Lecture #5

The reciprocal lattice

Def. If we have lattice vectors $\bar{a}_1, \bar{a}_2, \bar{a}_3$

$$\bar{R} = n_1 \bar{a}_1 + n_2 \bar{a}_2 + n_3 \bar{a}_3 \qquad \text{(Bravais lattice)}$$

$\Longrightarrow$ Reciprocal lattice vectors $\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$

Such that $\bar{a}_i \cdot \bar{b}_j = 2\pi \delta_{ij} = \begin{cases} 2\pi & i=j \\ 0 & i \neq j \end{cases}$

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

Set $\bar{b}_1 = C \cdot \underbrace{\bar{a}_2 \times \bar{a}_3}_{\text{vector perp. to both}}$

$$\bar{b}_1 \cdot \bar{a}_1 = 2\pi = C \cdot \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)$$

$$\Longrightarrow \quad C = \frac{2\pi}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)}$$

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

cell volume

Similarly $\bar{b}_2 = 2\pi \dfrac{\bar{a}_3 \times \bar{a}_1}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)}$

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

note: $\bar{a}_2$ and $\bar{a}_3$ do not need to be perp. to each other.

The reciprocal lattice is also a Bravaislattice

Lattice planes

A lattice plane is defined from 3 Bravais lattice points that are not all aligned.

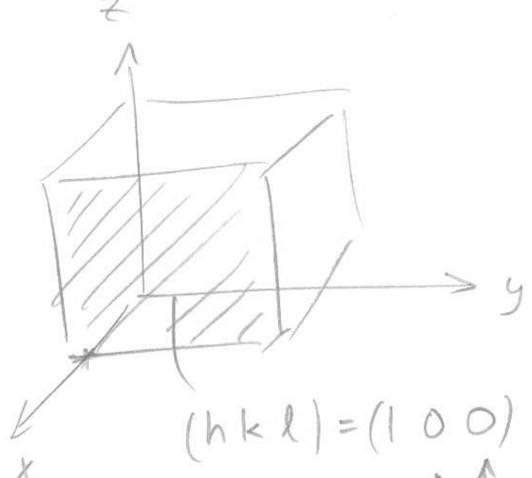
Parallel planes (infinite amount) $\Rightarrow$ family of lattice planes

The $\boxed{\text{Miller indices}}$ $(h\,k\,l)$ are used to describe a family of lattice planes.

Construction

1. Determine where a plane cuts the axes, expressed in lattice parameters $\bar{a}_1, \bar{a}_2, \bar{a}_3$
2. Invert the three numbers
3. Multiply by a common number to reach the lowest possible integer numbers

$$\Longrightarrow (h\,k\,l)$$

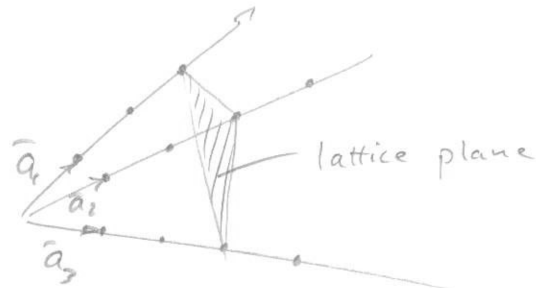


$(h\,k\,l) = (1\,0\,0)$

plane does not cross $\hat{y}, \hat{z}$

$\bar{a}_1$, $\bar{a}_2$ and $\bar{a}_3$ do not need to be $\perp$ to each other.

Ex



① Intercepts $\bar{a}_1$: 3

a_2 : 3

a_3 : 3

② Invert $\frac{1}{3}\ \frac{1}{3}\ \frac{1}{3}$

③ Multiply by 3: $(1\,1\,1) = (h\,k\,l)$

Miller index for all planes parallel with this

× Distance between planes decrease with increasing M.I.

× Atomic/lattice point density increase with decreasing M.I.

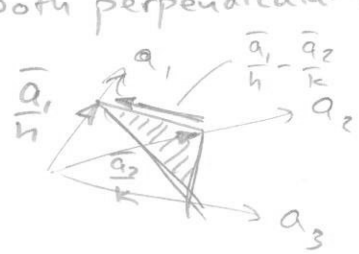
× Important planes: High density $\Longleftrightarrow$ low Miller Indices

IMPORTANT

The reciprocal lattice vector $\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$ is perpendicular to the (real space) lattice plane with Miller index $(h\,k\,l)$

Proof: Construct two different vectors in the lattice plane and show that they are both perpendicular to $\bar{G}$.

$\frac{\bar{a}_1}{h} - \frac{\bar{a}_2}{k}$ is one vector



$$\bar{G}(hkl) \cdot \left(\frac{\bar{a}_1}{h} - \frac{\bar{a}_2}{k}\right) =$$

$$= (h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3) \cdot \left(\frac{\bar{a}_1}{h} - \frac{\bar{a}_2}{k}\right) = 2\pi + 0 + 0 - 0 - 2\pi - 0 = 0$$

$\left(\frac{\bar{a}_1}{h} - \frac{\bar{a}_3}{l}\right)$ is another vector $\Longrightarrow$ ... Same thing

$\Longrightarrow \bar{G} \perp (h\,k\,l)$

Reciprocal lattice - properties

1) $\bar{G}(hkl) = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$ is $\perp$ to (hkl)

2) The distance between planes (hkl)

$$d(hkl) = \frac{2\pi}{|\bar{G}(hkl)|}$$

3) If a function $f(\bar{r})$ is periodic in the direct lattice

$f(\bar{r}) = f(\bar{r}+\bar{R})$, then

$$f(\bar{r}) = \sum_{\bar{G}} a_{\bar{G}} e^{i\bar{G}\cdot\bar{r}}$$

sum only over reciprocal lattice points

4) The cell volume of the reciprocal lattice

$$V_g = \frac{(2\pi)^3}{V_c}$$

5) The reciprocal lattice of a reciprocal lattice is the direct lattice

6) The reciprocal lattice is the fourier transform of the direct lattice

7) R.L of bcc is an fcc-lattice with side $\frac{4\pi}{a}$

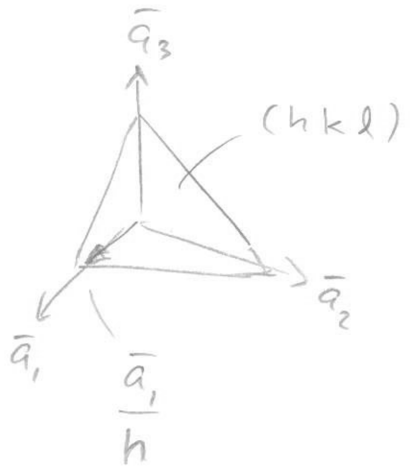
— " — fcc is a bcc — " —

Conventional Cell

Show property 2) $d(hkl) = \frac{2\pi}{|G(hkl)|}$

One plane goes through the origin

Determine distance between origin and plane (hkl)

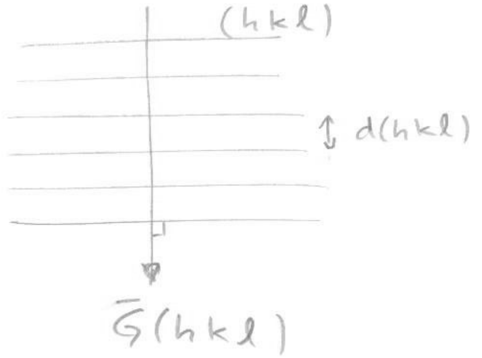


A unit vector normal to (hkl) is $\hat{n} = \frac{\bar{G}(hkl)}{|\bar{G}(hkl)|}$

$$d(hkl) = \frac{\bar{a}_1}{h} \cdot \hat{n} =$$

$$= \frac{\bar{a}_1}{h} \cdot \frac{h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3}{|\bar{G}(hkl)|} =$$

$$= \frac{2\pi}{|\bar{G}(hkl)|}$$



The planes act like "wavefronts" of the planewave

Wavelength $\lambda = \frac{2\pi}{k} = d$, $k = |\bar{G}|$ $\quad e^{i\bar{G}\cdot\bar{r}}$

Show property 3)

If $f(\bar{r}) = f(\bar{r}+\bar{R})$ then $f(\bar{r}) = \sum_{\bar{G}} a_{\bar{G}} e^{i\bar{G}\cdot\bar{r}}$

Proof

$$\left.\begin{aligned} \text{Write } f(\bar{r}) &= \sum_{\bar{k}} a_{\bar{k}} e^{i\bar{k}\cdot\bar{r}} \\ f(\bar{r}+\bar{R}) &= \sum_{\bar{k}} a_{k} e^{i\bar{k}\cdot(\bar{r}+\bar{R})} \end{aligned}\right\} \Rightarrow e^{i\bar{k}\cdot\bar{R}} = 1$$

$\bar{k}\cdot\bar{R} = n\cdot 2\pi$

integer

(fourier series)

But the definition of $\bar{G} \Rightarrow \bar{G}\cdot\bar{R} = n\cdot 2\pi$

since $\bar{a}_i\cdot\bar{b}_j = 2\pi\,\delta_{ij}$

If $\bar{k}$ other than $\bar{G}$:

assume that $\bar{k}$ contains $c\,\bar{b}_1$, $c < 1$

$$\bar{k}\cdot\bar{R} = \ldots + \underbrace{n_1\cdot c}_{\neq \text{ integer for any } n_1}\cdot 2\pi$$

$\Longrightarrow$ only $\bar{k} = \bar{G}$ needed and required.

$\bar{G}$ - points spaced $\sim \frac{2\pi}{a} \sim 2\cdot 10^{10}\ m^{-1}$

Electrons $k = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L} \Longrightarrow$ space $\sim 600\ m^{-1}$

sample size $\sim$ 1cm

$\Longrightarrow$ Saves a lot to sum only over $\bar{G}$

to describe electron properties

since these are periodic in the lattice.

Show property 4) $$V_g = \frac{(2\pi)^3}{V_c}$$

$$V_c = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)$$

$$V_g = \bar{b}_1 \cdot (\bar{b}_2 \times \bar{b}_3)$$

use $$\bar{b}_3 = 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)} = 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{V_c}$$

$$V_g = \bar{b}_1 \cdot \left(\bar{b}_2 \times \left(\frac{2\pi}{V_c} \bar{a}_1 \times \bar{a}_2 \right) \right) =$$

$$= \frac{2\pi}{V_c} \bar{b}_1 \cdot \left\{ (\bar{b}_2 \cdot \bar{a}_2)\, \bar{a}_1 - (\bar{b}_2 \cdot \bar{a}_1)\, \bar{a}_2 \right\}$$

since $\bar{B} \times (\bar{C} \times \bar{D}) = (\bar{B} \cdot \bar{D})\,\bar{C} - (\bar{B} \cdot \bar{C})\,\bar{D}$

but $\bar{b}_2 \cdot \bar{a}_2 = 2\pi$ and $\bar{b}_2 \cdot \bar{a}_1 = 0$

$$\Rightarrow V_g = \frac{2\pi}{V_c} \bar{b}_1 \cdot (2\pi \bar{a}_1) = \frac{(2\pi)^3}{V_c} \qquad (\bar{b}_1 \cdot \bar{a}_1 = 2\pi)$$

Show property 5) RL of RL is direct lattice

Calculate reciprocal lattice $\bar{c}_1, \bar{c}_2, \bar{c}_3$ of $\bar{b}_1, \bar{b}_2, \bar{b}_3$

$$\bar{c}_1 = 2\pi \frac{\bar{b}_2 \times \bar{b}_3}{\bar{b}_1 \cdot (\bar{b}_2 \times \bar{b}_3)} = \frac{2\pi}{V_g} (\bar{b}_2 \times \bar{b}_3) =$$

$$= \frac{2\pi}{\frac{(2\pi)^3}{V_c}} \cdot \bar{b}_2 \times \left(\frac{2\pi}{V_c} \bar{a}_1 \times \bar{a}_2 \right) = \frac{1}{2\pi} \bar{b}_2 \times (\bar{a}_1 \times \bar{a}_2) = \left\{ \begin{matrix} \text{as} \\ \text{above} \end{matrix} \right\} =$$

$$= \frac{1}{2\pi} \left\{ \underbrace{(\bar{b}_2 \cdot \bar{a}_2)}_{2\pi} \bar{a}_1 - \underbrace{(\bar{b}_2 \cdot \bar{a}_1)}_{0} \bar{a}_2 \right\} = \bar{a}_1$$

etc.

Brillouin zones

The Wigner-Seitz cell of the reciprocal lattice is called the <u>first Brillouin zone</u>.

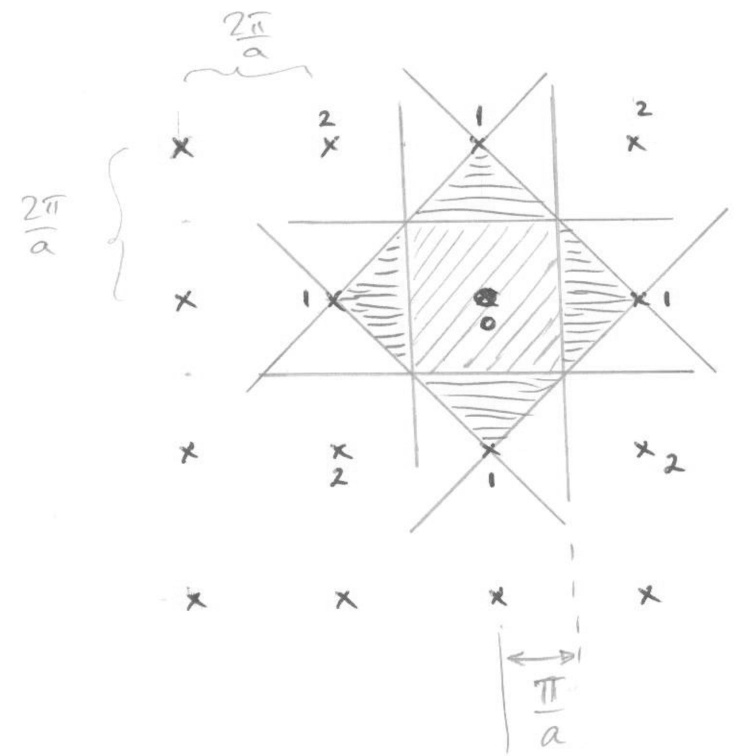
Ex. Sketch 1:st and 2:nd Brillouin zones of a quadratic lattice, 2D

Solution Do calc. for 3D with a help vector or find $\bar{b}_1$ and $\bar{b}_2$ from $\bar{a}_i \cdot \bar{b}_j = 2\pi \delta_{ij}$

Set $\bar{a}_1 = a\hat{x}$, $a_2 = a\hat{y}$ help vector $\bar{a}_3 = a\hat{z}$ $V_c = a^3$

$$\Rightarrow \bar{b}_1 = \frac{2\pi}{V_c} \bar{a}_2 \times \bar{a}_3 = \frac{2\pi}{a^3} a^2 \hat{x} = \frac{2\pi}{a} \hat{x} \quad ; \quad \bar{b}_2 = \frac{2\pi}{a} \hat{y}$$

$\Rightarrow$ quadratic lattice with lattice param $\frac{2\pi}{a}$



0 : $\bar{k} = 0$

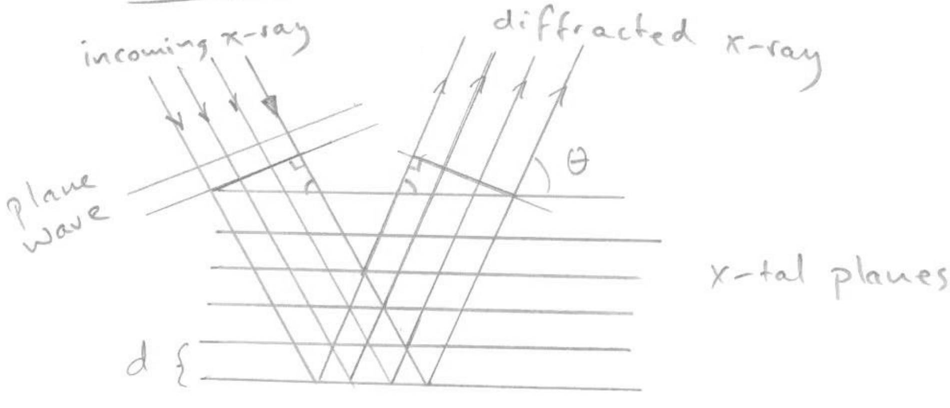
1 : nearest neighbor

2 : 2nd nearest

First Brillouin zone

Second Brillouin zone

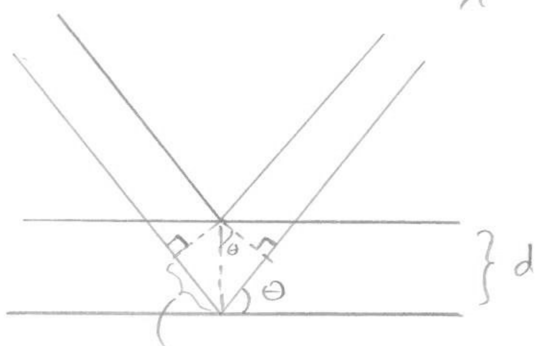
X-ray diffraction



Diffraction $\Longleftrightarrow$ constructive interference

Planewave $e^{i\bar{k}\cdot\bar{r}}$ $\longrightarrow$ diffracted $e^{i\bar{k}'\cdot\bar{r}}$

$$|\bar{k}| = |\bar{k}'| = \frac{2\pi}{\lambda} \qquad \lambda \text{ wavelength}$$



$d\cdot\sin\theta$

Bragg's law

$$\boxed{2d\cdot\sin\theta = n\cdot\lambda} \qquad n = 1, 2, 3\ldots$$

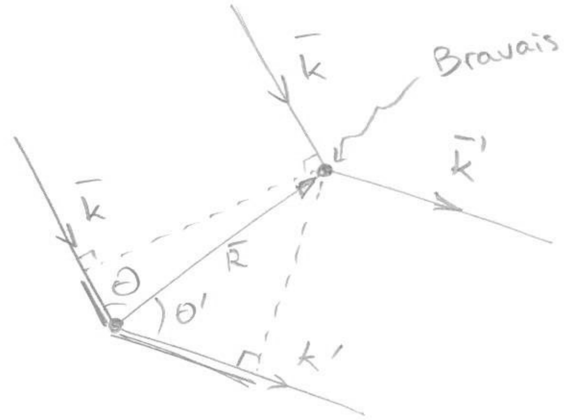
Condition for const. int.

$$\frac{n\cdot\lambda}{2d} \leq 1 \Rightarrow \underline{\lambda_{max} = 2d}$$

In a crystal: Any family of lattice planes may give x-ray diffraction

d is given by Miller index (hkl):

$$d = \frac{2\pi}{|\bar{G}(hkl)|}$$



$$\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$$

$$|\bar{k}| = |\bar{k}'| = \frac{2\pi}{\lambda}$$ Elastic scattering

$$R\cdot\cos\theta + R\cos\theta' = n\cdot\lambda \quad \Big|\cdot\frac{2\pi}{\lambda}$$

$$\underbrace{\frac{2\pi}{\lambda}R\cos\theta}_{-\bar{k}\cdot\bar{R}} + \underbrace{\frac{2\pi}{\lambda}R\cos\theta'}_{\bar{k}'\cdot\bar{R}} = n\cdot\frac{2\pi}{\cancel{\lambda}}\cdot\cancel{\lambda}$$

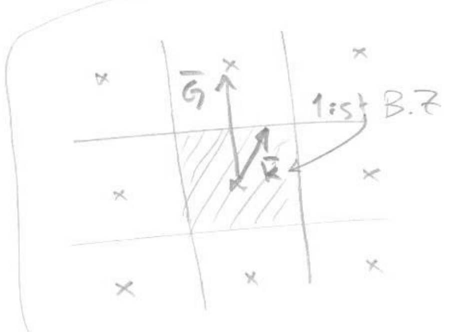
Define $\Delta\bar{k} = \bar{k}' - \bar{k} \implies \Delta\bar{k}\cdot\bar{R} = n\cdot 2\pi$

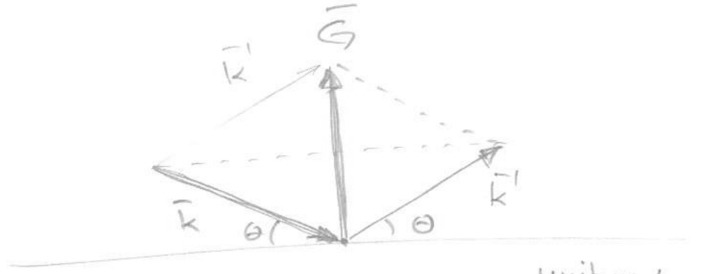
But $\bar{G}$ are defined by $\bar{k}\cdot\bar{R} = n\cdot 2\pi$

$\implies \Delta\bar{k} \in \bar{G}$ reciprocal lattice vector

$$\boxed{\Delta\bar{k} = \bar{G}}$$ Condition for diffraction of Bravaislattice

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





(h k l) crystal plane

From the figure: $\boxed{\bar{k}\cdot\hat{G} = \frac{1}{2}G}$ Laue condition

unit vector

or $\bar{k}\cdot\bar{G} = \frac{1}{2}G^2$

Scattering when $\bar{k}$ touches surface to Brillouin zone

Diffraction conditions

1. $\Delta \bar{k} = \bar{G}$ Bravais lattice

2. For lattice + basis <u>also</u>:

$$s = \sum_j f_j e^{i\bar{G}\cdot\bar{r}_j} \neq 0$$

sum over the basis

Here $f_j \approx Z_j$ atomic number

atomic form factor

Case 2) The scattered wave is sum of individual rays and contains a factor from the cell / basis

$$s_{\bar{G}} = \sum_{j=1}^{N} f_j e^{i\bar{G}\cdot\bar{r}_j}$$

N ions in basis

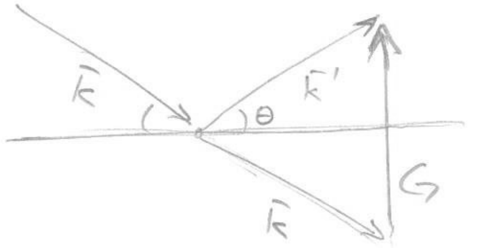
Geometric structure factor

electron density

The atomic form factor $f_j = \underbrace{\int_{\text{ion } j} \rho(\bar{r}) e^{i\bar{G}\cdot\bar{r}} d^3r}_{\text{includes all electrons...}}$

Intensity $\sim |s_{\bar{G}}|^2$

Quadratic expression



$$|\bar{G}| = 2|\bar{k}|\sin\theta = \frac{4\pi}{\lambda}\sin\theta$$

$$G^2 = \frac{16\pi^2}{\lambda^2}\sin^2\theta$$

For the cubic case: $\bar{G} = h\cdot\frac{2\pi}{a}\hat{x} + k\cdot\frac{2\pi}{a}\hat{y} + l\cdot\frac{2\pi}{a}\hat{z}$

$$G^2 = \left(\frac{2\pi}{a}\right)^2(h^2+k^2+l^2)$$

$$\Rightarrow \quad \frac{16\pi^2}{\lambda^2}\sin^2\theta = \frac{4\pi^2}{a^2}(h^2+k^2+l^2)$$

$$\boxed{\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+k^2+l^2)}$$

Basis $\Rightarrow$ additional conditions on $h\,k\,l$ for diffraction.