Lattice plane:

Consider a plane containing at least three non-collinear lattice points in BVK cell.
You can draw many planes parallel to it to contain all lattice points in the BVK cell.
Now consider the BVK cell to expand to ∞ large.
So now you have a Bravais lattice and need ∞ number of parallel planes to contain all the ∞ number of lattice points.

Parallel lattice plane: family of ∞ number of lattice planes.

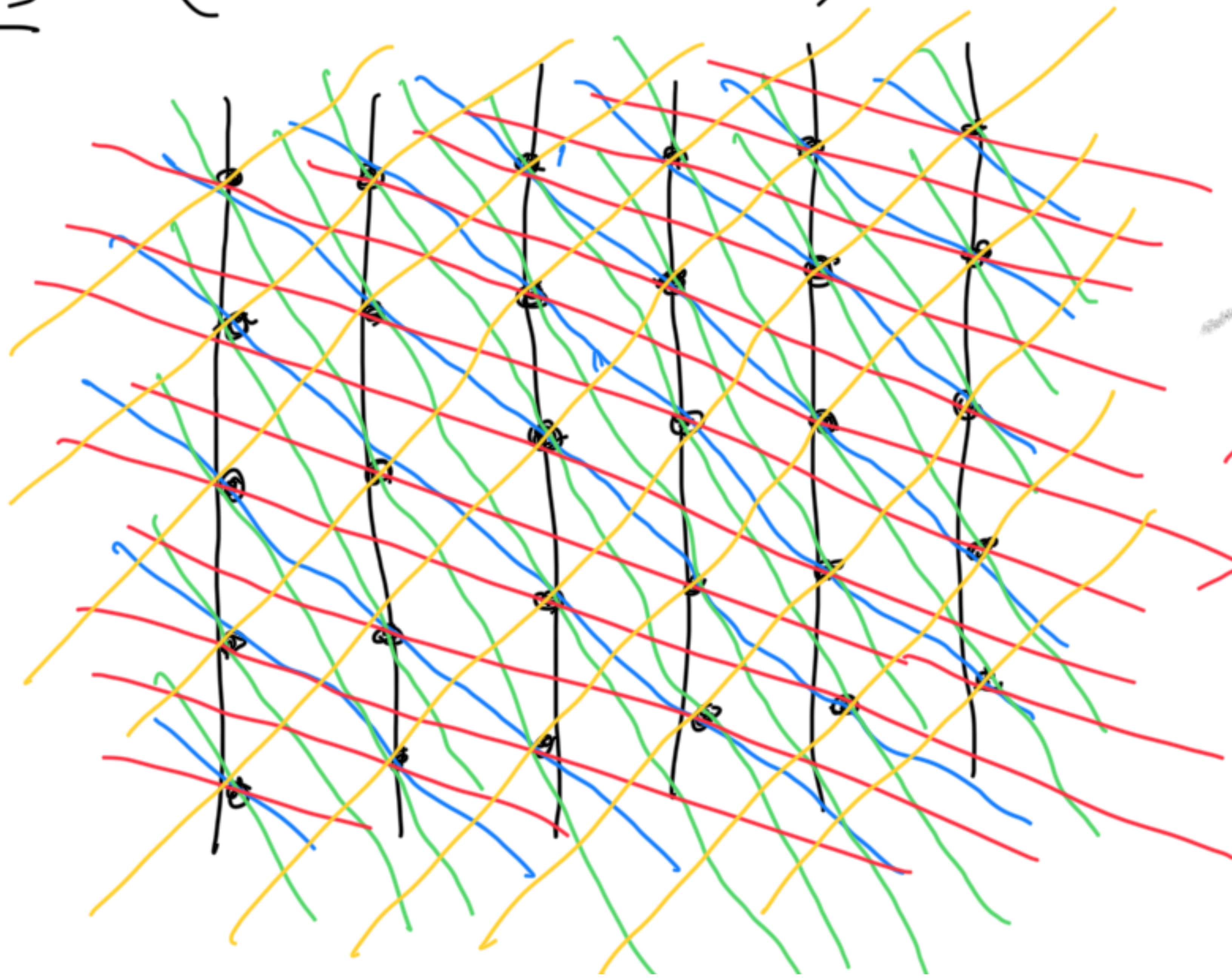
To each family of lattice planes we can associate of family of collinear $\vec{G}$ vectors:

$$\left\{ \vec{G} = l\,\vec{G}_{min} \;;\; l = \pm 1, \pm 2, \cdots \pm \infty \right\}$$

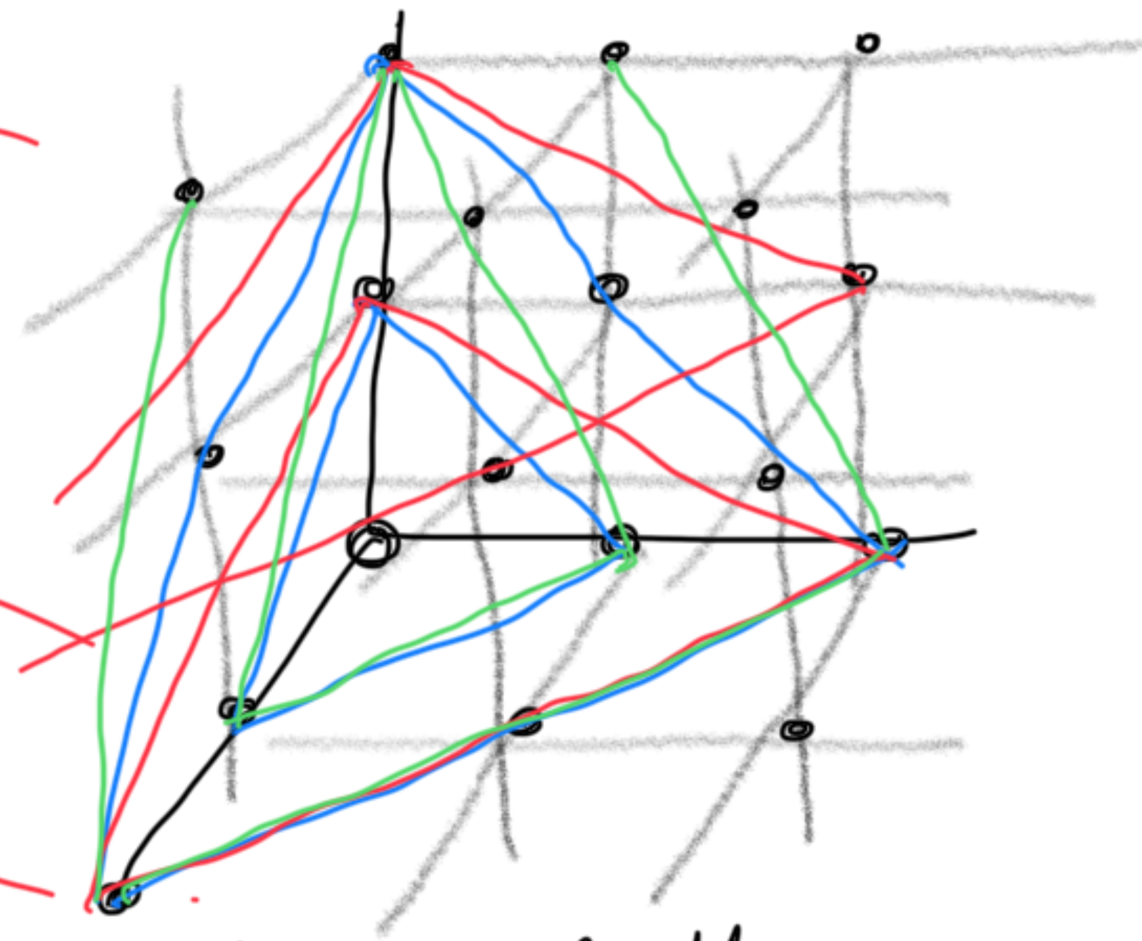
let $\vec{G}_{min} = h\,\vec{b}_1 + k\,\vec{b}_2 + l\,\vec{b}_3$

such that $\left\{ \vec{R} : \vec{G}\cdot\vec{R} = 0 \right\}$ defines set of coplanar lattice vectors.

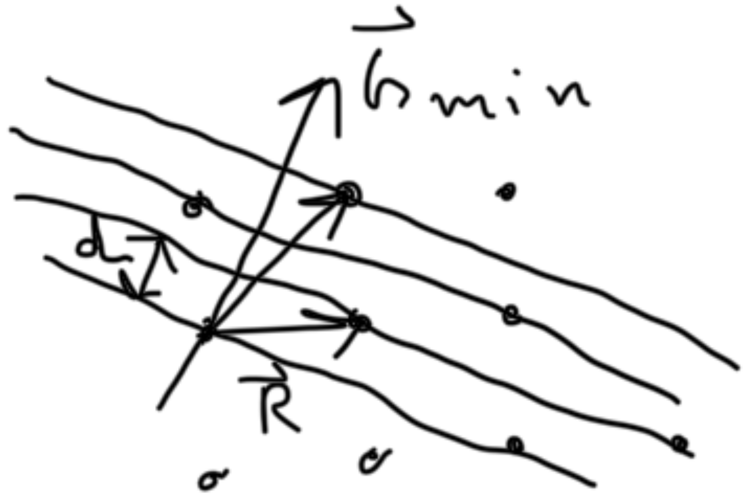
<u>In 2D</u> (plane → line)



<u>3D</u>

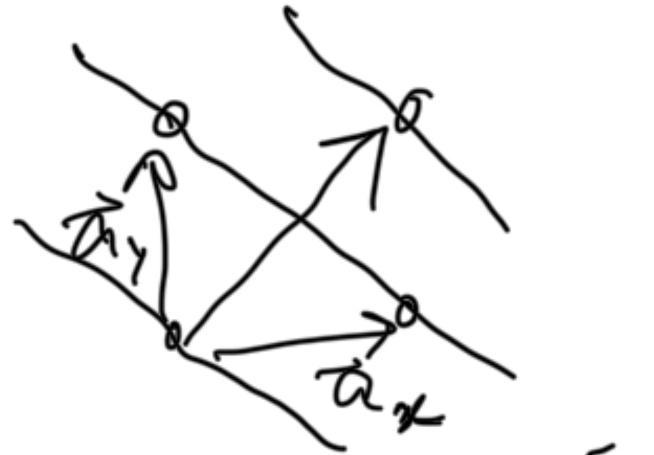


Note $\parallel^{l}$ planes.



For any interplanar $\vec R$:

$$\vec G_{min} \cdot \vec R = m\, 2\pi$$



$$\therefore \left| \vec G_{min} \cdot \vec R \right|_{min} = 2\pi$$

$$\Rightarrow |\vec G_{min}|\, d = 2\pi \quad \text{(see figure)}$$

$$|G_{min}| = \frac{2\pi}{a}\sqrt{2}$$

$$d = \frac{2\pi}{2\pi\sqrt{2}/a} = a/\sqrt{2}$$

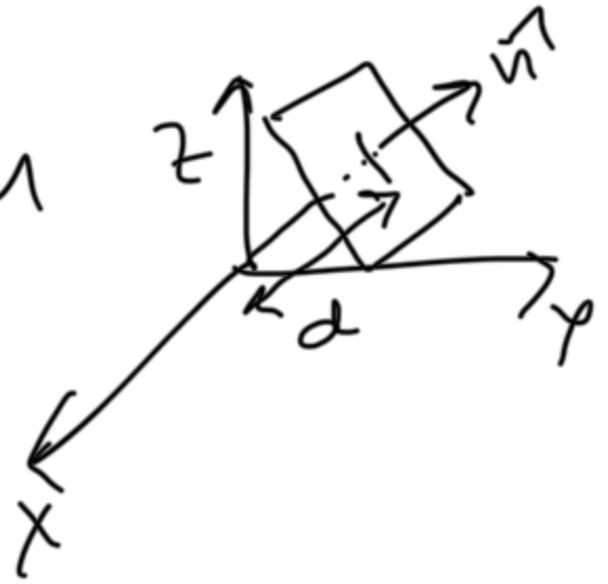
$$\Rightarrow d = \frac{2\pi}{|\vec G_{min}|}$$

In orthogonal unit cell: $\hat a_i \perp \vec a_j$ $\; i \neq j \Rightarrow \vec b_i \perp \vec b_j$ $\; i \neq j$

$$d = \frac{2\pi}{\sqrt{h^2|\vec b_1|^2 + k^2|\vec b_2|^2 + l^2|\vec b_3|^2}} = \frac{1}{\sqrt{h^2/a_1^2 + k^2/a_2^2 + l^2/a_3^2}}$$

For a general Bravais lattice (orthogonal or not)

$\vec{G}_{min} \cdot \vec{R} = 2\pi \longrightarrow$ Eq^n of plane $\perp$ to $\vec{G}_{min}$ in space spanned by $\vec{R}$.

[Recall 

$\hat{n}\cdot\vec{r} = d \rightarrow$ Eq^n of plane $\perp$ $\hat{n}$ at a distance d from origin.]

Note that $\vec{G}$ and $\vec{R}$ are vectors, so they are expressable in the same Cartesian 3D space but their components have different interpretations.

$$\vec{G}_{min} \cdot \vec{R} = 2\pi \longrightarrow$$

$$\Rightarrow (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\cdot(l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3) = 2\pi$$

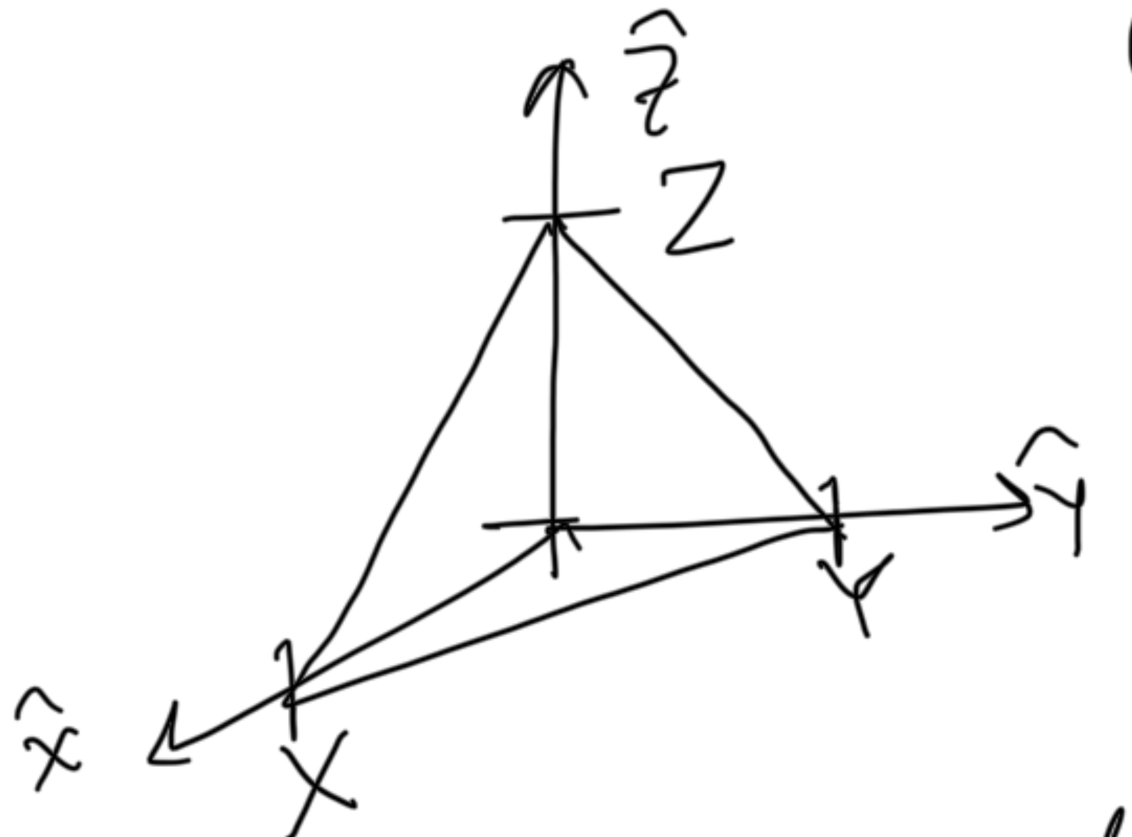
$$\Rightarrow hl_1 + kl_2 + ll_3 = 1, \quad \because \vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

Note that the above equation denotes a plane in the Cartesian coordinate system where $l_1\ l_2\ l_3$ are measured along the three axes.

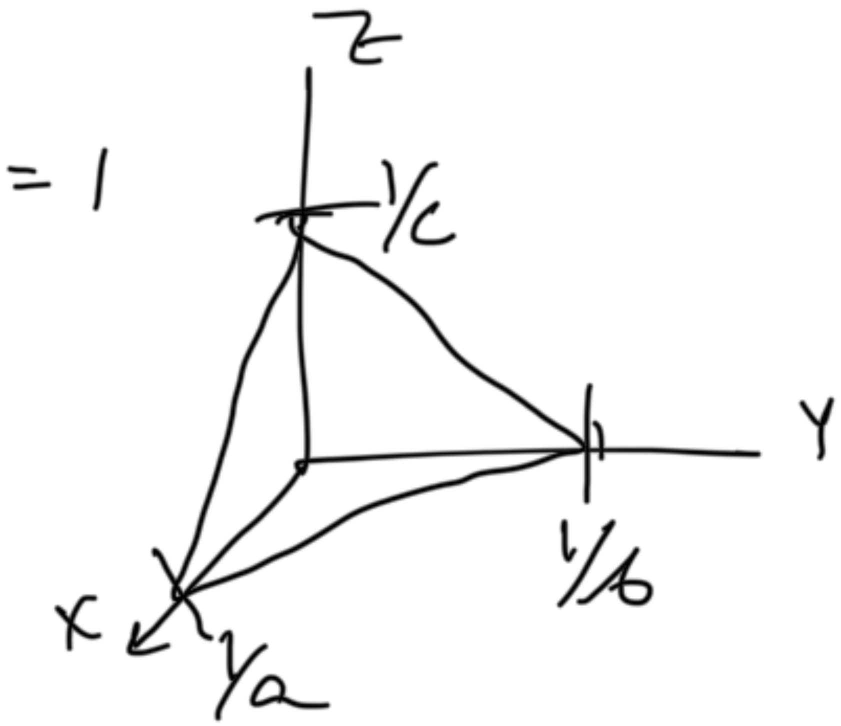
The ratio of the intercepts of the plane on the three Cartesian axes are $\frac{1}{h} : \frac{1}{k} : \frac{1}{l}$ respectively.

(hkl) thus denote an infinite set of parallel planes such that for all such planes : $\frac{1}{X} : \frac{1}{Y} : \frac{1}{Z} = h : k : l$

X Y Z being intercepts on the three axis.

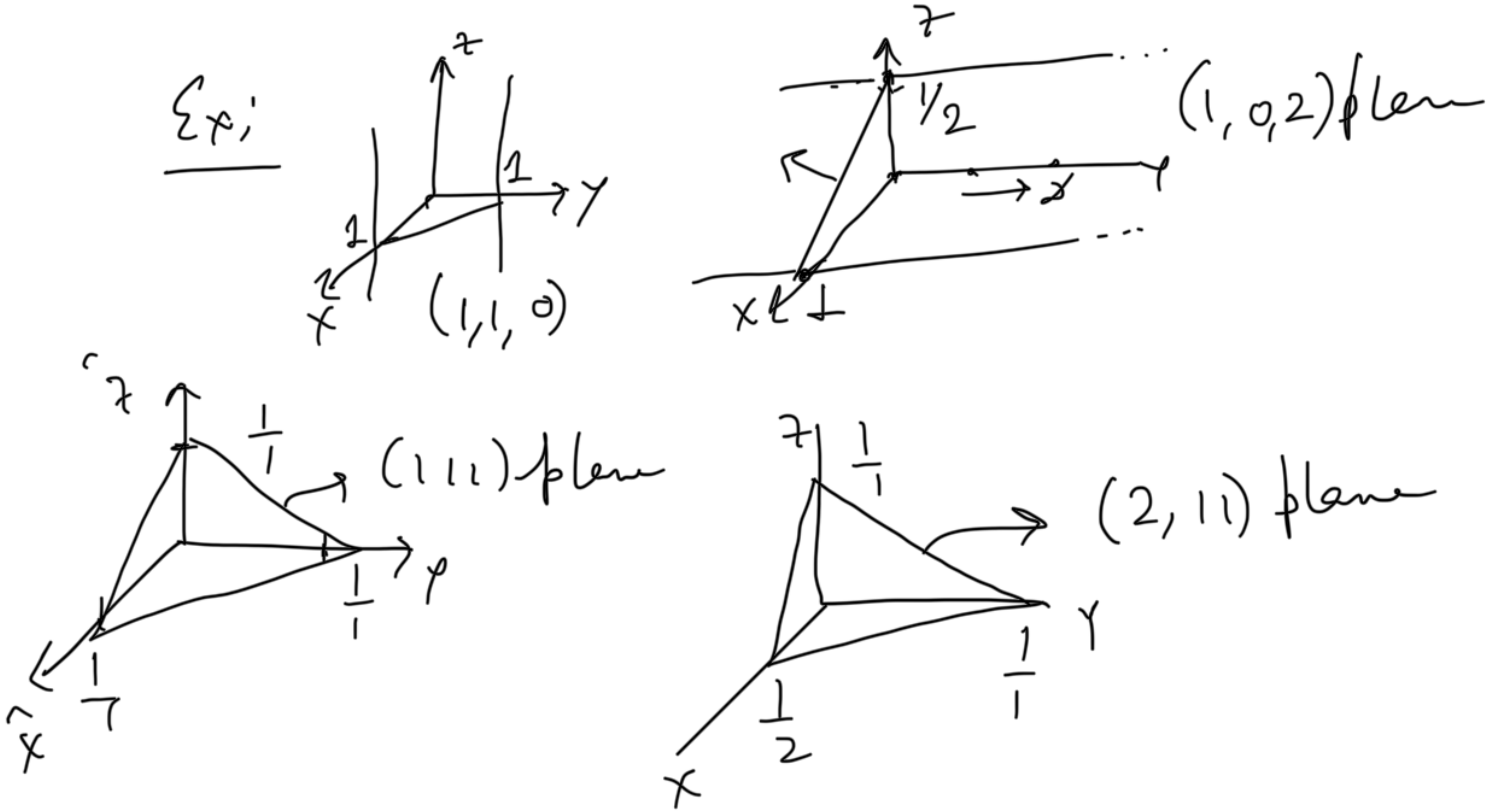


Recall
$ax + by + cz = 1$

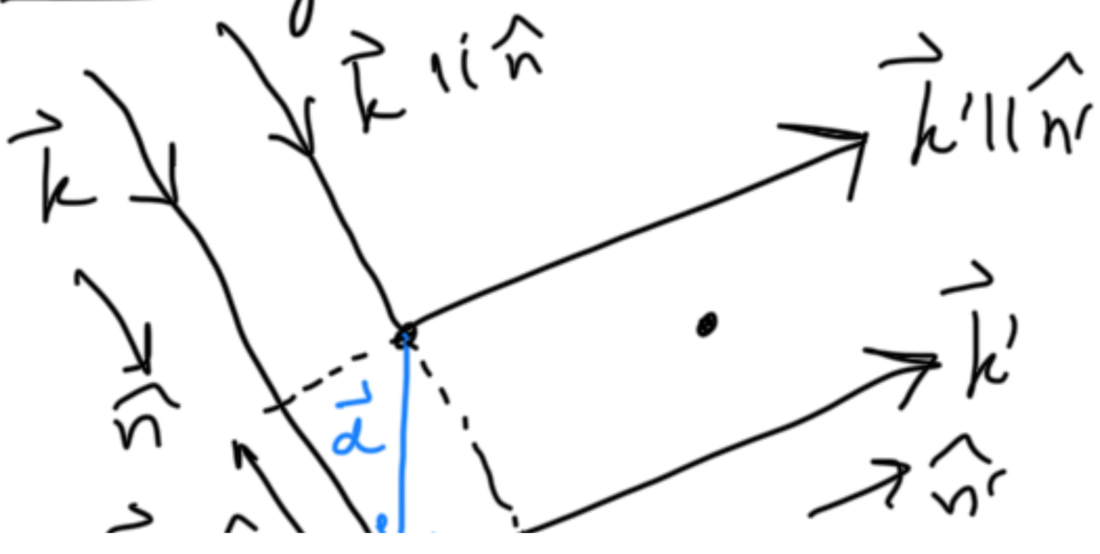


for cubic lattice these planes are the real crystal plane. [Cubic lattice: $\vec{a}_1 \perp \vec{a}_2 \perp \vec{a}_3$, $|\vec{a}_1| = |\vec{a}_2| = |\vec{a}_3|$]

Ex:



X-ray diffraction:



Constructive interference:

$$\vec{d}\cdot\hat{n} + (-\vec{d})\cdot\hat{n}' = m\lambda \qquad \underline{\lambda \to \text{X ray}}$$

$$\Rightarrow \vec{d}\cdot(\hat{n} - \hat{n}') = m\lambda$$

$\vec d\cdot\hat n$

$-\vec d\cdot\hat n'$

$$\Rightarrow \vec d\cdot\left(\frac{2\pi}{\lambda}\hat n - \frac{2\pi}{\lambda}\hat n'\right) = m2\pi$$

$$\Rightarrow \vec d\cdot(\vec k - \vec k') = m2\pi$$

$\vec d$ can be generalized to $\vec R$ to account for constructive interference from all pairs of lattice points.

$$\Rightarrow \vec R\cdot(\vec k - \vec k') = m2\pi$$

$$\Rightarrow \vec k - \vec k' = \vec G \longrightarrow \text{Von Laue condition.}$$

Note that no specific notion of specular reflection has been introduced in Von Laue treatment.

Now assume elastic scattering $\Rightarrow |\vec k|^2 = |\vec k'|^2$ no loss of energy.

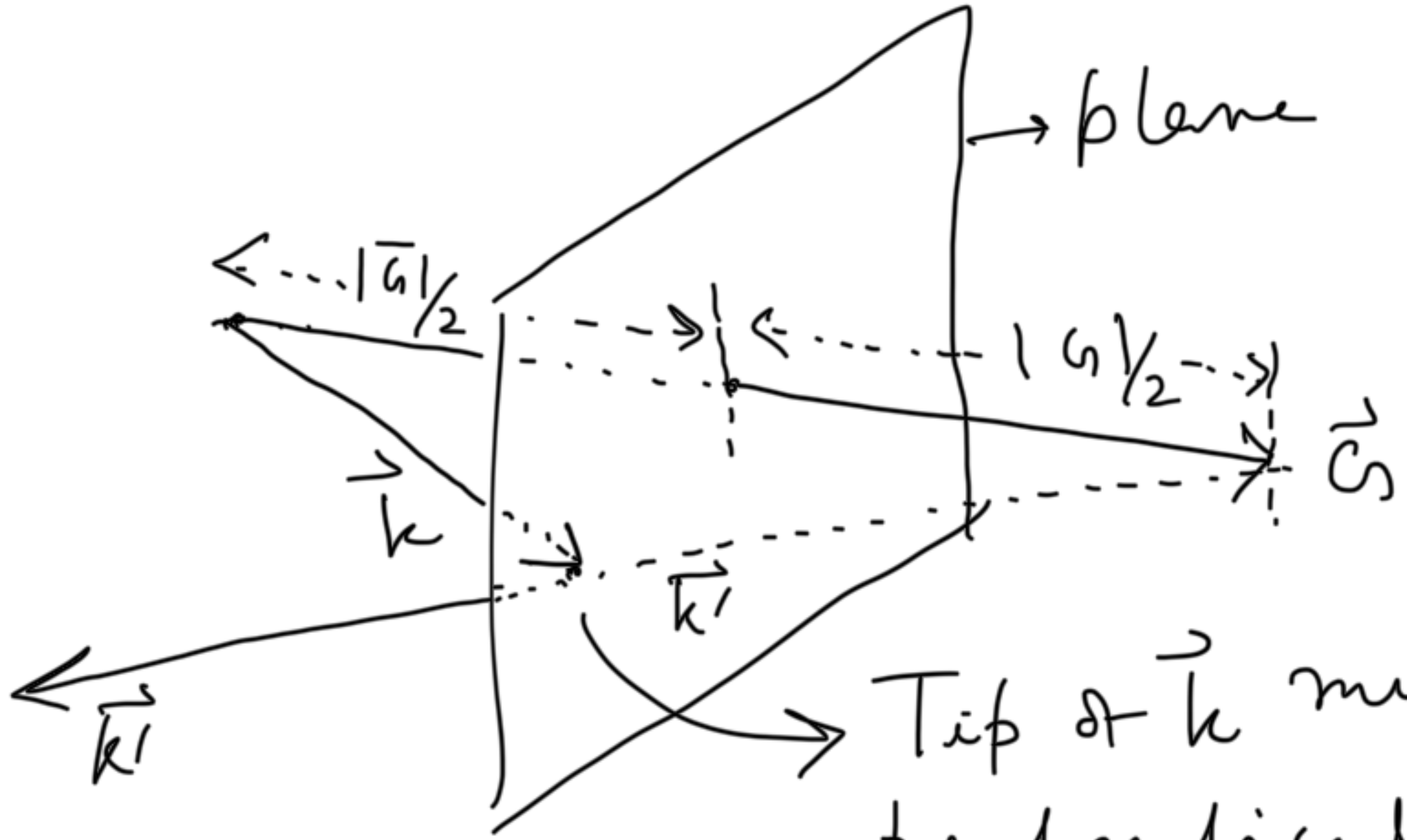
$$\therefore \vec k' = \vec k - \vec G$$

$$\Rightarrow |\vec k'|^2 = |\vec k|^2 - 2\vec k\cdot\vec G + |\vec G|^2$$

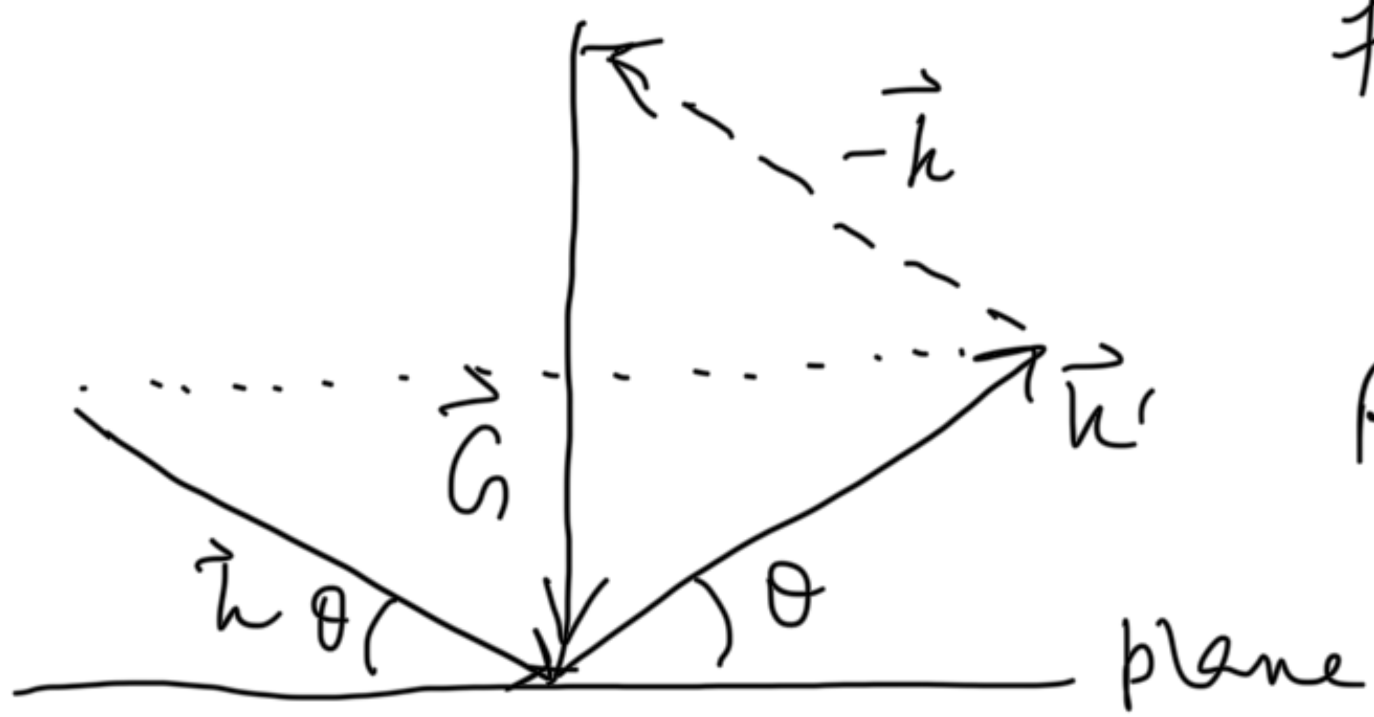
$$\Rightarrow \vec k\cdot\vec G = \frac{1}{2}|\vec G|^2 \Rightarrow \vec k\cdot\hat G = \frac{1}{2}|\vec G|$$

Similarly one can derive $\vec k'\cdot(-\hat G) = \frac{1}{2}|\vec G|$

$\Rightarrow$



Tip of $\vec{k}$ must be on the perpendicular bisector of $\vec{G}$ for constructive interference



Recall $\vec{G} = n\,\vec{G}_{min}$

$$|\vec{G}| = n\,\frac{2\pi}{d}$$

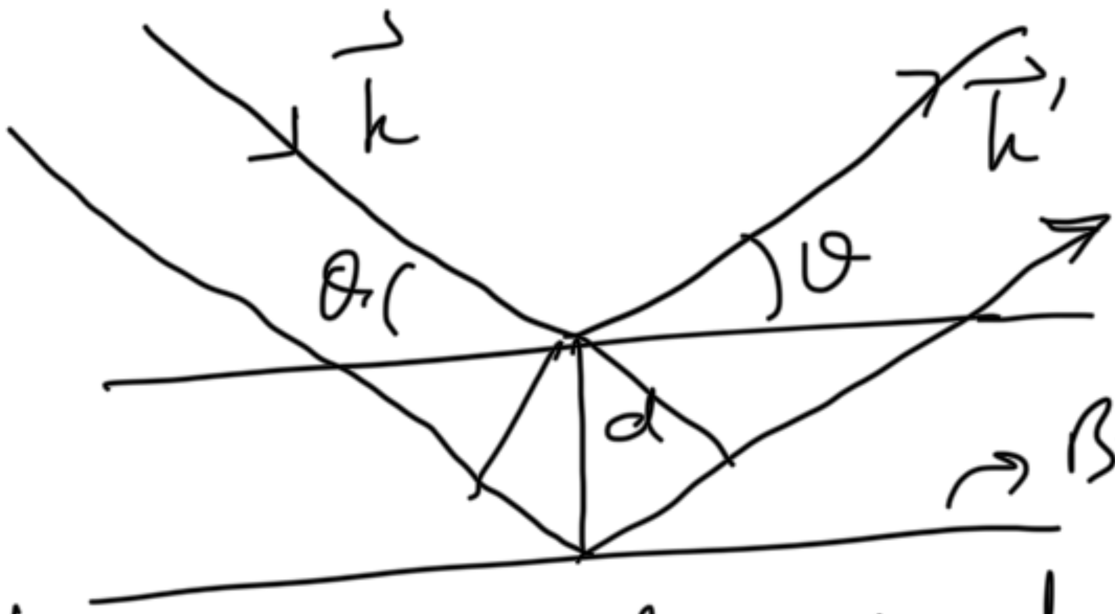
$$|G| = 2|k|\sin\theta$$

$$\therefore \underbrace{|k|}_{\frac{2\pi}{\lambda}}\sin\theta = n\,\frac{\pi}{d}$$

$$\Rightarrow \frac{2\pi}{\lambda}\sin\theta = n\,\frac{\pi}{d} \Rightarrow \boxed{2d\sin\theta = n\lambda}$$

Bragg condition.

simple picture of specular reflection.
$\theta = \theta'$



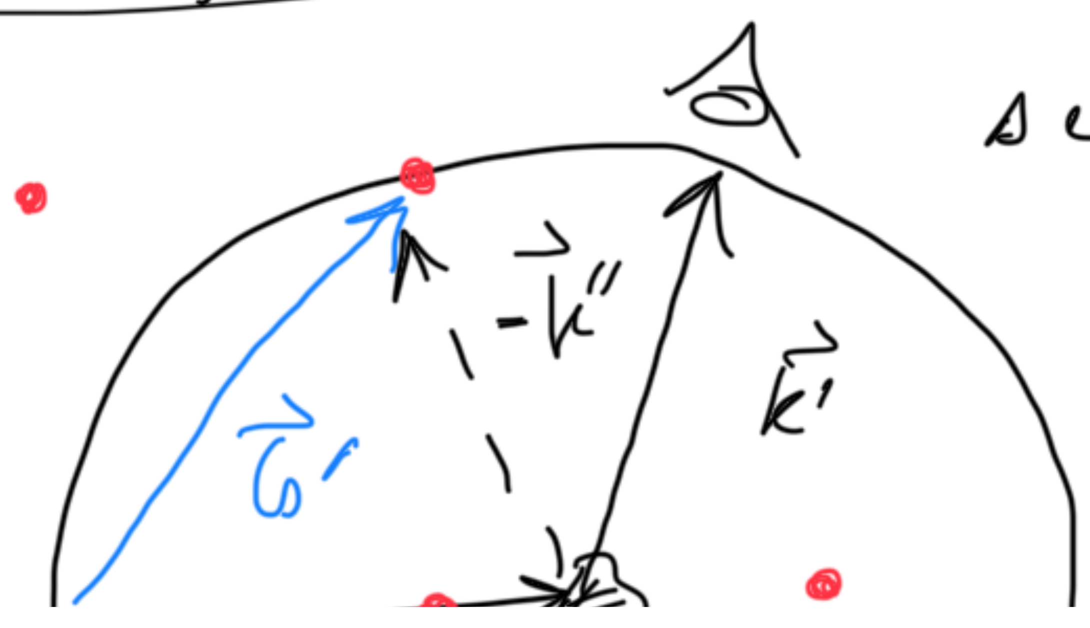
→ Bragg plane (crystal planes)

∴ Von Laue condition + elastic scattering = Bragg condition

∴ Periodic arrangement of scatterer + elastic scattery effectively lead to specular reflection from crystal planes.

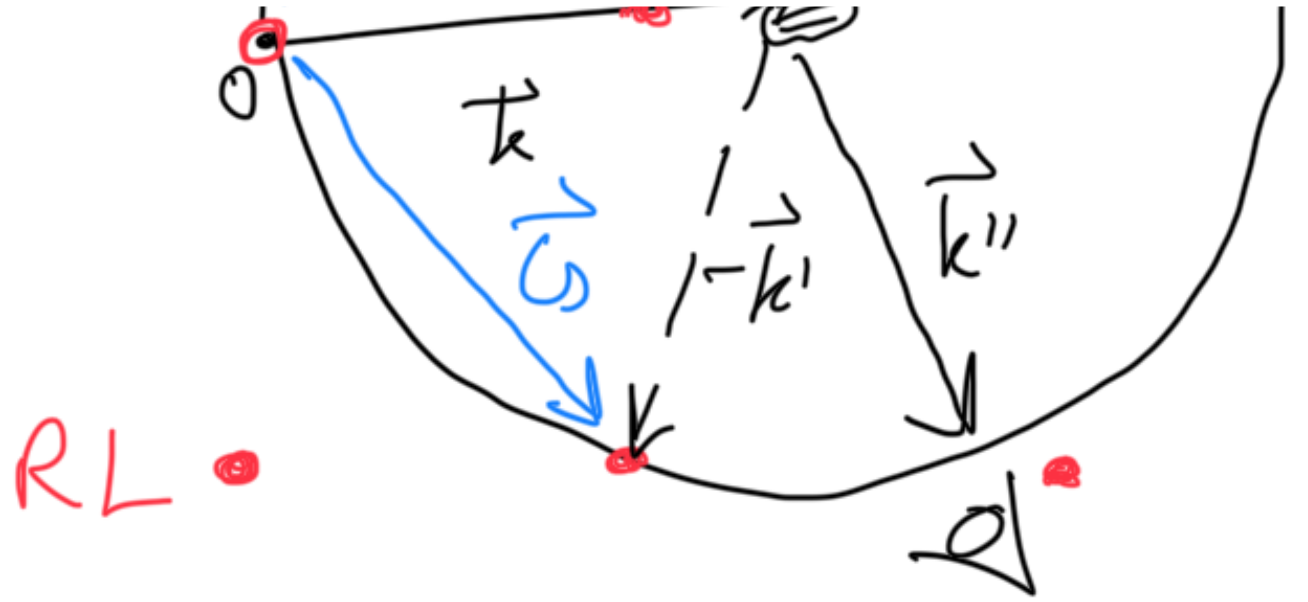
How to get the crystal structure.

(Bragg spot.)



search across the sph surface around crystal (single chunk) for bright spot.

Each time you find a bright spot you get a $\vec{G}$.

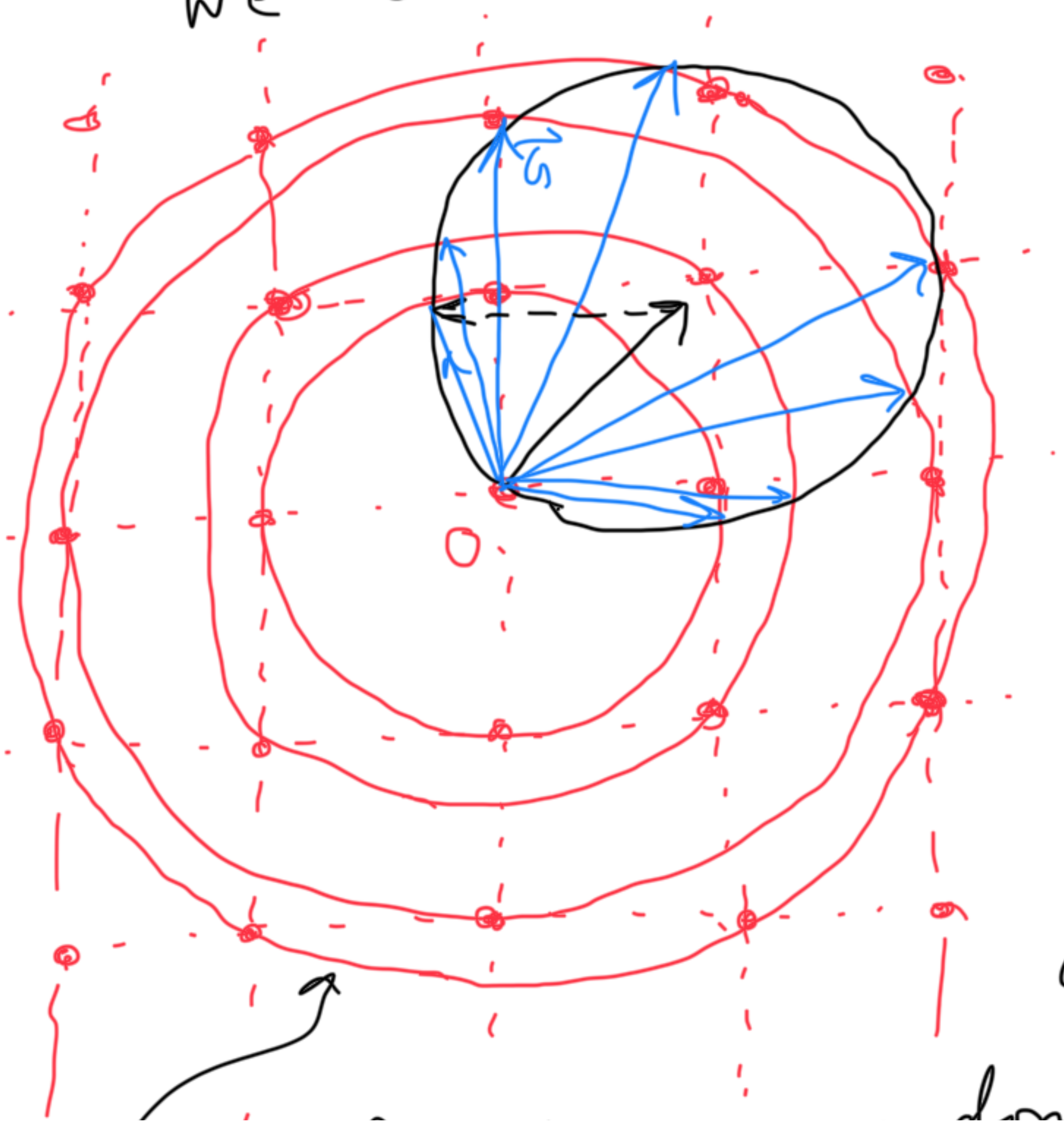


spot ...

However you are not sure to get a spot.

So we can vary $\vec{k}$ $\left(= \frac{2\pi}{\lambda}\right)$ ie λ.

We can also rotate the crystal about some axis $\parallel$ to $\vec{k}$



This way we can get a selection of $\{|\vec{G}|\}$.

However single crystals are difficult to get.

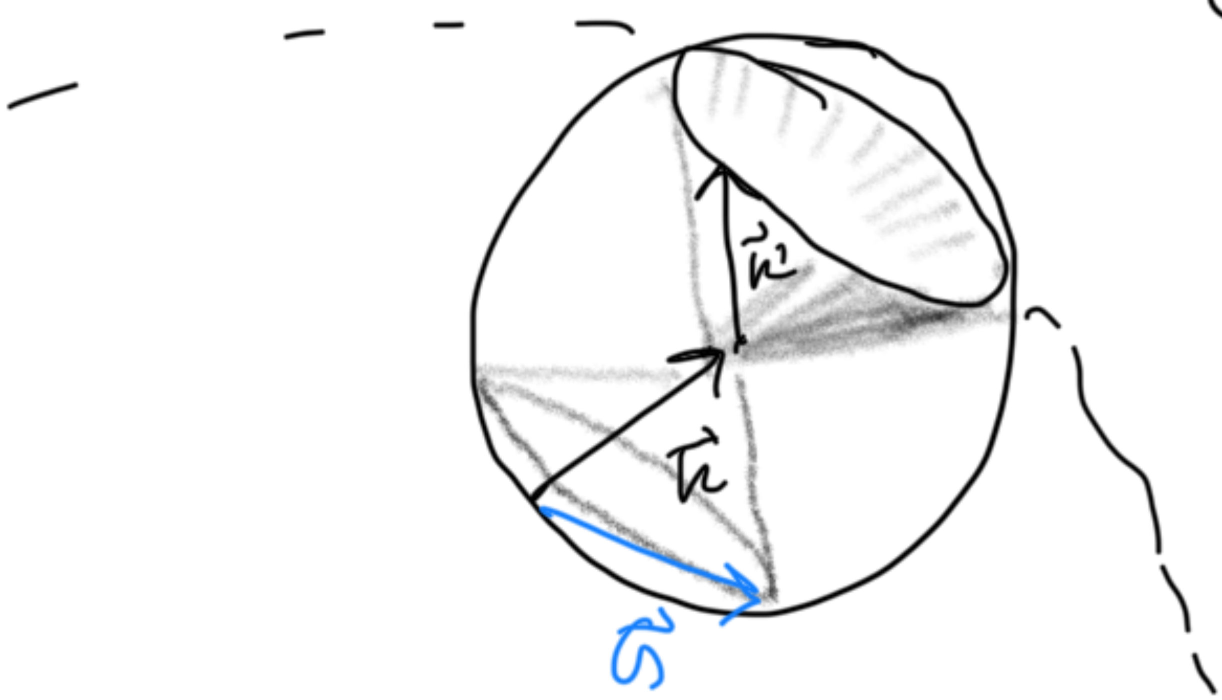
We use powder made of crystalline grains.

Each grain is a single crystal chunk.

... randomly oriented in a crystal.

Grain are randomly ...

No need of rotation. We will get spheres instead of circles which will cut the Ewald sph. in circles.



Once we have the $\{|\vec{G}|\}$ we can then go back to single crystal and fix $\vec{k}$ as per $|\vec{G}|$ to find orientation of $\vec{G}$ and find full reciprocal lattice (RL)

Recall: $FT(RL) \rightarrow BL \rightarrow$ the Bravais lattice.