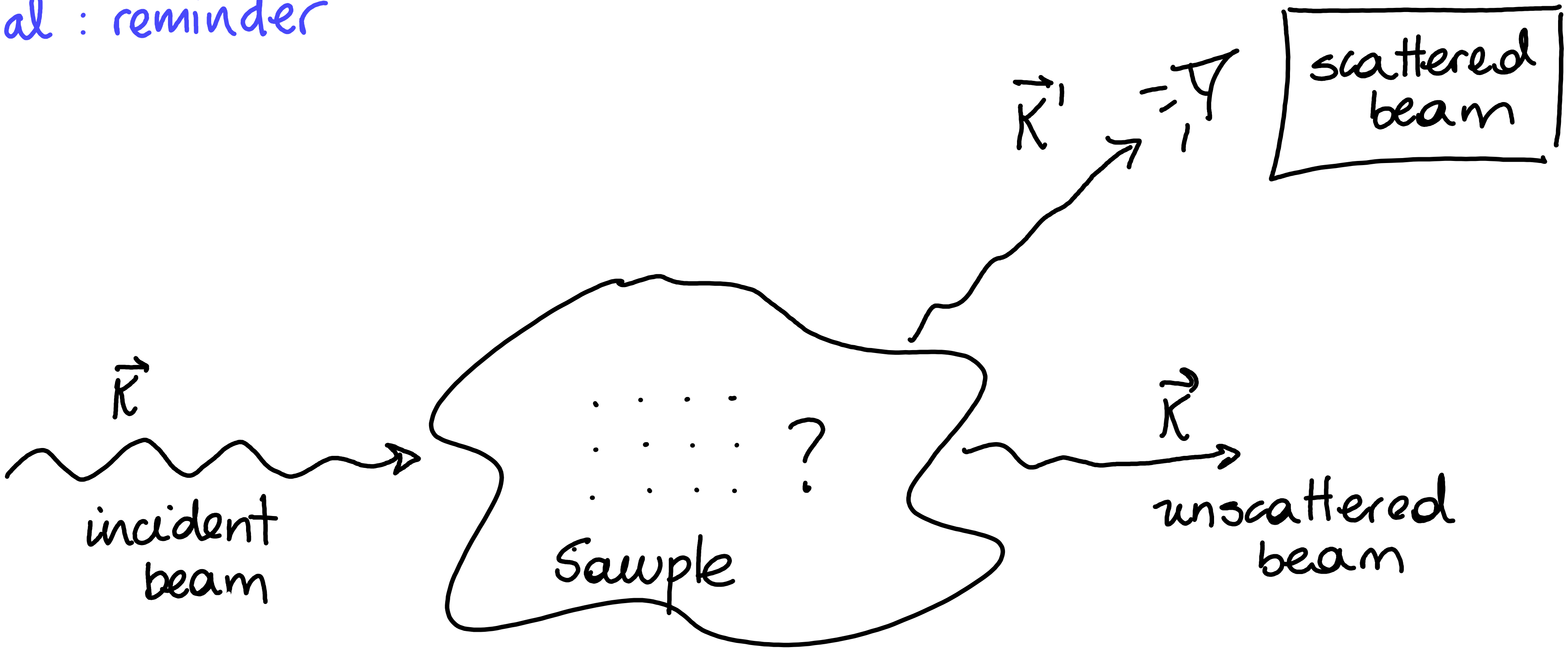
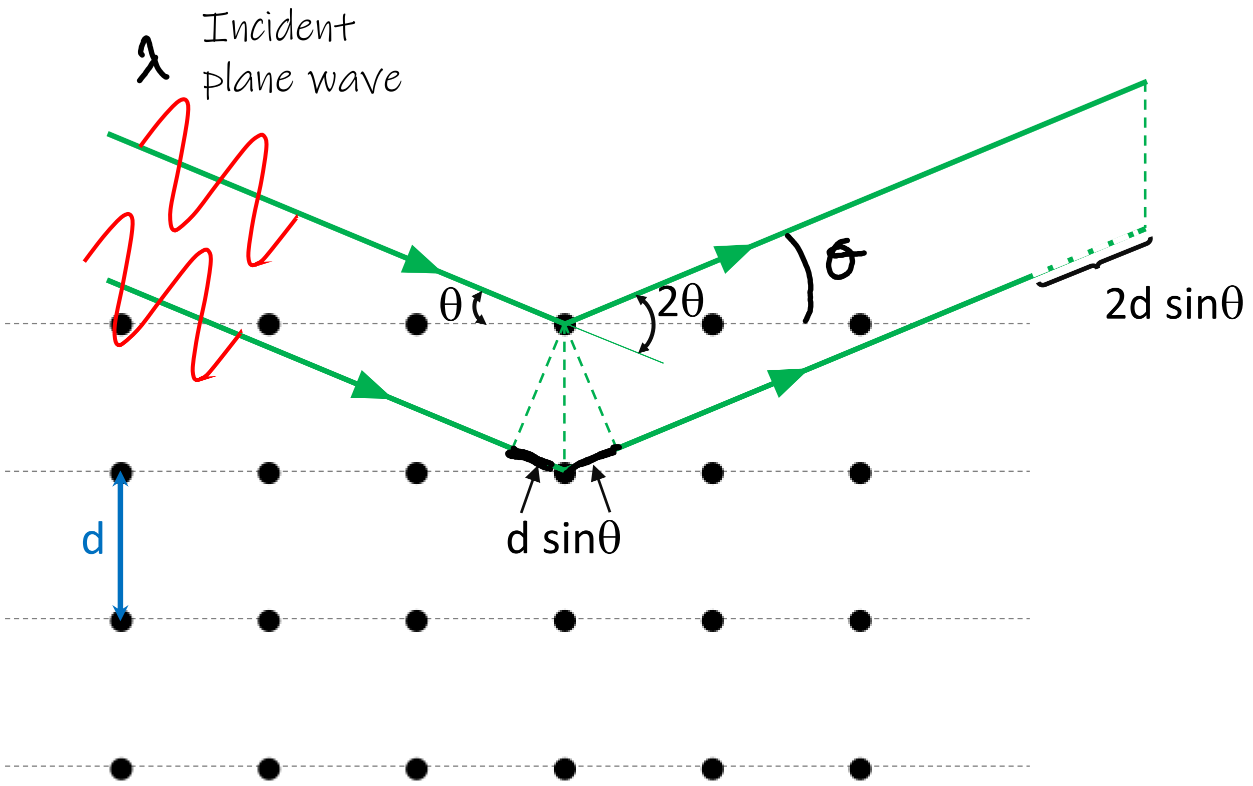
Scattering

see, for instance, Kittel chapter 2

Our goal : reminder



Recap - Bragg Law



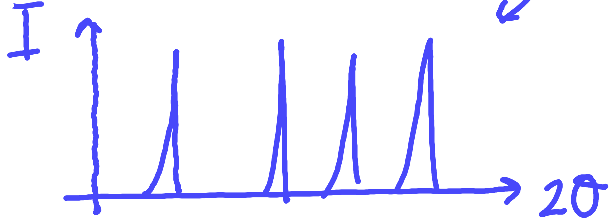
Bragg law is very useful but it is an oversimplification ⇐

Constructive Interference

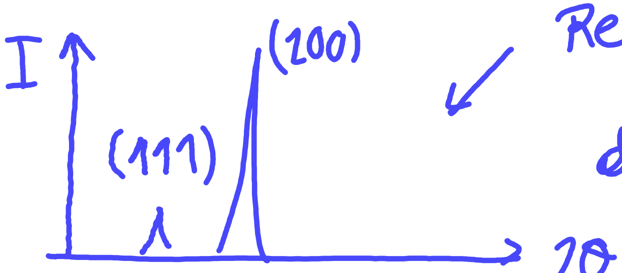
$$2 \cdot d \sin\theta = n\lambda$$

↑ integer

we saw



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

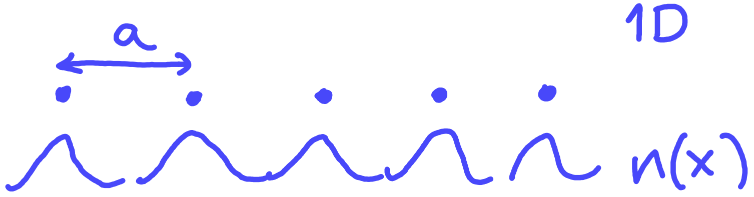


Real example NaCl diffraction pattern

Recap - Reciprocal lattice

Crystal : translation symmetry $\vec{T} = u_1\bar{a}_1 + u_2\bar{a}_2 + u_3\bar{a}_3$: $\vec{r}\,' = \vec{r} + \vec{T}$

Physical properties, i.e. $n(\vec{r}) = n(\vec{r} + \vec{T})$



$\Longrightarrow n(\bar{r}) = \sum_{\bar{G}} n_{\bar{G}} \exp(i\bar{G}\cdot\bar{r})$ $\qquad \boxed{e^{i\bar{G}\cdot\vec{T}} = 1}$

$\bar{G}$: <u>reciprocal lattice vectors</u> : $\bar{G} = h\bar{b}_1 + k\bar{b}_2 + \ell\bar{b}_3$

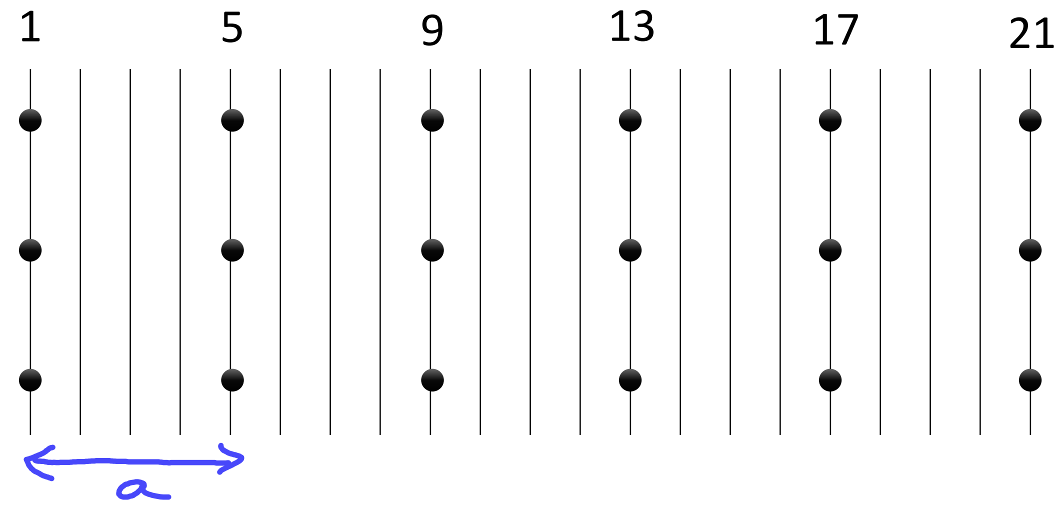
$\bar{b}_1 = 2\pi \dfrac{\bar{a}_2 \times \bar{a}_3}{\bar{a}_1 \cdot \bar{a}_2 \times \bar{a}_3} \longrightarrow \vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij} \quad (\delta_{ij} = 0 \;\; i \neq j \; ; \; \delta_{ij} = 1 \;\; i = j)$

$= \dfrac{2\pi}{V_c} \, \bar{a}_2 \times \bar{a}_3$

* Each crystal has a Real Lattice [length] and a reciprocal Lattice [length^{-1}]

* Direct lattice : Miller Indices $(hk\ell)$ $\longrightarrow$ $d_{hk\ell} = \dfrac{2\pi}{|\bar{G}|}$

Quiz



- Determine the reciprocal lattice vectors associated to $\nexists \vec{G} \in R.L.$

a) 1, 9, 17, … $K = \frac{2\pi}{d} = \frac{2\pi}{2a} = \frac{1}{2}\frac{2\pi}{a}$

b) 1, 5, 9, … $\longrightarrow \exists \vec{G} \in R.L.$ $\vec{K} = 2\pi/a$ $\left\{ \begin{array}{l} \vec{T} = u_1 \bar{a}_1 \\ \vec{G} = h \bar{b}_1 \end{array} \right.$ $\bar{a}_1 = a(1\,0\,0)$, $\bar{b}_1 = \frac{2\pi}{a}(1\,0\,0)$

c) 1, 3, 5, …

d) 1, 2, 5, 6, …. not equidistant planes

Reminder last lecture:

Ex. 1: $\vec{G} = \vec{b}_1$ $(hkl) = (100)$

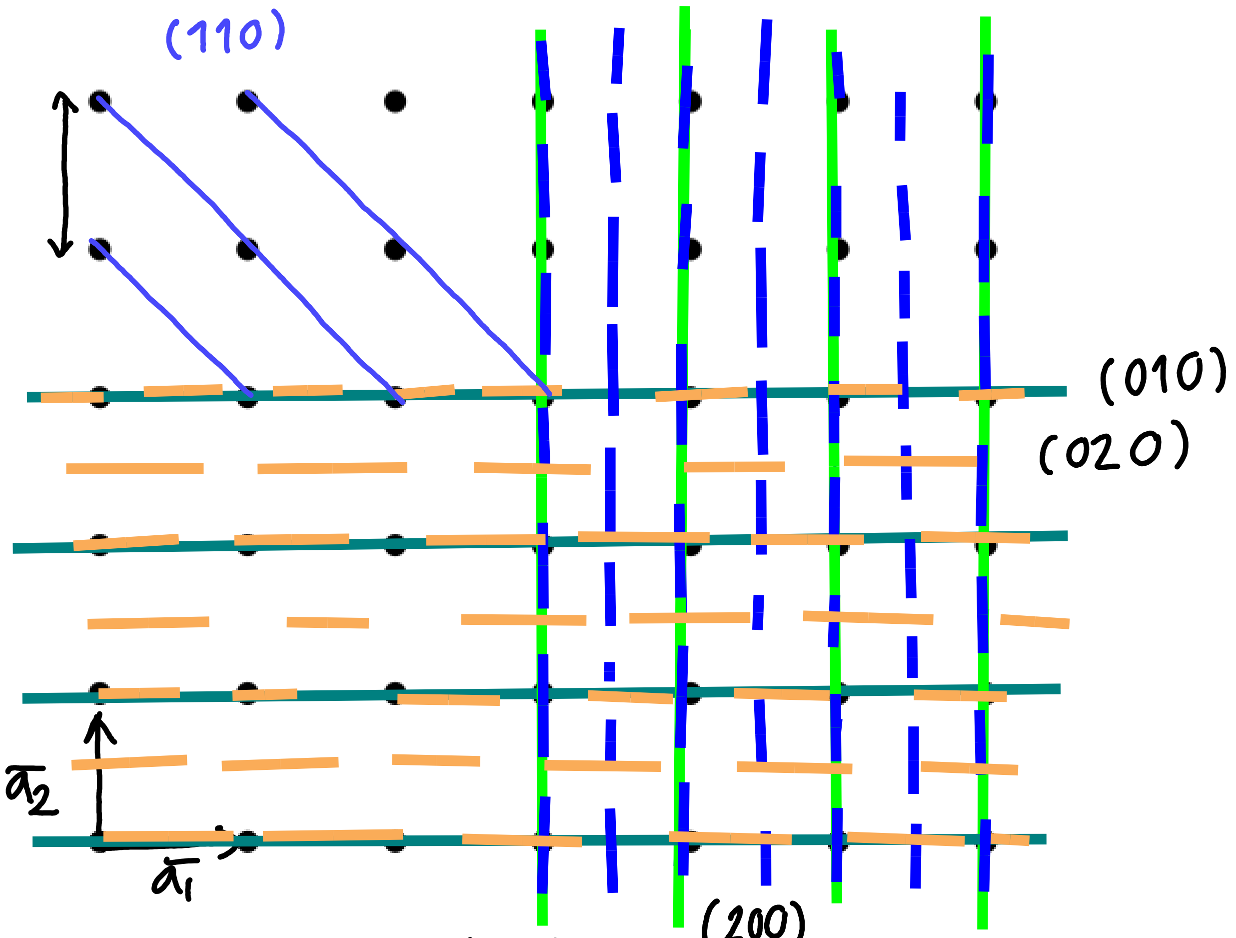
$$d = \frac{2\pi}{|G|} = \frac{2\pi}{2\pi/a} = a$$

Ex. 2: $\vec{G}_2 = \vec{b}_1 + \vec{b}_2$ $(hkl) \Rightarrow (110)$

$$d_{hkl} = \frac{2\pi}{|G|} = \frac{2\pi}{\frac{2\pi\sqrt{2}}{a}} = \frac{a\sqrt{2}}{2}$$

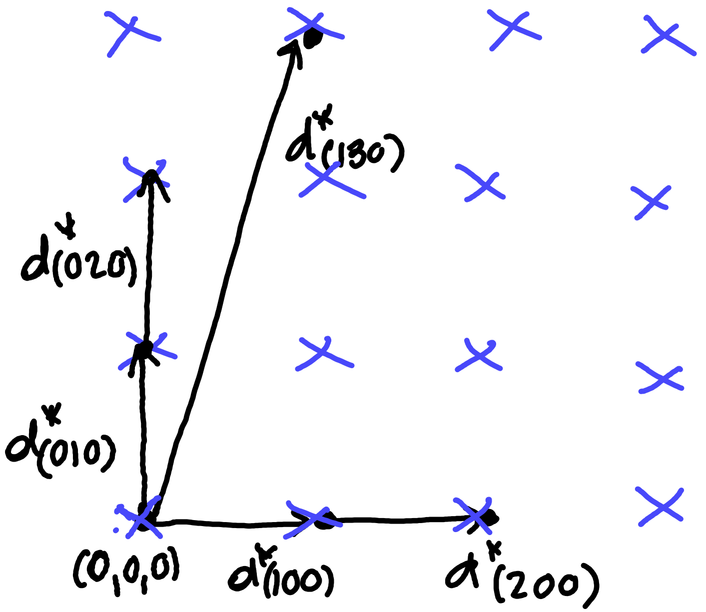
Reciprocal Lattice for the simple cubic lattice

Draw the reciprocal lattice vectors for the (100), (010), (200), (020), (130) set of planes



Real Lattice $\otimes z$

$$d_{hkl} = \frac{2\pi}{|G_{min}|}$$



Reciprocal Lattice

$$\vec{b}_1 = \frac{2\pi}{a}(10)$$

$$\vec{b}_2 = \frac{2\pi}{a}(01)$$

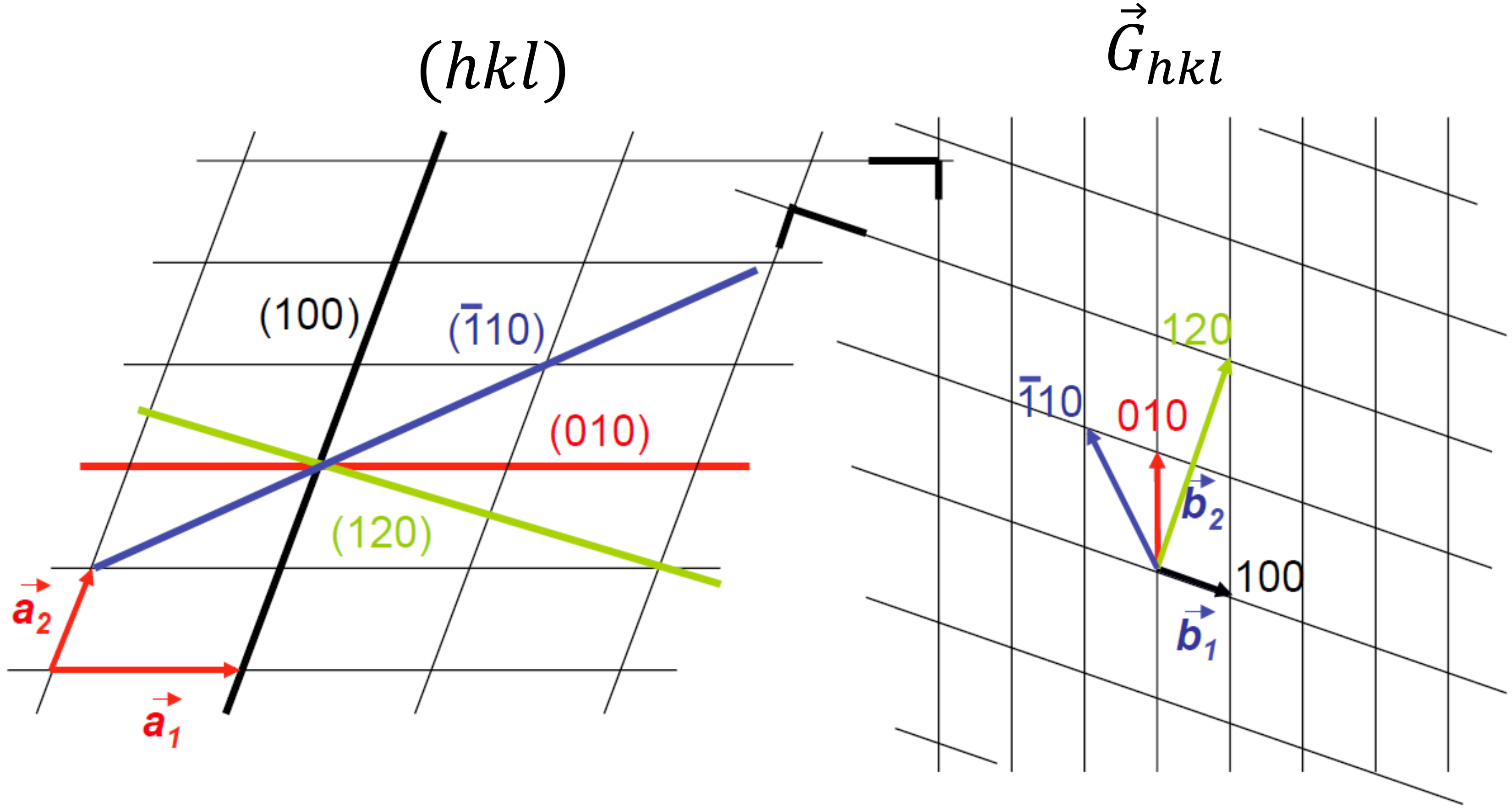
Monoclinic with $a_3 \to \infty$

$$\vec{b}_1 = 2\pi \frac{\bar{a}_2 \times \bar{a}_3}{\bar{a}_1 \cdot \bar{a}_2 \times \bar{a}_3}$$

$\vec{b}_1 \perp \bar{a}_2, \bar{a}_3$

$b_1 \parallel \bar{a}_2 \times \bar{a}_3$

($\vec{b}_1 \parallel \bar{a}_1$ for orthogonal vectors only)



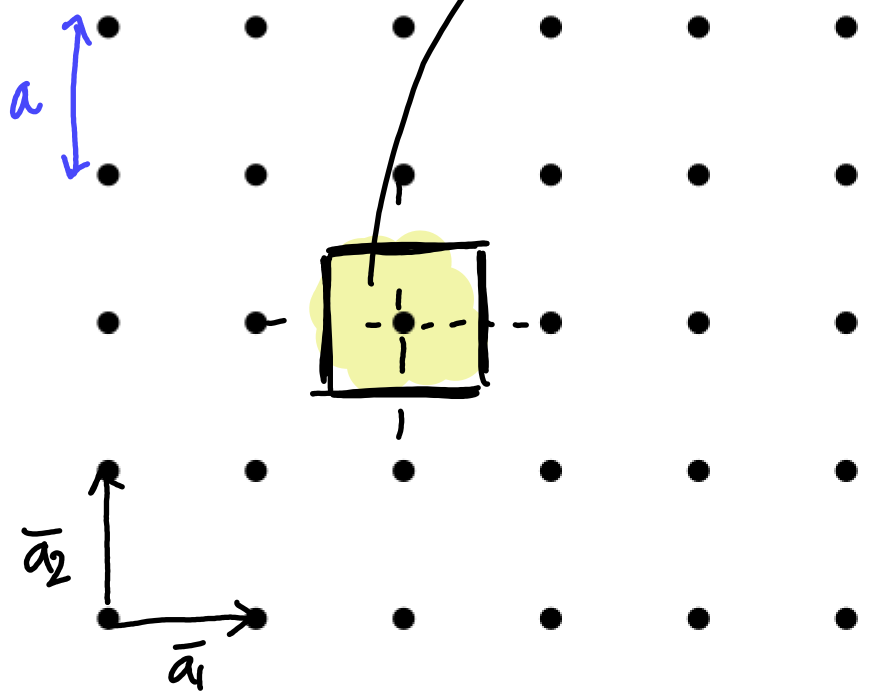
Direct Lattice

Reciprocal Lattice

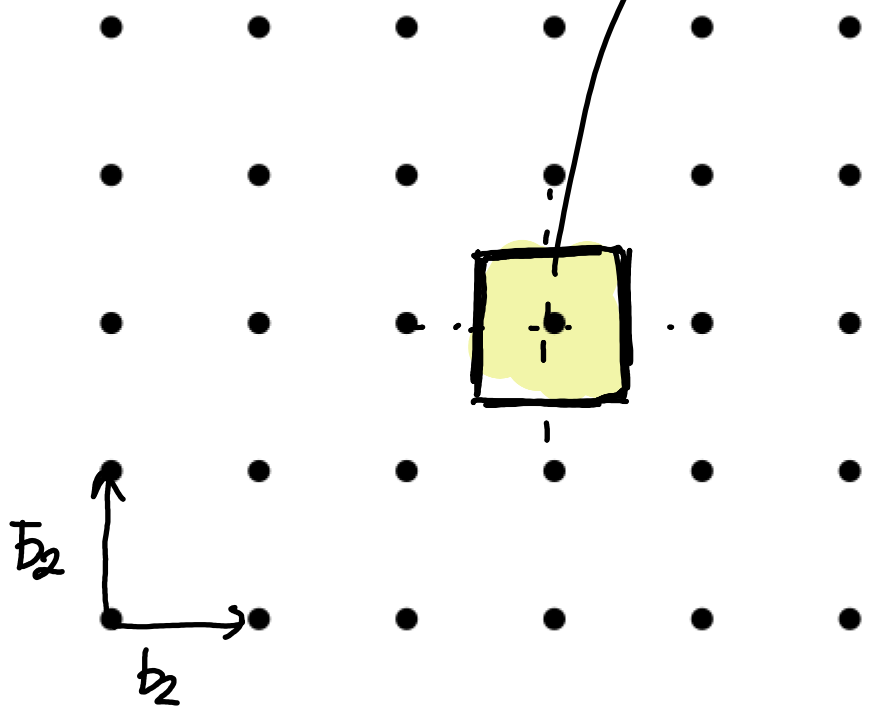
Each crystal has a real and reciprocal lattice associated

Square Lattice

Wigner-Seitz (primitive unit cell)



Wigner-Seitz in the reciprocal lattice $\equiv$ <u>1rst Brillouin zone</u>



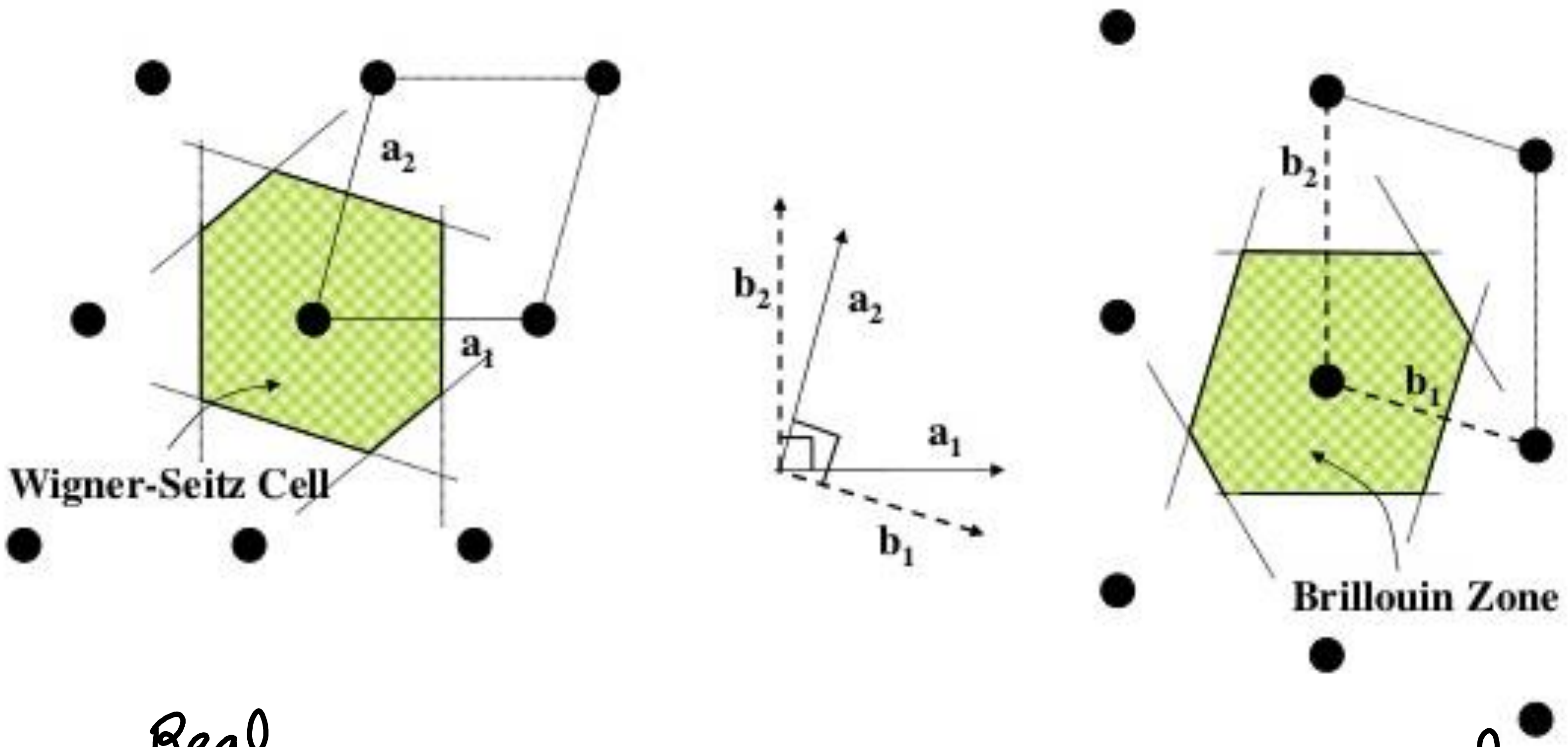
Real Lattice

$$\bar{a}_1 = a\,(1,0,0)$$
$$\bar{a}_2 = a\,(0,1\,0)$$

$$\bar{b}_1 = \frac{2\pi}{a}(1,0,0)$$
$$\bar{b}_2 = \frac{2\pi}{a}(0,1,0)$$

Reciprocal Lattice

Another example.

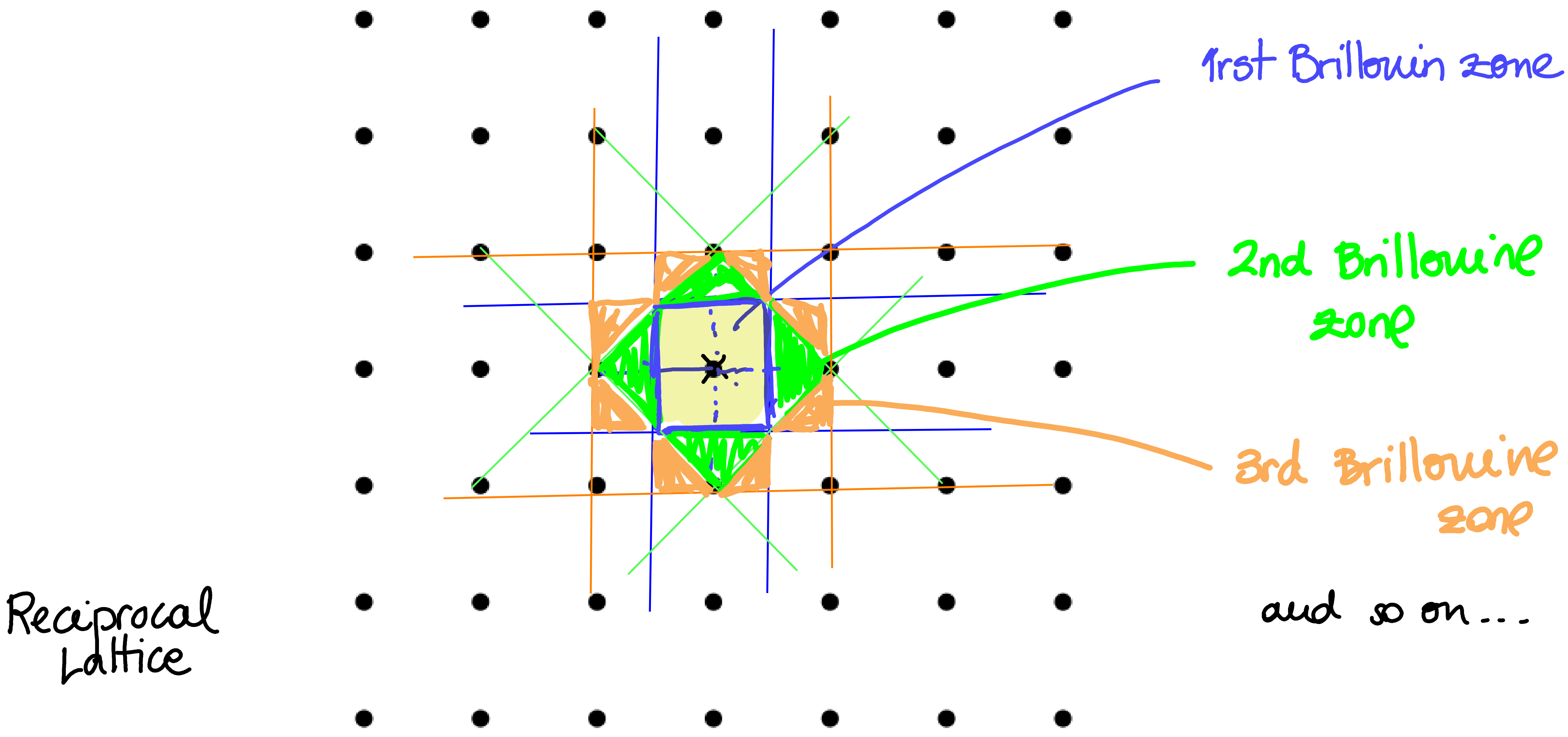


Real Lattice

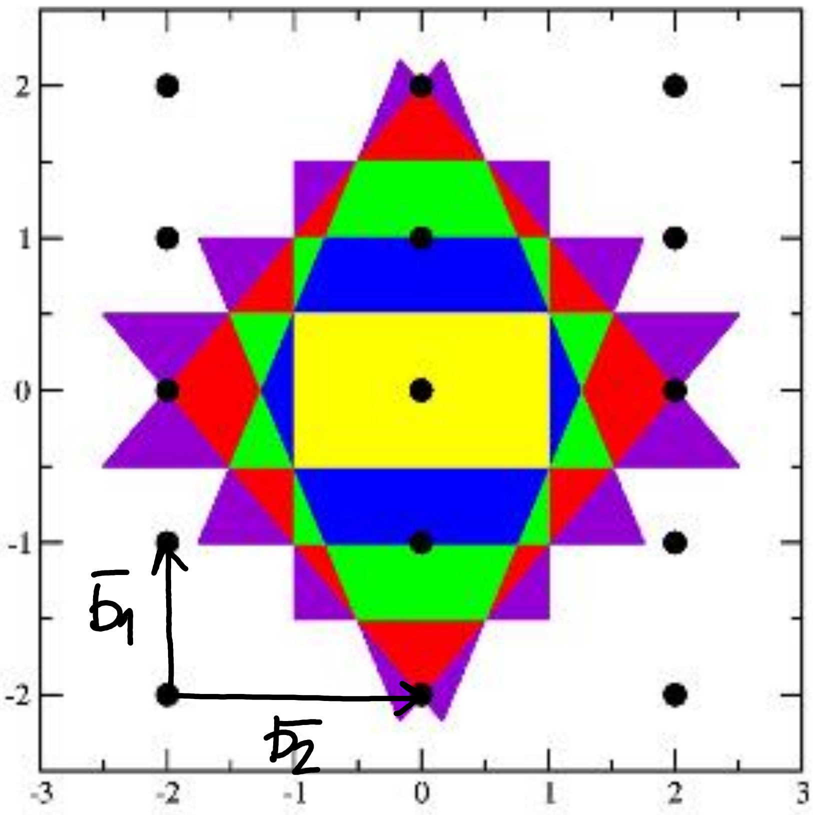
Reciprocal lattice

Brillouin zone

A **Brillouin zone** is defined as a Wigner-Seitz primitive cell in the reciprocal lattice



Brillouin zones



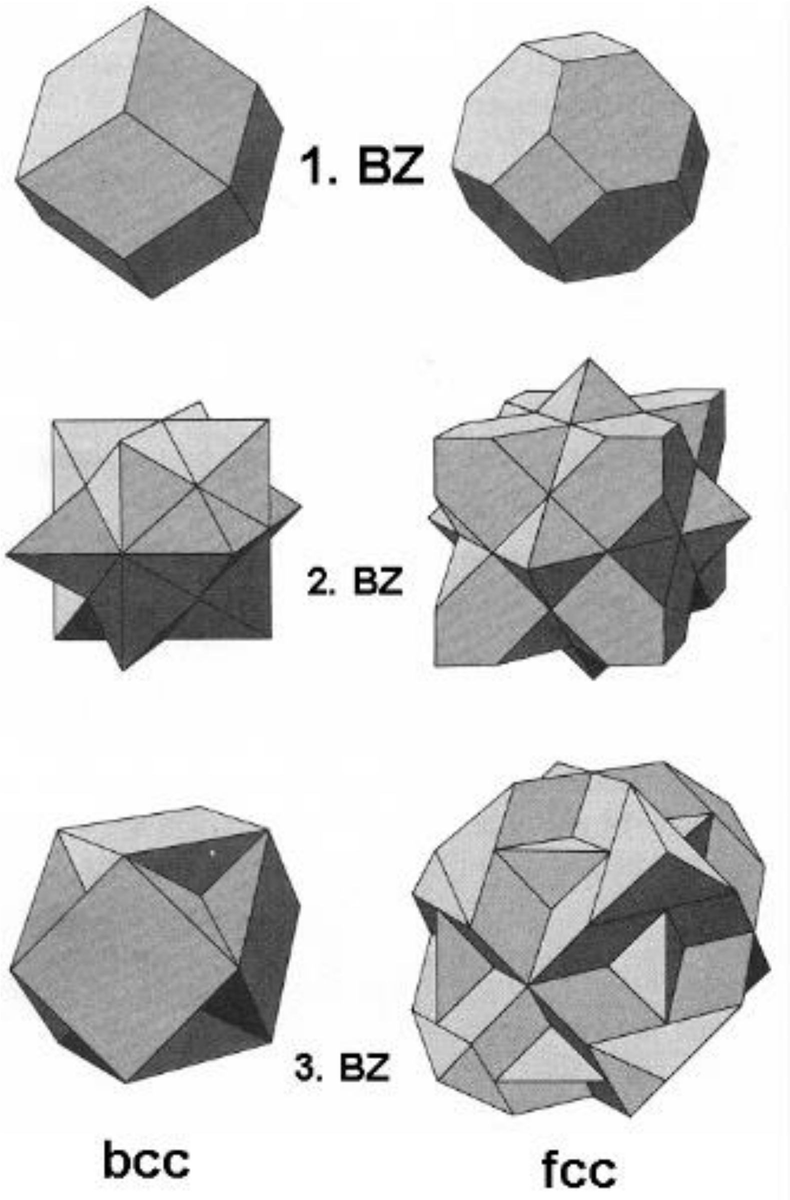
(b) Rectangular lattice $b/a = 2$

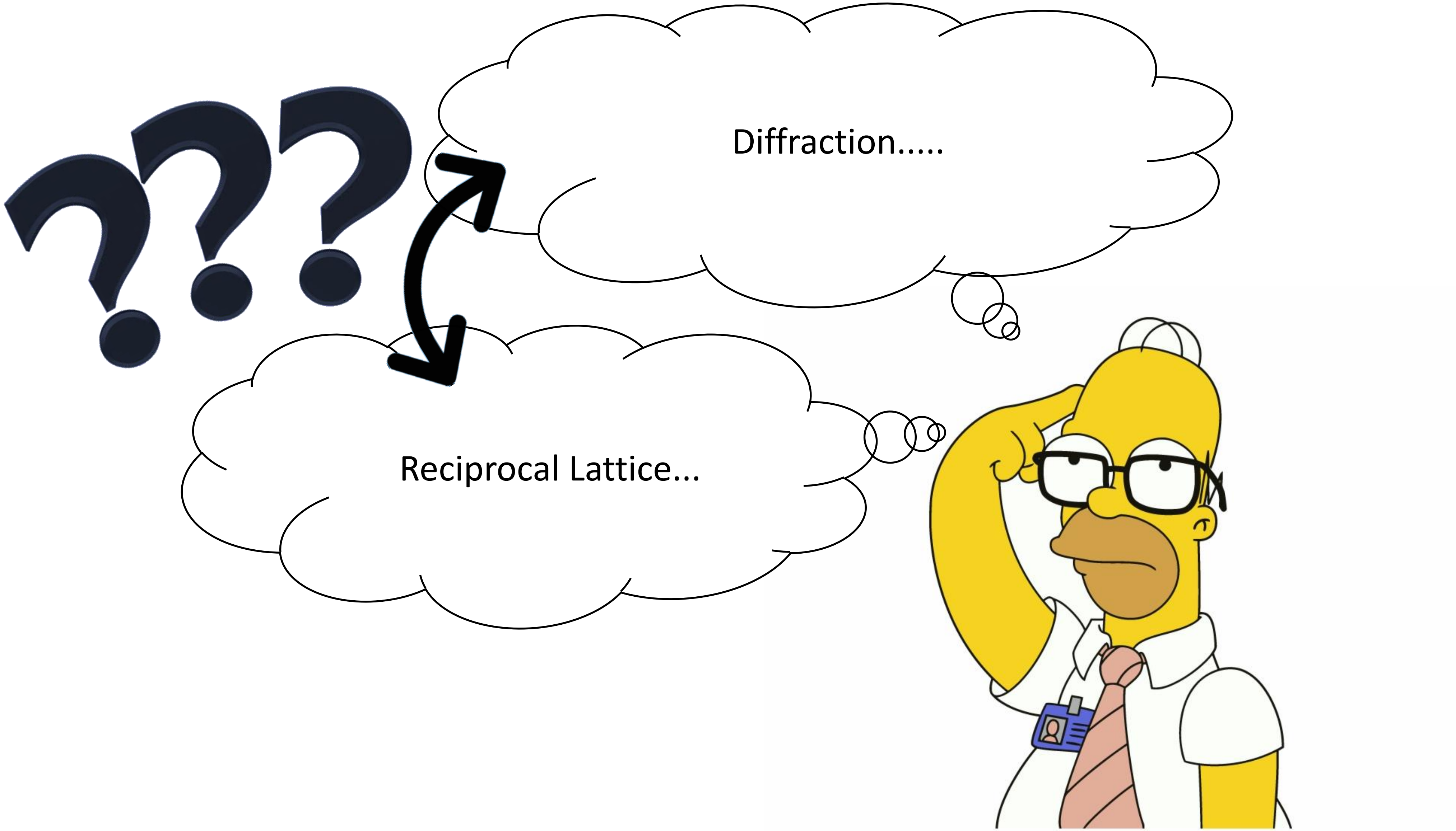
* First Brillouin zone is connected, but the higher B.Z. typically not

* Each B.Z. has exactly the same area (or volume in 3D)

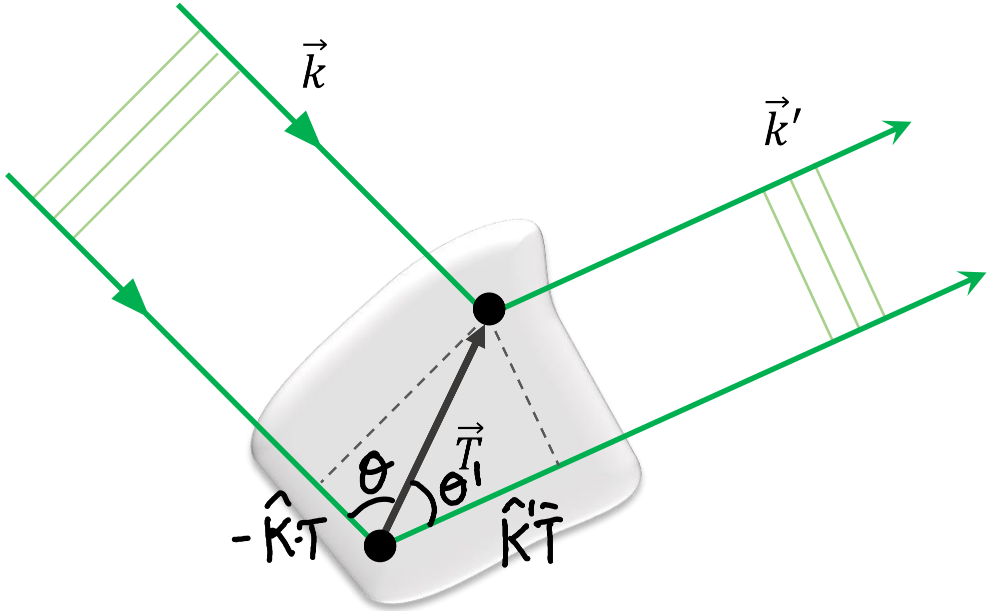
* Zone boundaries occur in parallel pairs symmetric around 0 and they are separated by a reciprocal lattice vector.

Brillouin zones in 3D




Diffraction.....
Reciprocal Lattice...

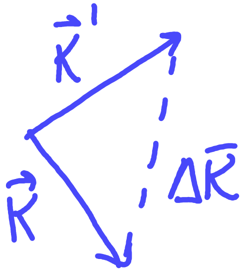
Diffraction condition and reciprocal lattice



Crystal: identical atoms separated $\vec{T}$
(real space)

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

$\hat{K} = \frac{\vec{K}}{|\vec{K}|}$ $\quad \hat{K}' = \frac{\vec{K}'}{|\vec{K}'|}$



Constructive Interference:

$$T\cdot\cos\theta + T\cos\theta' = n\lambda$$ integer

$$(\hat{K}' - \hat{K})\cdot\vec{T} = n\lambda$$

Elastic scattering: $|\vec{K}| = |\vec{K}'| = \frac{2\pi}{\lambda}$

$$(\vec{K}' - \vec{K})\cdot\vec{T} = n2\pi$$

$$e^{i(\vec{K}'-\vec{K})\cdot\vec{T}} = 1$$

- Remember reciprocal lattice def.: $e^{i\vec{G}\cdot\vec{T}} = 1$
- Define scattering vector $\Delta\vec{K} = \vec{K}' - \vec{K}$

$\Rightarrow \boxed{\Delta\vec{K} = \vec{G}}$ Laue Equation

(⇒ Diffraction maxima gives us the R.L. of the crystal)
not an image

Diffraction condition

$$\boxed{\Delta\vec{K} = \vec{G}} \quad \text{with} \quad \Delta\bar{K} = \bar{K}' - \bar{K}$$

Elastic scattering $\longrightarrow$ Energy $E = \hbar\omega$ is conserved

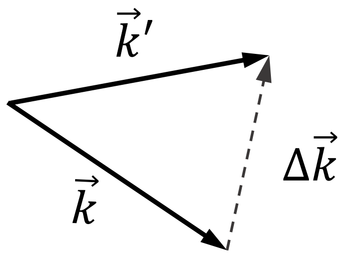
$$\omega = cK = \omega' = cK'$$
$$K^2 = K'^2$$

$$\Rightarrow \quad \Delta\vec{K} = \vec{G} \longrightarrow (\vec{K} + \vec{G})^2 = (\vec{K}')^2$$

$$\boxed{2\bar{K}\cdot\bar{G} + G^2 = 0}$$

If $\bar{G}$ is a reciprocal lattice vector, $-\bar{G}$ too:

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



Condition for diffraction

the set of reciprocal lattice vectors $\bar{G}$ determine the possible x-ray reflections

Geometric construction of diffraction conditions

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

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

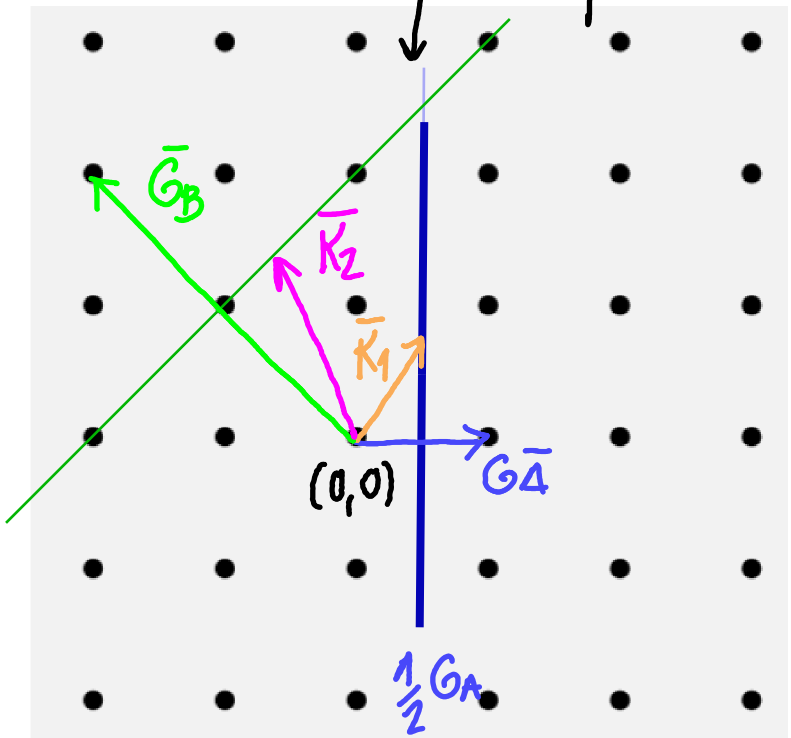
- select $\bar{G}$ from origin to R.L. point
- construct plane $\perp \bar{G}$ at its midpoint
- any vector $\bar{k}$ from the origin and ending in that plane (i.e. $\bar{k}_1$) will satisfy the condition

$$\bar{k}_1\cdot\left(\tfrac{1}{2}\bar{G}_A\right) = \left(\tfrac{1}{2}G_A\right)^2$$

$$\bar{k}_2\cdot\left(\tfrac{1}{2}\bar{G}_B\right) = \left(\tfrac{1}{2}G_B\right)^2$$

Notice that this plane is part of a B.Z. boundary

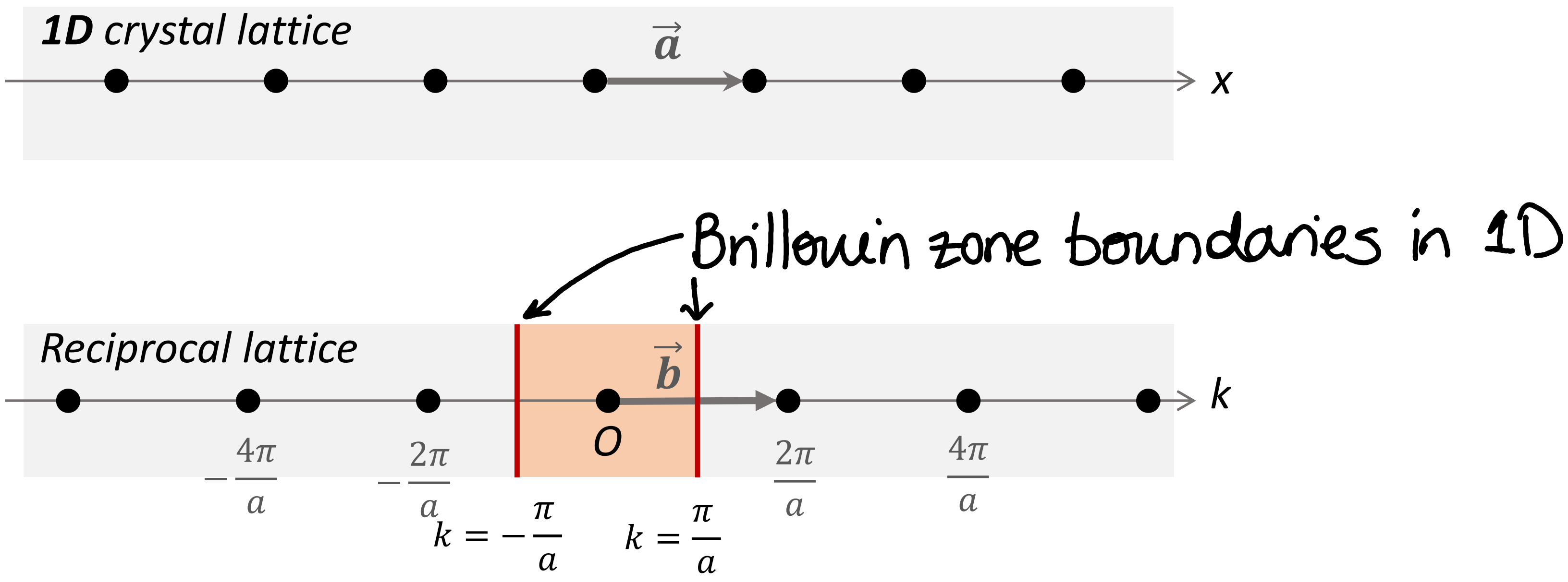
$\Rightarrow$ special role of B.Z. compared to any primitive unit cell of the reciprocal Lattice!



***2D** reciprocal lattice*

Diffraction and Brillouin zone

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



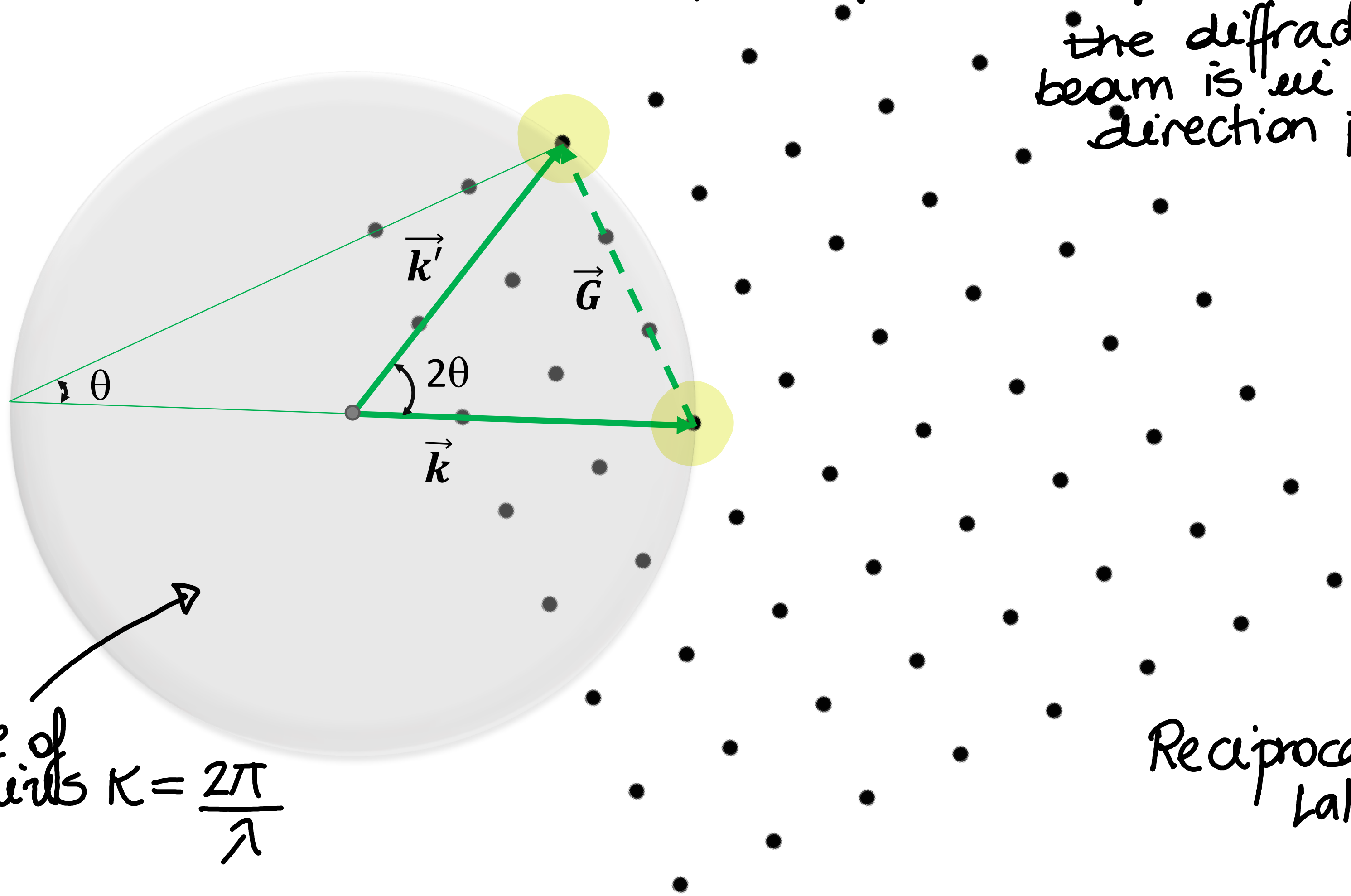
Ewald construction for diffraction

③ → A diffracted beam will be form if the sphere intersects another point of the reciprocal lattice

Diffraction condition:

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

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



the diffracted beam is in the direction $\vec{K'}=\vec{K}+\vec{G}$

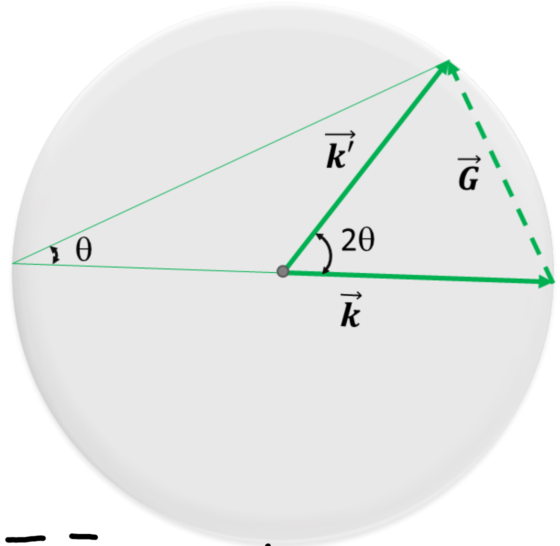
① $\vec{K}$: origin chosen it terminates at any reciprocal lattice point

② sphere of radius $K = \frac{2\pi}{\lambda}$

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

Equivalence of Laue and Bragg conditions

$$\left.\begin{array}{ll} \text{Laue Eq.} & 2\vec{k}\cdot\vec{G} = G^2 \\ \text{Bragg Eq.} & 2d\sin\theta = n\lambda \end{array}\right\}$$



$$2\vec{K}\cdot\vec{G} = 2KG\sin\theta$$

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

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

$$2\left(\frac{2\pi}{\lambda}\right)\sin\theta = \frac{2\pi}{d_{hkl}}$$

$$2d_{hkl}\sin\theta = \lambda \implies 2d\sin\theta = n\lambda$$

in the definition of the index hkl we devided the distances between the common factor n