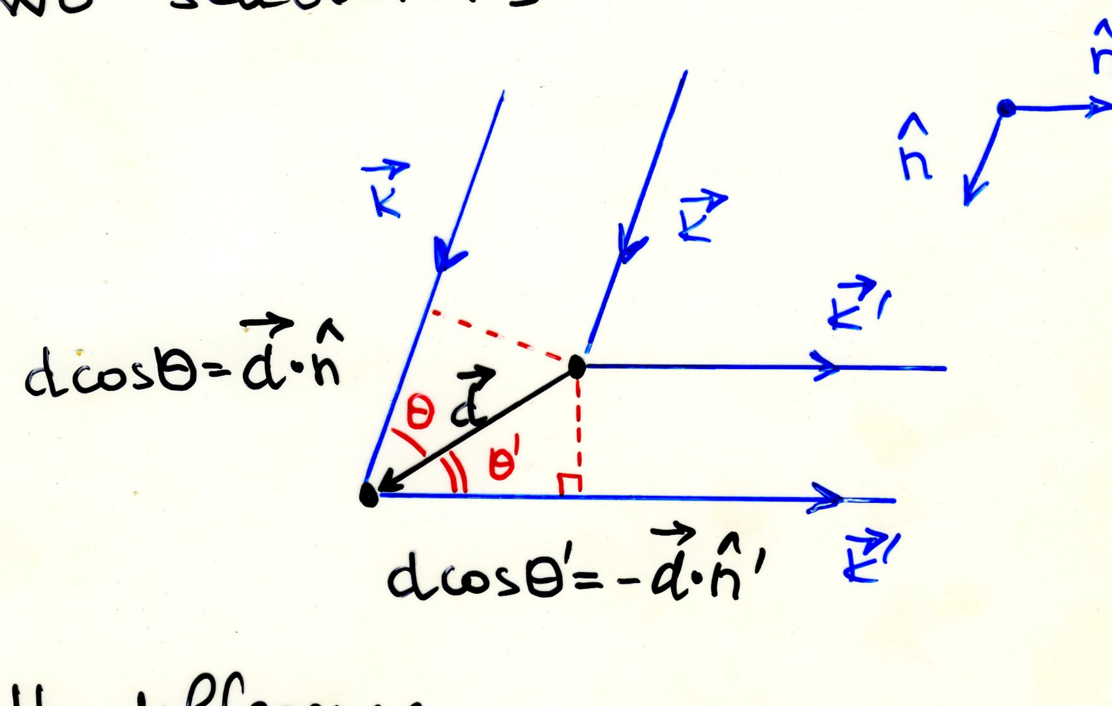
different energies $\Rightarrow$ different λ

$\Rightarrow$ constructive interference at various Θ

Von Laue formulation

- crystal as a set of identical microscopic scatterers (atoms, ions) placed at sites $\vec{R}$ of a BL
- Each scatters radiation in all directions
- Sharp peaks: in directions and wavelengths for which rays interfere constructively

Two scatterers



Path difference

$$d\cos\theta + d\cos\theta' = \vec{d}\cdot(\hat{n}-\hat{n}')$$

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

For constructive interference

$$\vec{d}\cdot(\hat{n}-\hat{n}') = m\lambda \qquad m = 1, 2, \dots$$

or (mult. by $2\pi/\lambda$)

(*) $$\boxed{\vec{d}\cdot(\vec{k}-\vec{k}') = 2\pi m}$$ for a <u>pair</u> of atoms

For ∞ number of atoms in a BL?

(*) be satisfied simultaneously
for <u>all</u> $\vec{d}$'s that are BL vectors $\vec{R}$

$$\vec{d} \dashrightarrow \vec{R} :$$

$$\vec{R}\cdot(\vec{k}-\vec{k}') = 2\pi m$$

let $\Delta\vec{K} = \vec{k}-\vec{k}' = -\vec{K}$ change in the wave vector

$$\boxed{\vec{R}\cdot\vec{K} = 2\pi m} \qquad \forall\, \vec{R}\in BL$$

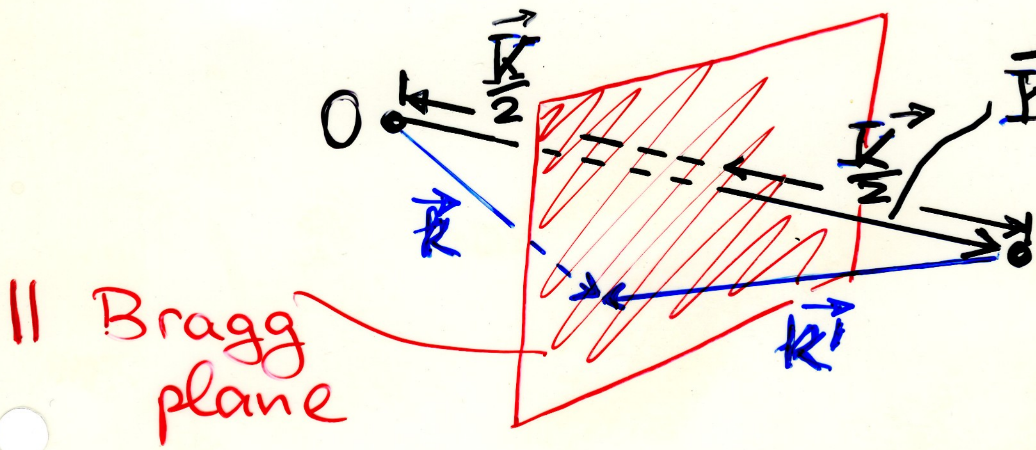
Equivalent form $\exp(i\,\vec{K}\cdot\vec{R}) = 1$

$\vec{K}$ is a RL vector!

Laue Condition

In terms of incident wave vector

$$\boxed{\vec{k}\cdot\frac{\vec{K}}{|\vec{K}|}=\frac{1}{2}K}$$



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

or

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

$$\vec{k}'^2=\vec{k}^2-2\vec{k}\cdot\vec{K}+\vec{K}^2$$

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

Incident wave vector $\vec{k}$ will satisfy Laue Condition if and only if the tip of $\vec{k}$ lies in a plane that is a $\perp$ Bisector of some RL vector $\vec{K}$

Equiv. of Bragg and von Laue Formulations

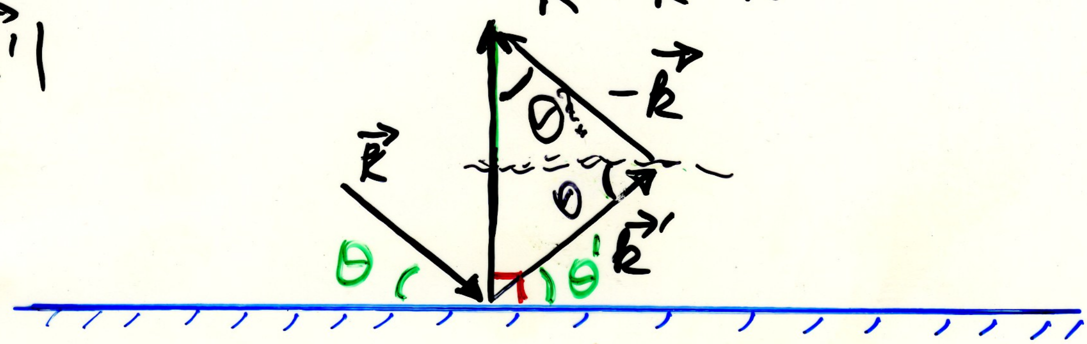
$$\vec{K} = \vec{k}' - \vec{k}$$

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

elastic

$\Downarrow$

$\theta = \theta'$



$\vec{K} \perp$ to the plane

$\vec{K}$ is a RL vector $\boxed{\vec{K} = n\vec{K}_0}$

$\vec{K}_0$ shortest RL vector

$\vec{K}_0$ determines a family of crystal planes $\hat{n} = \frac{\vec{K}_0}{|\vec{K}_0|} = \frac{\vec{K}}{|\vec{K}|}$

$$d = \frac{2\pi}{|\vec{K}_0|}$$

$$|\vec{K}| = n|\vec{K}_0| = \frac{2\pi n}{d}$$

$$|\vec{K}| = 2k\sin\theta$$

$$k\sin\theta = \frac{\pi n}{d} \qquad k = \frac{2\pi}{\lambda}$$

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

Bragg condition

Laue diffraction peak:
change in the wave vector $\vec{k}' - \vec{k} = \vec{K} \in R$

$\Updownarrow$

Bragg diffraction peak:
a family of crystal planes

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

$\vec{K} = n\,\vec{K}_0$

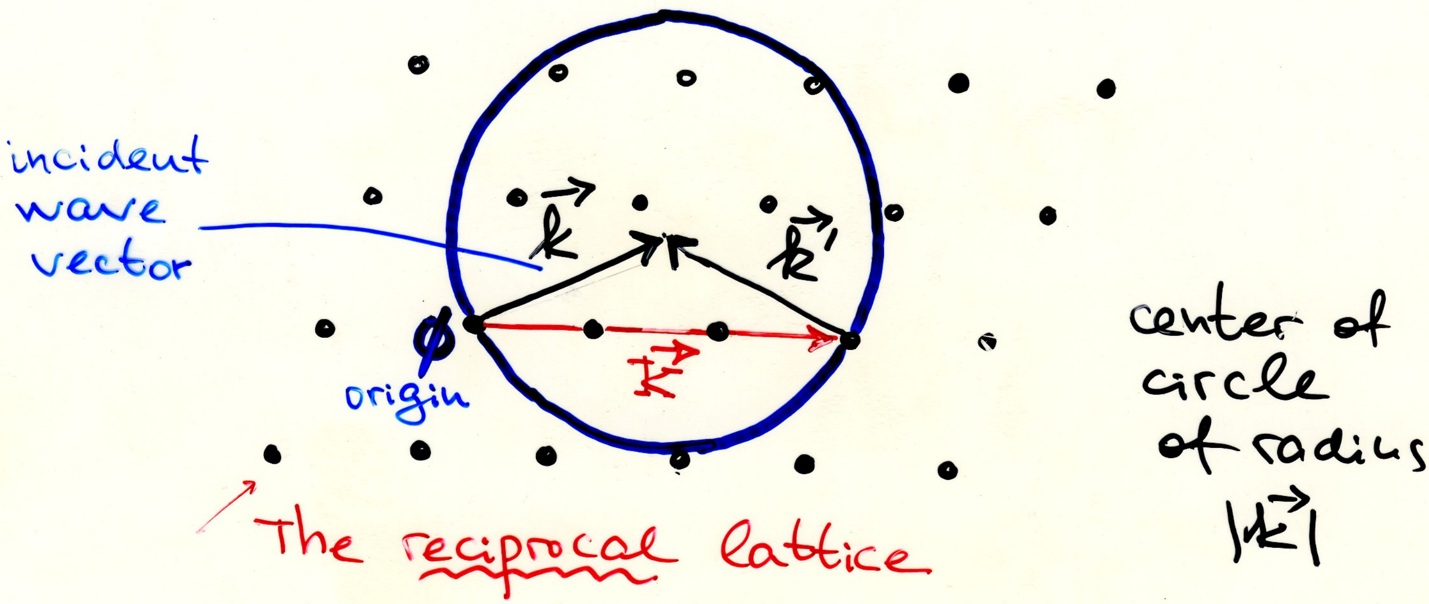
gives the order of reflection

$\vec{K}_0$ is the shortest RL in a given direction

$$|\vec{K}_0| = \frac{2\pi}{d}$$

Much easier to work with RL $\vec{K}$ than to visualize various possible families of crystal planes

The Ewald Construction



Laue: $\vec{K} = \vec{k} - \vec{k}'$ must be a RL vector

For elastic scattering $|\vec{k}| = |\vec{k}'|$

some RL points must lie on the surface of the sphere

Generally, there are no points on a sphere when $\vec{k}$ is fixed.

① using $k_0 < |\vec{k}| < k_1$ with $\frac{\vec{k}}{|\vec{k}|} = \hat{n}$ fixed

② fix $|\vec{k}|$ use various directions $\hat{n}$