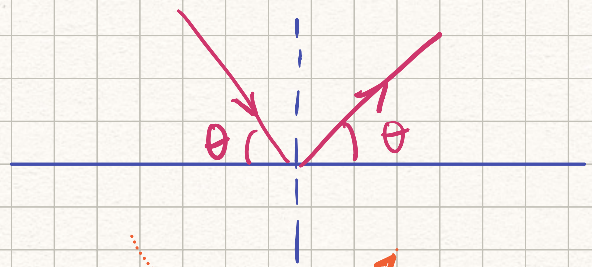
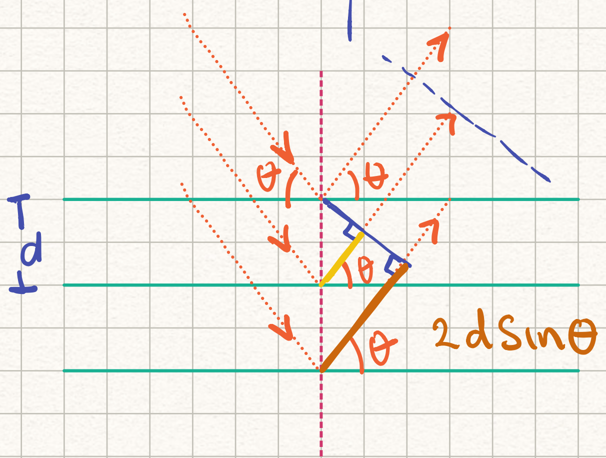
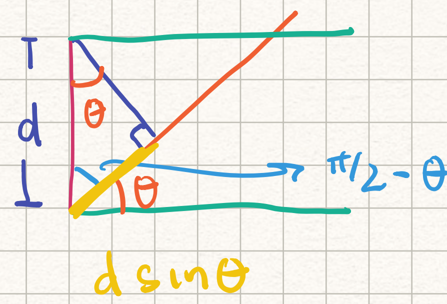
Bragg law and Diffraction Conditions



Lawrence Bragg



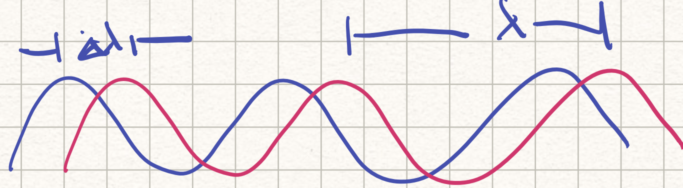


$\Delta\lambda_1 = 2d\sin\theta$

$\Delta\lambda_2 = 4d\sin\theta$

$\vdots$

$\Delta\lambda_m = 2md\sin\theta$



Interference

Const. interf. $\Delta\lambda = n\lambda$

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

n: order of diffraction

d: lattice constant

$\sin\theta \leq 1$

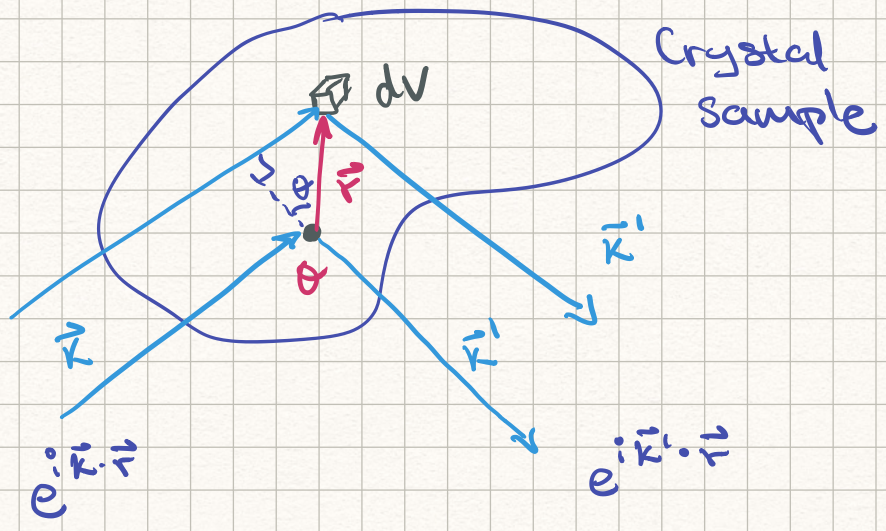
$n\lambda \leq 2d \Rightarrow \lambda \leq 2d$

Typically $d = 1\,\text{Å} = 10^{-10}\,m$

λ : x-rays

Micro waves

↳ what's d?



Change in phase of the wave is
$e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}$

F : Scattering amplitude

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

$\Delta\vec{k} = \vec{k} - \vec{k}'$ $\qquad \vec{k}' = \vec{k} + \Delta\vec{k}$

$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}$$

$$F = \int_V \sum_{\vec{G}} n_G\, e^{i\vec{G}\cdot\vec{r}}\, e^{-i\Delta\vec{k}\cdot\vec{r}}\, dV$$

$$= \sum_{\vec{G}} n_{\vec{G}} \int_V e^{i(\vec{G}-\Delta\vec{k})\cdot\vec{r}}\, dV$$

Particular case $\underline{\vec{G} = \Delta\vec{k}}$ $\qquad F = n_G V$

⇒ If the maximum of Scatt. $\Delta\vec{k} = \vec{G}$

$\Delta\vec{k} = \vec{k} - \vec{k}' = \vec{G}$

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

$\hbar\omega$: energy of incoming photon

$\omega = cK \qquad K = |\vec{K}|$

$\hbar\omega'$: energy of outcoming photon

$\omega' = cK' \qquad K' = |\vec{K}'|$

Scattering is ellastic : $\omega = \omega'$

$cK = cK' \Rightarrow K = K'$

$\vec{K}' = \vec{K} - \vec{G} \qquad \vec{K}' \cdot \vec{K}' = K'^2$

$(\vec{K} - \vec{G}) \cdot (\vec{K} - \vec{G}) = K'^2$

$$(\vec{K} - \vec{G}) \cdot (\vec{K} - \vec{G}) = K^2 - 2\vec{K} \cdot \vec{G} + G^2 = K'^2$$

$$K^2 - K'^2 + G^2 - 2\vec{K} \cdot \vec{G} = 0$$

$$G^2 - 2\vec{K} \cdot \vec{G} = 0$$

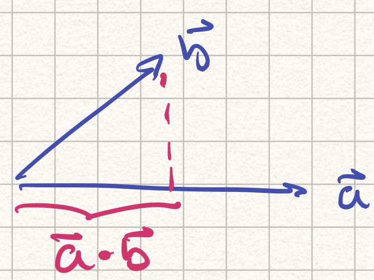
$$\boxed{G^2 = 2\vec{K} \cdot \vec{G}}$$

Analogous version of Bragg law

$$\frac{G^2}{4} = \frac{2\vec{K}}{2} \cdot \frac{\vec{G}}{2}$$

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

Dot product :



Find the Wigner-Seitz cell of the reciprocal space

Brillouin Zone : Wigner-Seitz cell of reciprocal space

contains all $\vec{K}$ that yield diffraction