Chap 2 Wave diffraction and the reciprocal lattice

- Braggs' theory of diffraction (1913)
- Reciprocal lattice
- Laue's theory of diffraction (June 1912)
- Bragg theory = Laue theory

Later than Laue's theory, but simpler.

The analysis of diffraction here applies to the diffraction of EM wave, electron, neutron … etc

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Laue thought that X-ray might scatter off crystals in the way that ordinary light scatters off a diffraction grating.

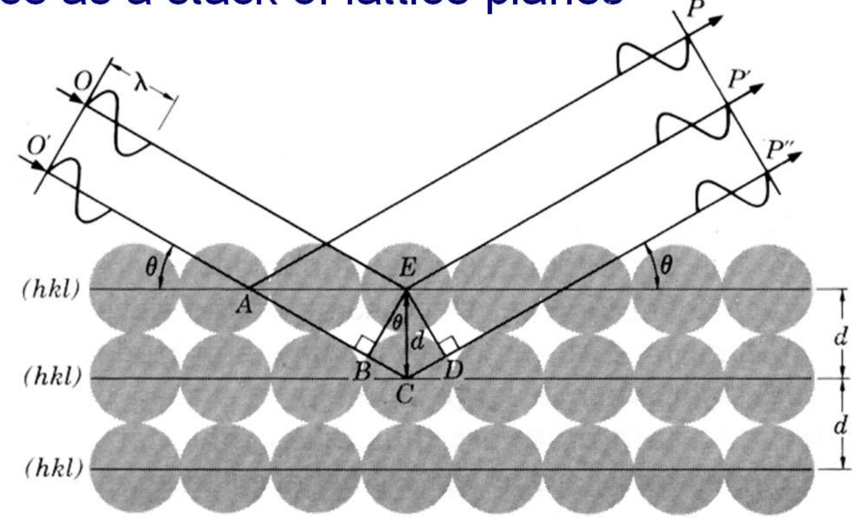
He discussed

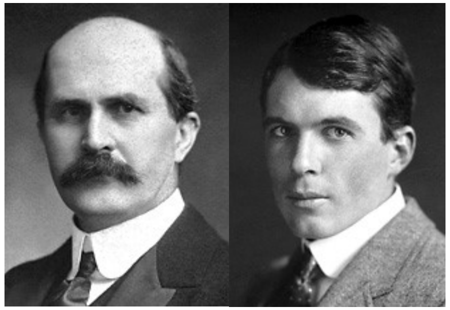
his idea with colleagues Sommerfeld, Wien and others with the result of encountering a strong disbelief in a significant outcome of any diffraction experiment based upon the regularity of the internal structure of crystals. It was argued that the inevitable temperature motion of the atoms would impair the regularity of the grating to such an extent that no pronounced diffraction maxima could be expected. —Ewald (1962), p. 42

- For example, For NaCl, the thermal fluctuation is expected to be $2 \cdot 10^{-9}$ cm ~ the wavelength of X-ray 10^{-9} cm (Marder, p.43)
- Now we know that thermal fluctuation would only broaden the diffraction peaks, but not distroy them.

Braggs' view of the diffraction (1913, father and son)

Treat the lattice as a stack of lattice planes





1915

- Specular reflection from crystal planes when

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

(typically $10^3 \sim 10^5$ planes)

- Difference from the usual reflection:

  $\lambda > 2d$, no reflection

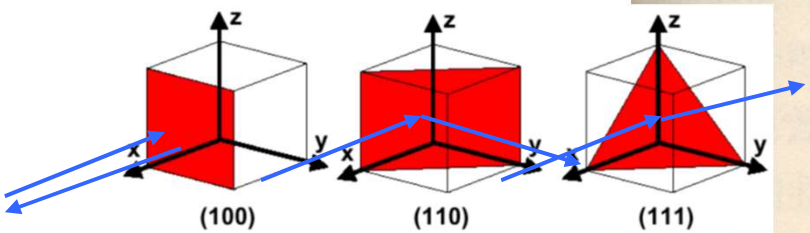
  $\lambda < 2d$, reflection only at certain angles

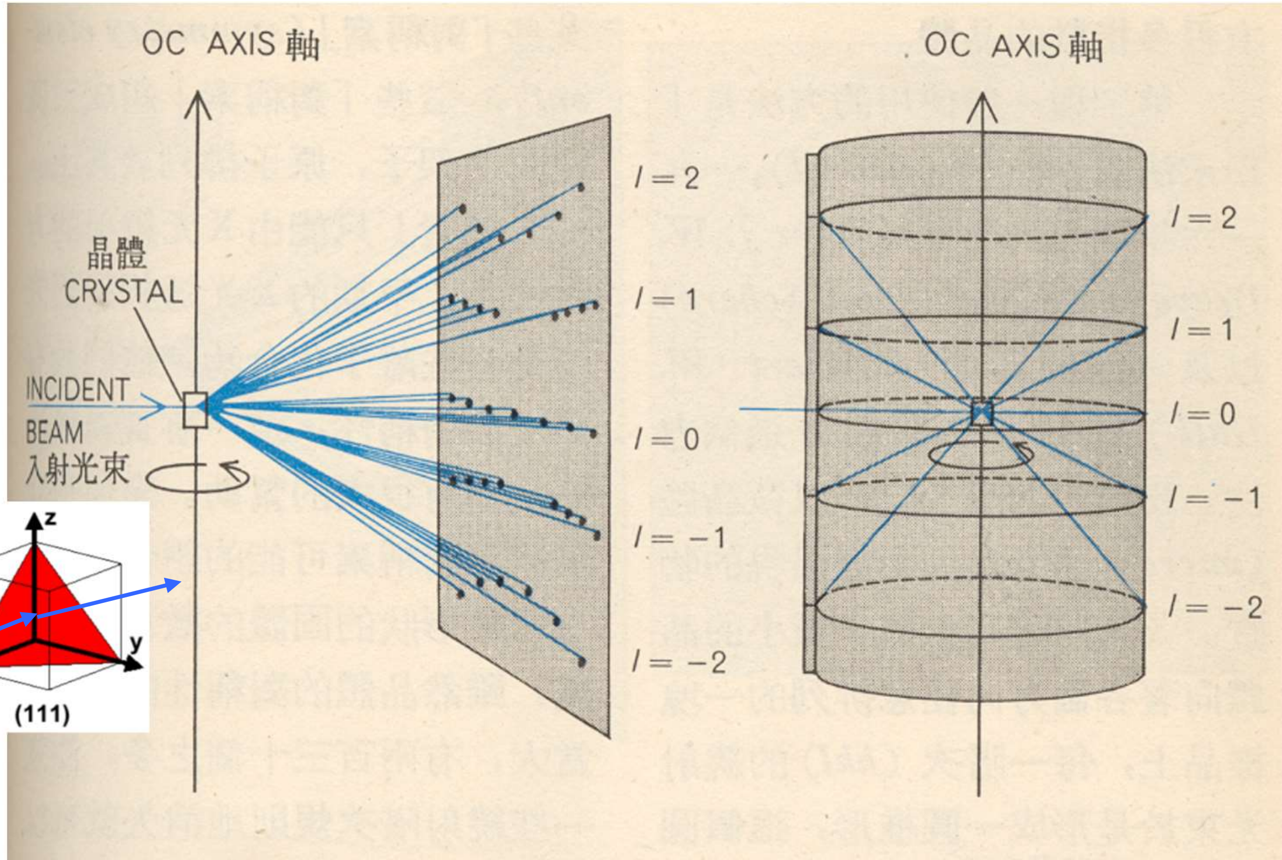
- Measure λ, θ → get distance between crystal planes d

The Bragg derivation is simple but convincing only because it produces the correct result -- Kittel

Single-crystal diffraction

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





〔圖七〕旋轉式攝影（ROTATION PHOTOGRAPHS）

作旋轉式攝影時，將X光對準一小塊晶體，這塊晶體繞著與一主晶軸平行之軸旋轉，繞射光束可由一平的感光板(左)或圓柱形的感光片（右）記錄，所有反射光束的像都排在層線上，本圖之晶軸沿 OC，層線對應於 $l=0$, $l=1$, $l=2$；所有的點 對應於 全部不同的 h 及 k。

- Braggs' theory of diffraction
- **Reciprocal lattice** **(for Bravais lattice)**
- Laue's theory of diffraction
- Bragg theory = Laue theory

important

Reciprocal lattice (倒晶格) in *k*-space

Bravais Lattice primitive vectors $\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3$	↔	Reciprocal lattice primitive vectors $\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3$

Def. 1

$$\vec{b}_1\cdot\vec{a}_1 = 2\pi,\ \vec{b}_1\cdot\vec{a}_2 = \vec{b}_1\cdot\vec{a}_3 = 0,$$
$$\vec{b}_2\cdot\vec{a}_2 = 2\pi,\ \vec{b}_2\cdot\vec{a}_3 = \vec{b}_2\cdot\vec{a}_1 = 0,$$
$$\vec{b}_3\cdot\vec{a}_3 = 2\pi,\ \vec{b}_3\cdot\vec{a}_1 = \vec{b}_3\cdot\vec{a}_2 = 0.$$

$\vec{b}_1 \propto \vec{a}_2\times\vec{a}_3$ because of orthogonality, then use $\vec{b}_1\cdot\vec{a}_1 = 2\pi$ to determine the constant.

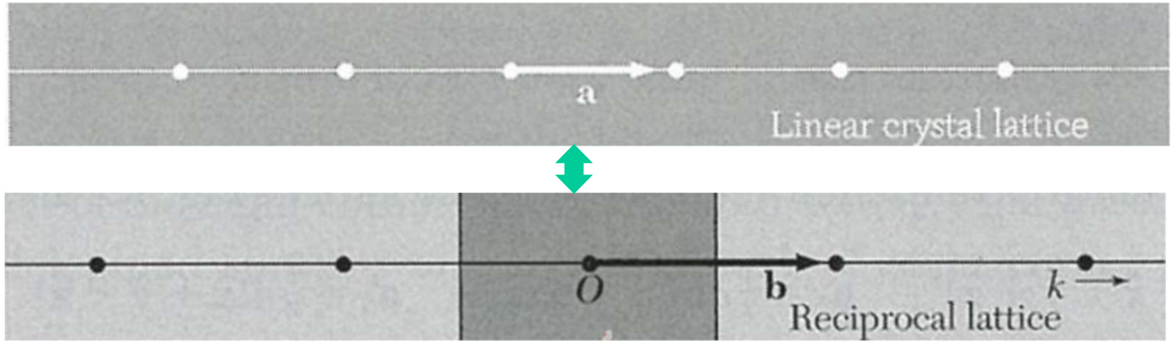
Def. 2

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

- Every Bravais lattice has a reciprocal lattice
- The reciprocal lattice of a reciprocal lattice is the original lattice
- $\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3) = \dfrac{(2\pi)^3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} = \dfrac{(2\pi)^3}{V_{cell}}$ ← volumn of a unit cell in reciprocal lattice

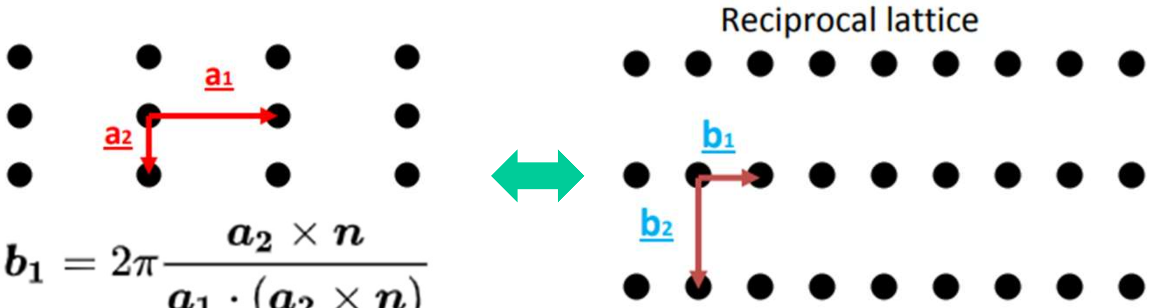
Example of reciprocal lattice

1-dim



$$\boldsymbol{b} = 2\pi\frac{\boldsymbol{a}}{a^2}$$

2-dim



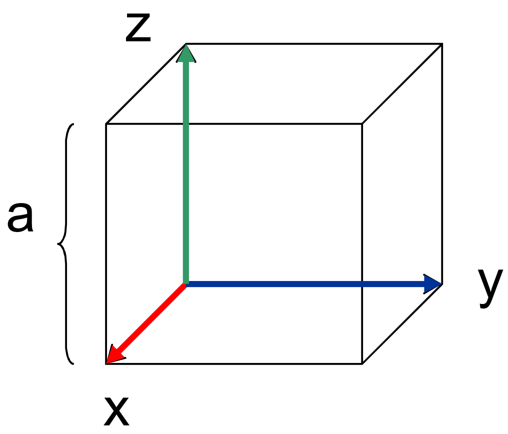
$$\boldsymbol{b}_1 = 2\pi\frac{\boldsymbol{a}_2 \times \boldsymbol{n}}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{n})}$$

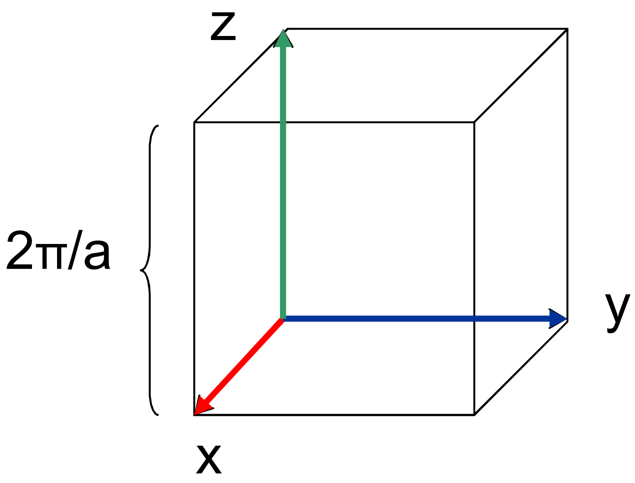
$$\boldsymbol{b}_2 = 2\pi\frac{\boldsymbol{n} \times \boldsymbol{a}_1}{\boldsymbol{a}_2 \cdot (\boldsymbol{n} \times \boldsymbol{a}_1)}$$

- Reciprocal lattice has unit [1/L], the same as wave vector ***k***'s
- When one lattice shrinks, the other expand (but you can't compare their size since they have different units)
- When we rotate a crystal, both lattices rotate with the same angle

3-dim

Simple cubic lattice



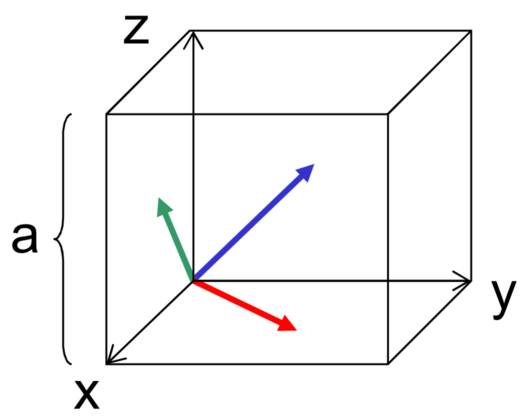


$$\vec{a}_1 = a\hat{x},$$
$$\vec{a}_2 = a\hat{y},$$
$$\vec{a}_3 = a\hat{z}.$$
$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = a^3$$

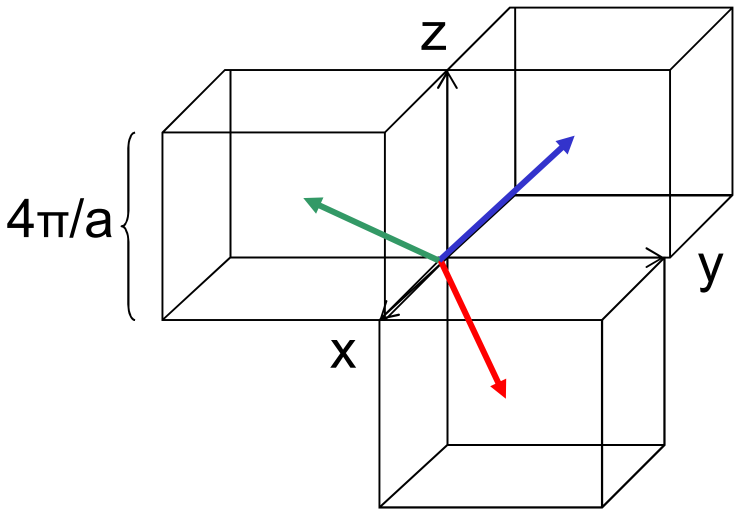
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{a}\hat{x},$$
$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{a}\hat{y},$$
$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{a}\hat{z}.$$

$$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \left(\frac{2\pi}{a}\right)^3$$

FCC lattice



BCC lattice



$$\vec{a}_1 = \frac{a}{2}\left(\hat{x}+\hat{y}\right),$$

$$\vec{a}_2 = \frac{a}{2}\left(\hat{y}+\hat{z}\right),$$

$$\vec{a}_3 = \frac{a}{2}\left(\hat{z}+\hat{x}\right).$$

$$\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = \frac{a^3}{4}$$

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} = \frac{4\pi}{a}\frac{1}{2}\left(\hat{x}+\hat{y}-\hat{z}\right),$$

$$\vec{b}_2 = 2\pi\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} = \frac{4\pi}{a}\frac{1}{2}\left(-\hat{x}+\hat{y}+\hat{z}\right),$$

$$\vec{b}_3 = 2\pi\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} = \frac{4\pi}{a}\frac{1}{2}\left(\hat{x}-\hat{y}+\hat{z}\right).$$

$$\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3) = \frac{1}{2}\left(\frac{4\pi}{a}\right)^3$$

Two simple properties:

1. $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \ (n_1, n_2, n_3 \in Z) \quad \in \text{direct lattice}$

$\vec{G} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3 \ (k_1, k_2, k_3 \in Z) \quad \in \text{reciprocal lattice}$

$\Rightarrow \vec{G}\cdot\vec{R} = 2\pi(n_1k_1 + n_2k_2 + n_3k_3) = 2\pi \times \text{integer.}$

$\left(\therefore \ \exp(i\vec{G}\cdot\vec{R}) \ \text{ is always equal to 1}\right)$

2. Conversely, assume **G** · **R**=2π×integer for all **R**,

then **G** must be a reciprocal lattice vector.

For example, if

$$\boxed{\begin{aligned} &\vec{G}\cdot\vec{a}_1 = 2\pi h, \\ &\vec{G}\cdot\vec{a}_2 = 2\pi k, \\ &\vec{G}\cdot\vec{a}_3 = 2\pi l, \quad (h, k, l \in Z) \\ \text{then} \quad &\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 (\equiv \vec{G}_{hkl}). \end{aligned}}$$

Application of reciprocal lattice:

important

If f(**r**) has lattice translation symmetry, that is, f(**r**)=f(**r**+**R**) for any lattice vector **R**, then it can be expanded as,

$$f(\vec{r}) = \sum_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} f_{\vec{G}}\,,$$ where **G** is the reciprocal lattice vector.

e.g., charge density

Pf: Fourier expansion

$$f(\vec{r}) = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} f(\vec{k}), \qquad \leftarrow \vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z), \quad n_x, n_y, n_z \in Z$$

$$\Rightarrow \quad f(\vec{r}+\vec{R}) = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} e^{i\vec{k}\cdot\vec{R}} f(\vec{k}) = f(\vec{r})$$

Orthogonality:

$$\sum_k a_k e^{ikx} = 0$$

$$\to a_k = 0 \ \text{ for } \forall k$$

$$\Rightarrow \quad \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \left(e^{i\vec{k}\cdot\vec{R}} - 1\right) f(\vec{k}) = 0$$

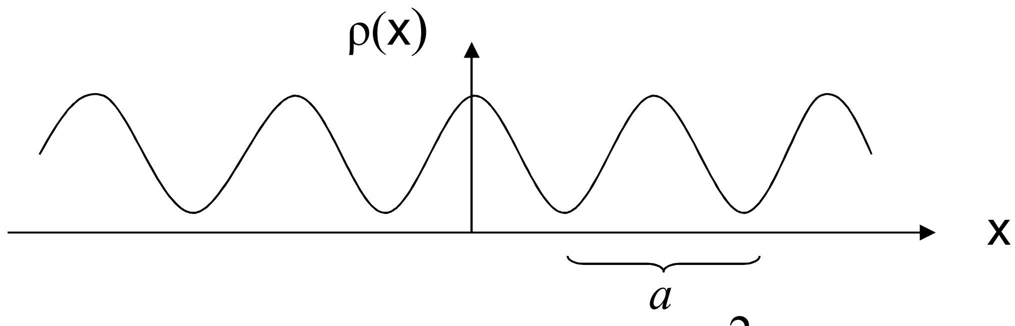
$$\Rightarrow \quad e^{i\vec{k}\cdot\vec{R}} = 1 \ \text{ for } \forall\ \vec{R} \quad \Rightarrow \quad \vec{k} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 = \vec{G}_{hkl} \quad \forall\ h, k, l$$

The expansion above is ***very*** general, it applies to

- every Bravais lattice (bcc, fcc, tetragonal, orthorombic...)
- every dimension (1, 2, and 3)

All you need to do is to find out the reciprocal lattice vectors **G.**

For example, charge density in a *1-dim* crystal



$$\rho(x)=\sum_k e^{ikx}\rho(k),\quad k=n\frac{2\pi}{L},\, n\in Z$$

$$\rho(x+a)=\sum_k e^{ikx}e^{ika}\rho(k)=\rho(x)$$

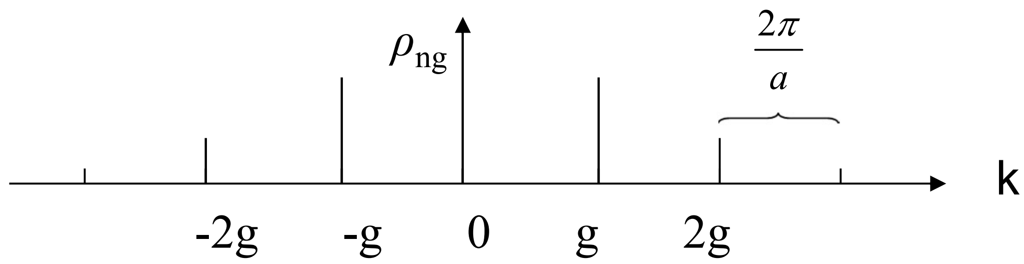
Therefore, $e^{ika}=1$

$$\rightarrow\quad k=n\frac{2\pi}{a}\equiv ng$$

$$\rho(x)=\sum_{n=-\infty}^{\infty} e^{ingx}\rho(ng)$$

$$\sum_k a_k e^{ikx}=0$$

$$\rightarrow a_k=0\ \text{ for } \forall k$$



reciprocal lattice points: ng

Summary

Direct lattice	Reciprocal lattice
cubic (a)	cubic ($2\pi/a$)
fcc (a)	bcc ($4\pi/a$)
bcc (a)	fcc ($4\pi/a$)
hexagonal (a,c)	hexagonal ($4\pi/\sqrt{3}a, 2\pi/c$) and rotated by 30 degrees

(See Prob.3)

The reciprocal lattice is useful in

- Fourier decomposition of a lattice-periodic function
- von Laue's diffraction condition **k**' = **k** + **G** (below)

- Braggs' theory of diffraction
- Reciprocal lattice
- **Laue's theory of diffraction**
- Bragg theory = Laue theory

A crystal = a collection of planes

A crystal = a collection of atoms

Bottom-up approach:

The analysis below concerns the scattering off

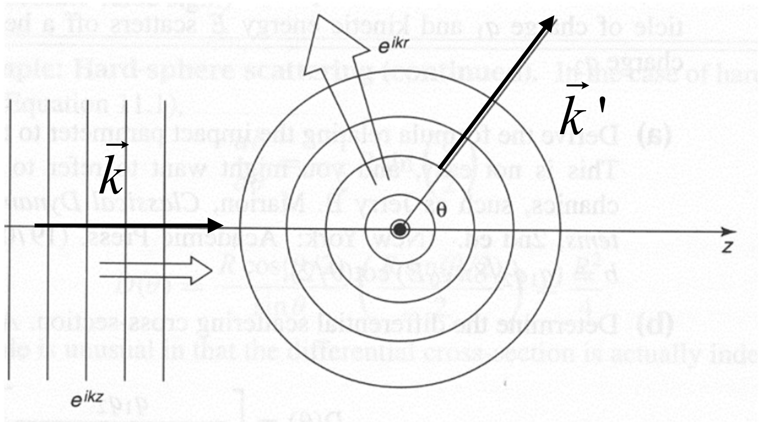
1. 1 atom, 2 atoms
2. *N* atoms (Bravais lattice in 1D)
3. Bravais lattice in 3D
4. Bravais lattice with basis in 3D

Note: Kittel uses a top-down approach, starting from the scattering of a whole crystal.

Scattering from an array of atoms (Laue, 1912)

1914

1. First, a wave scattering off an atom at the origin:

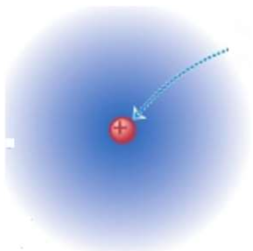


$$\text{scattered wave } \psi(\vec{r}) \sim f_a(\theta)\frac{e^{ikr}}{r} \quad \text{at large } r$$ (spherical wave)

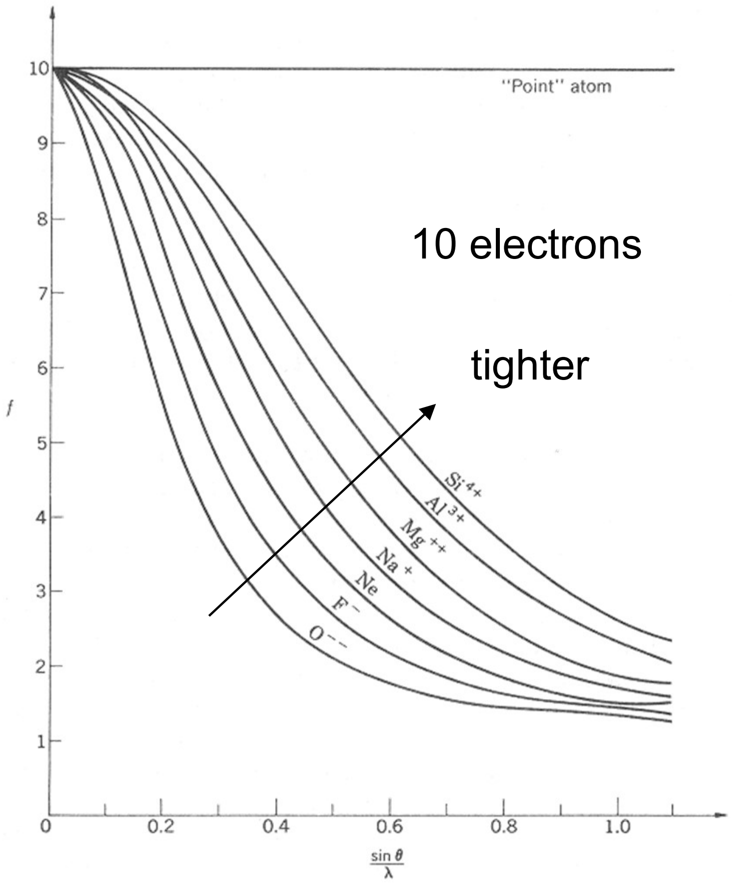
- Atomic form factor: Fourier transform of atom charge distribution $n(\rho)$

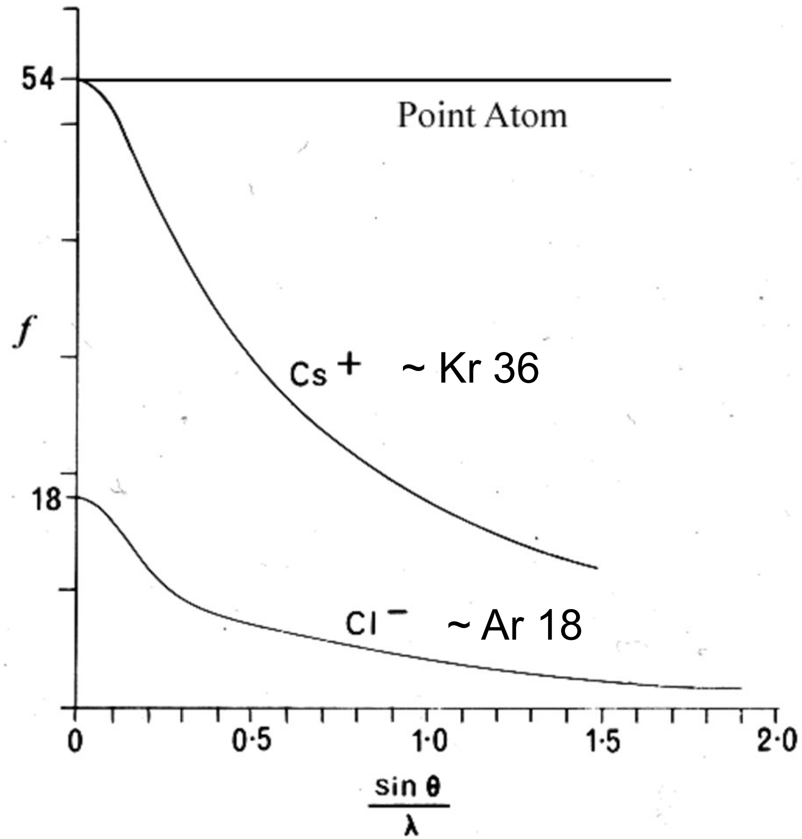
原子結構因子

$$f_a(\theta) = \int dV e^{-i\Delta\vec{k}\cdot\vec{\rho}} n(\vec{\rho}), \quad \Delta\vec{k} \equiv \vec{k}\,' - \vec{k}$$



Atomic form factor: $f_a(\theta) = \int dV e^{-i\vec{q}\cdot\vec{\rho}} n(\vec{\rho})$ (See Prob.9)





- Scattering off an atom not at the origin

$$\text{scattered wave } \psi(\vec{r}) \propto f_a \frac{e^{ik|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{i\vec{k}\cdot\vec{R}}$$

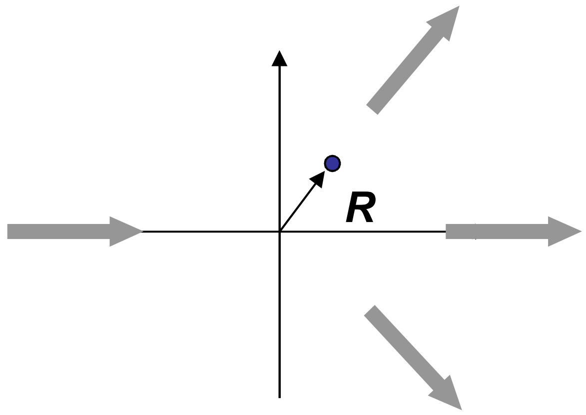
A relative phase w.r.t. an atom at the origin

$$|\vec{r}-\vec{R}| \approx r - \hat{r}\cdot\vec{R}$$

$$\frac{1}{|\vec{r}-\vec{R}|} \approx \frac{1}{r} + O\left(r^{-2}\right)$$

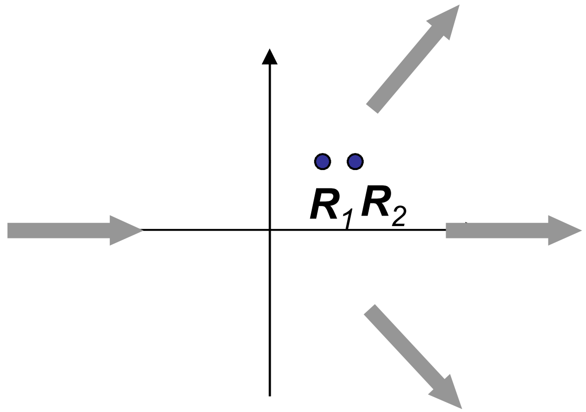
$$k\hat{r} = \vec{k}\,'$$

$$\therefore \psi(\vec{r}) \propto f_a \frac{e^{ikr}}{r} e^{-i\Delta\vec{k}\cdot\vec{R}}$$



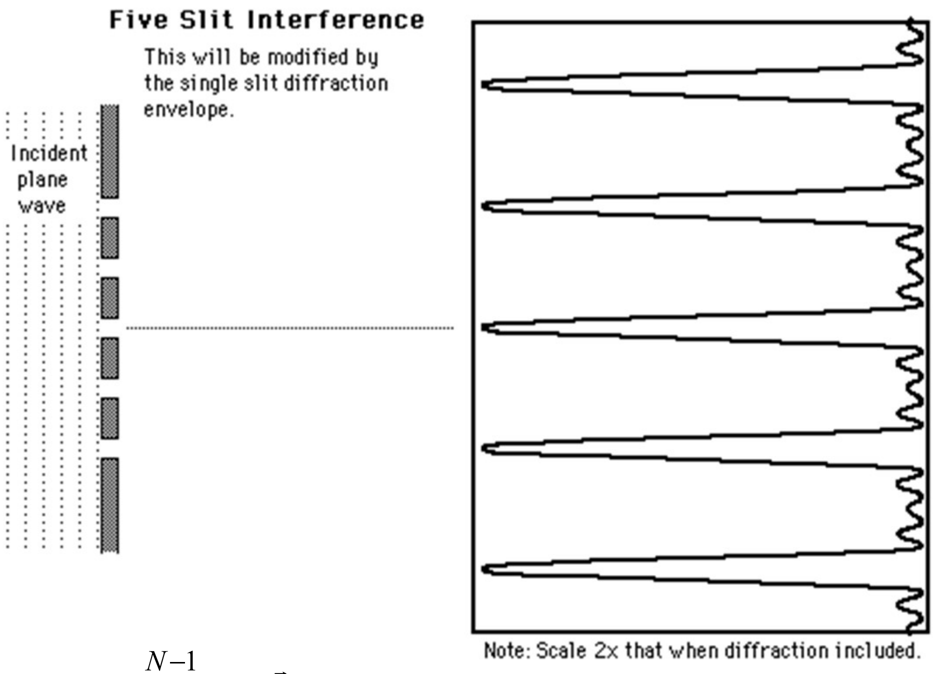
- Scattering off two atoms ($r >> R_1, R_2$)

$$\psi(\vec{r}) \propto f_a \frac{e^{ikr}}{r}\left(e^{-i\Delta\vec{k}\cdot\vec{R}_1} + e^{-i\Delta\vec{k}\cdot\vec{R}_2}\right)$$



2. Scattering off N-atoms: 1D lattice

$$\psi \approx e^{-i\Delta k\cdot 0} + e^{-i\Delta k\cdot a} + e^{-i\Delta k\cdot 2a} + e^{-i\Delta k\cdot 3a} + e^{-i\Delta k\cdot 4a}$$



2π

$a\Delta k$

$|\psi|^2$

http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html

$$\psi \approx \sum_{n=0}^{N-1} e^{-i\Delta\vec{k}\cdot n\vec{a}}$$

$$= \frac{1-\exp(-iN\Delta\vec{k}\cdot\vec{a})}{1-\exp(-i\Delta\vec{k}\cdot\vec{a})} \xrightarrow{N>>1} \sum_h \delta_{\Delta\vec{k}\cdot\vec{a},2\pi h}$$

See Prob. 7

For large N, ψ is nonzero only when

$\Delta\vec{k}\cdot\vec{a} = 2\pi h$ (h is an integer) ← Constructive interference

important

3. N-atom scattering: 3D Bravais lattice

For a Bravais lattice,

$$\psi(\vec{r}) \propto f_a \sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}}, \quad \vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3.$$

The lattice-sum can be separated,

$$\sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}} = \left(\sum_{n_1} e^{-i\Delta\vec{k}\cdot n_1\vec{a}_1}\right)\left(\sum_{n_2} e^{-i\Delta\vec{k}\cdot n_2\vec{a}_2}\right)\left(\sum_{n_3} e^{-i\Delta\vec{k}\cdot n_3\vec{a}_3}\right)$$

$\neq 0$ only when

$$\boxed{\begin{aligned} \Delta\vec{k}\cdot\vec{a}_1 &= 2\pi h, \\ \Delta\vec{k}\cdot\vec{a}_2 &= 2\pi k, \\ \Delta\vec{k}\cdot\vec{a}_3 &= 2\pi l. \end{aligned}} \Leftrightarrow \boxed{\Delta\vec{k} = \vec{G}_{hkl}}$$

Laue's diffraction condition

Δ***k*** forms a reciprocal lattice

i.e., $$\sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}} = N\sum_{hkl} \delta_{\Delta\vec{k}\cdot\vec{a}_1,2\pi h}\,\delta_{\Delta\vec{k}\cdot\vec{a}_2,2\pi k}\,\delta_{\Delta\vec{k}\cdot\vec{a}_3,2\pi l} = N\sum_{\vec{G}_{hkl}} \delta_{\Delta\vec{k},\vec{G}_{hkl}}$$

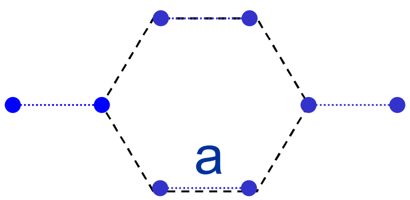
Number of atoms in the crystal

important

4. Previous calculation is for a Bravais lattice, now we calculate the scattering from a crystal with basis

***d**$_j$*: location of the *j*-th atom in a unit cell

Eg., honeycomb lattice



$$\vec{d}_1 = \vec{0}, \vec{d}_2 = a\hat{x}$$

atomic form factor for the *j*-th atom

$$\psi(\vec{r}) \propto \sum_{\vec{R}} \left(\sum_{j=1}^{p} f_{aj} e^{-i\Delta\vec{k}\cdot(\vec{R}+\vec{d}_j)} \right)$$

$$= \left(\sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}} \right) \left(\sum_{j=1}^{p} f_{aj} e^{-i\Delta\vec{k}\cdot\vec{d}_j} \right)$$

$$= N \sum_{\vec{G}_{hkl}} \delta_{\Delta\vec{k},\vec{G}_{hkl}} \cdot S(\Delta\vec{k})$$

Structure factor (of the basis)

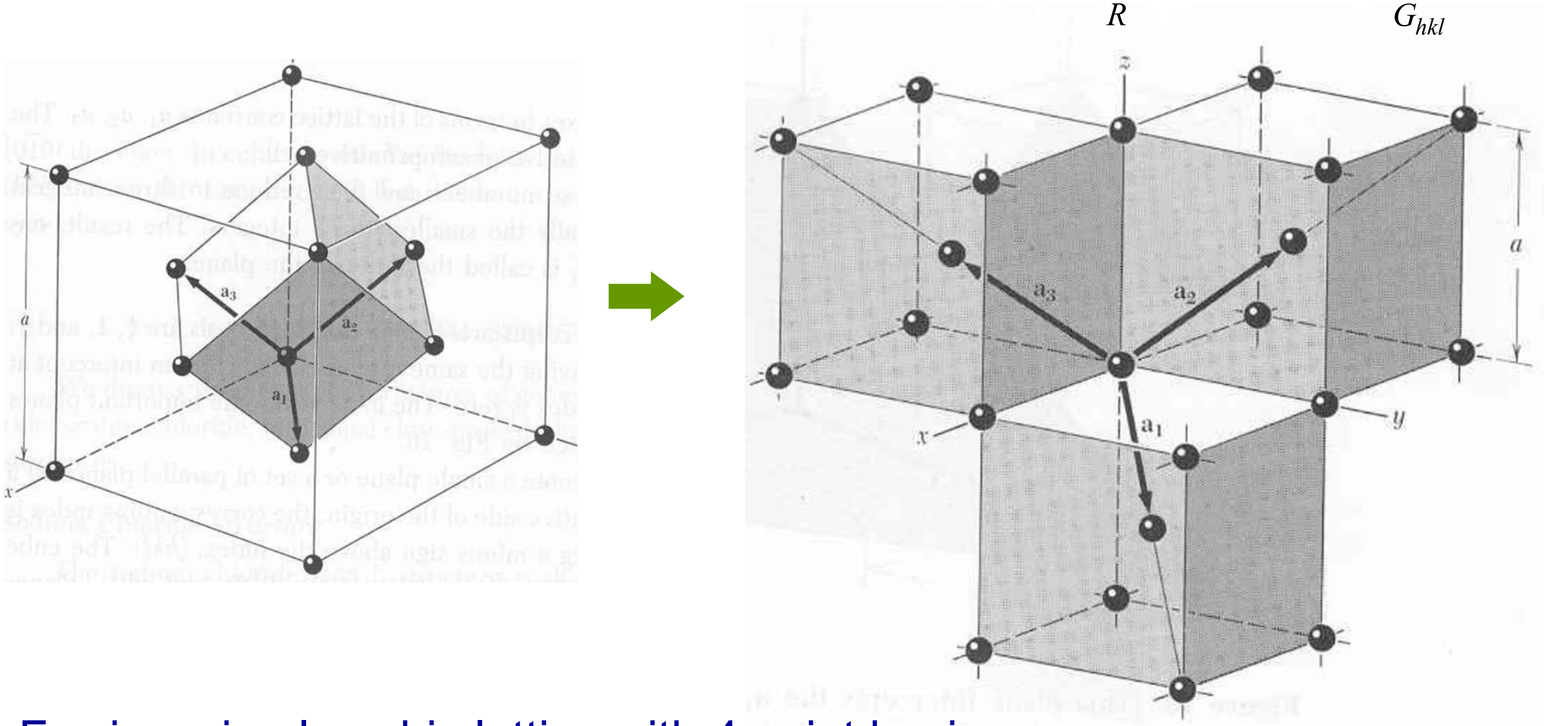
$$\boxed{S(h,k,l) \equiv \sum_{j=1}^{p} f_{aj} e^{-i\vec{G}_{hkl}\cdot\vec{d}_j}}$$

Example: Diffraction condition of fcc lattice

Method 1 Fcc is a Bravais lattice.

The Laue condition is determined by its reciprocal lattice, which is a bcc lattice.

$$\psi \sim \sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}} = N\sum_{\vec{G}_{hkl}} \delta_{\Delta\vec{k},\vec{G}_{hkl}}$$



Method 2 Fcc is a simple cubic lattice with 4 point basis

The Laue condition is determined by its reciprocal lattice, which is a sc lattice,
as well as the structure factor of 4-atom basis.

$$\psi \sim N\sum_{\vec{G}_{hkl}} \delta_{\Delta\vec{k},\vec{G}_{hkl}} \cdot S(\Delta\vec{k})$$

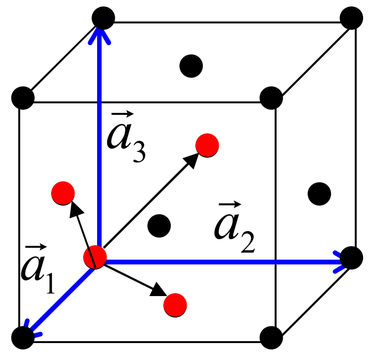
Method 2 (cont'd)

$$\psi \sim N \sum_{\vec{G}_{hkl}} \delta_{\Delta\vec{k},\vec{G}_{hkl}} \cdot S(\Delta\vec{k}) \qquad \vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

← A sc lattice

$$S(h,k,l) = \sum_{j=1}^{p} f_{aj} e^{-i\vec{G}_{hkl}\cdot\vec{d}_j}$$

A sc lattice



$$\vec{d}_1 = \vec{0},$$

$$\vec{d}_2 = \frac{\vec{a}_1}{2} + \frac{\vec{a}_2}{2}, \vec{d}_3 = \frac{\vec{a}_2}{2} + \frac{\vec{a}_3}{2}, \vec{d}_4 = \frac{\vec{a}_3}{2} + \frac{\vec{a}_1}{2}$$

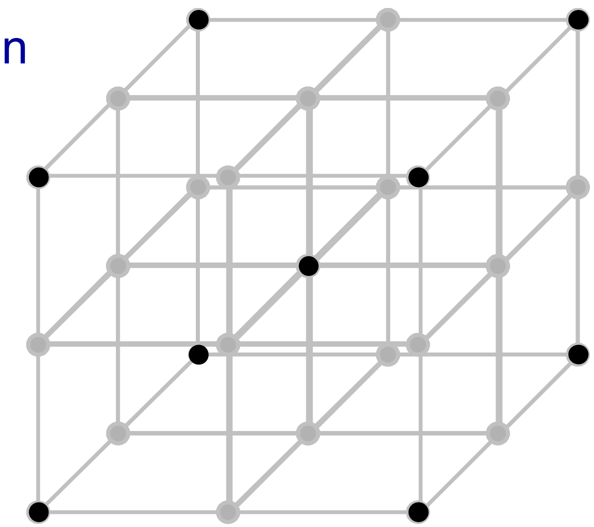
The structure factor for the 4-point basis

$$S(h,k,l) = f_a\left[1 + e^{-i\pi(h+k)} + e^{-i\pi(k+l)} + e^{-i\pi(l+h)}\right]$$

$$\begin{cases} = 4f_a \text{ when } h,k,l \text{ are all odd or all even} \\ = 0 \text{ otherwise} \end{cases}$$

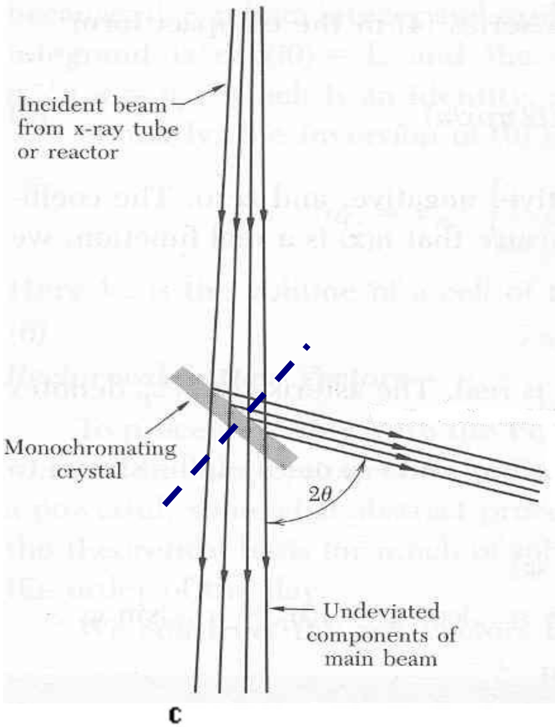
Destructive interference

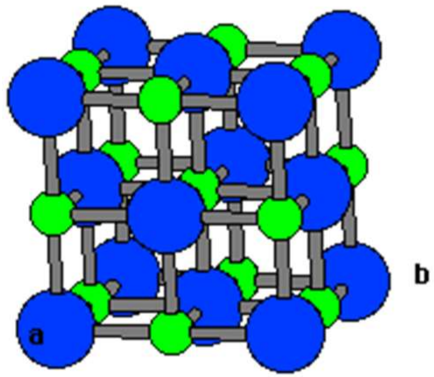
Reciprocal lattice, also a sc lattice



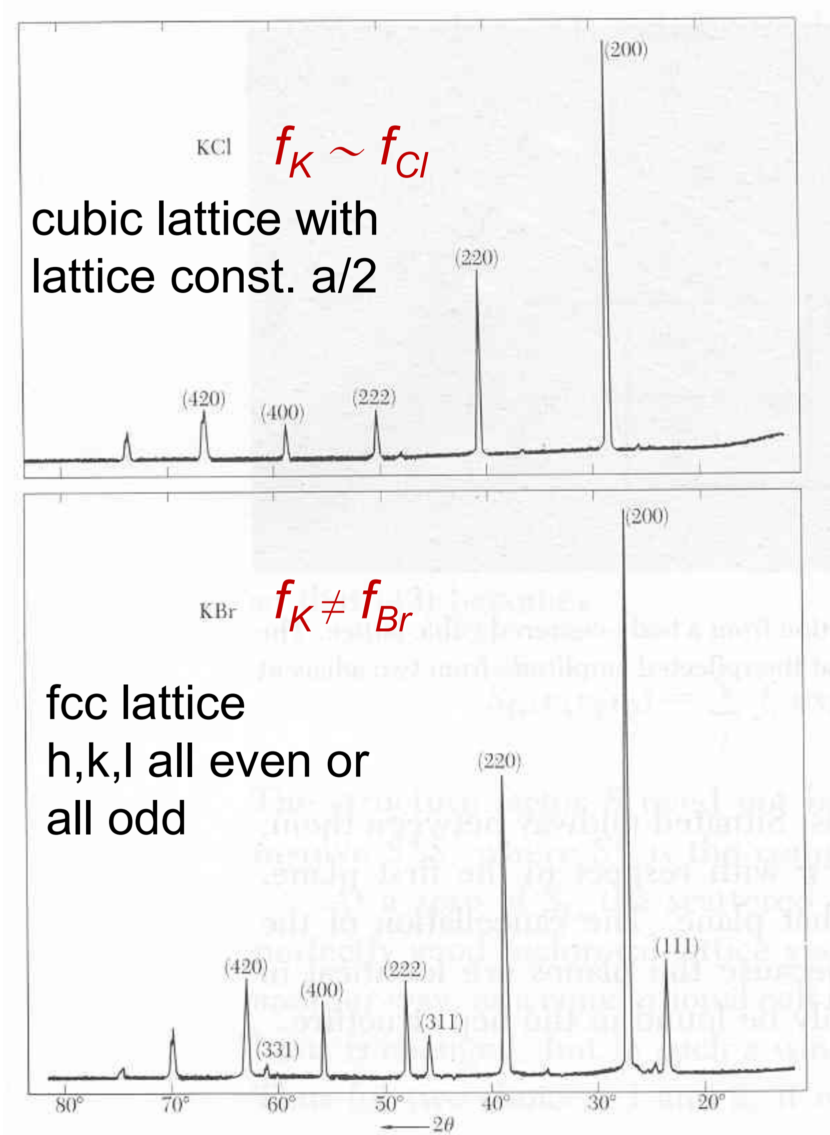
Eliminate the points in the reciprocal lattice with S=0.
The result is a bcc lattice, agrees with Method 1.

Atomic form factor and intensity of diffraction





SC with 2-atom basis



Summary

(Prob.8)

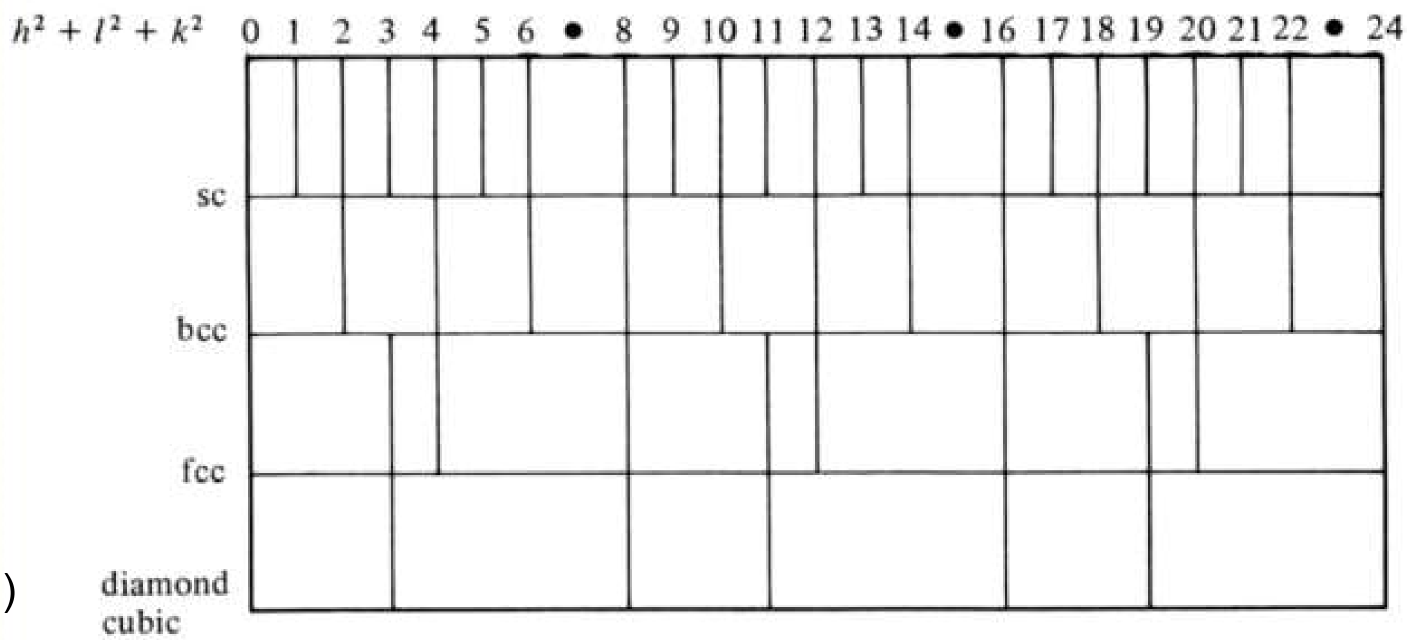


Fig. 3.4 Permitted diffracted beams in cubic systems are characterized by the values of $h^2 + k^2 + l^2$. The figure shows how the addition of a basis to the simple cubic primitive cell reduces the number of allowed beams, increasingly the more atoms in the basis. Note the regular sequence of each pattern. The correct angular separations are not reproduced in this diagram. *Myers*

• Find out the structure factor of the honeycomb structure, then draw its reciprocal structure. Different points in the reciprocal structure may have different structure factors. Draw a larger dots if the associated $|S|^2$ is larger.

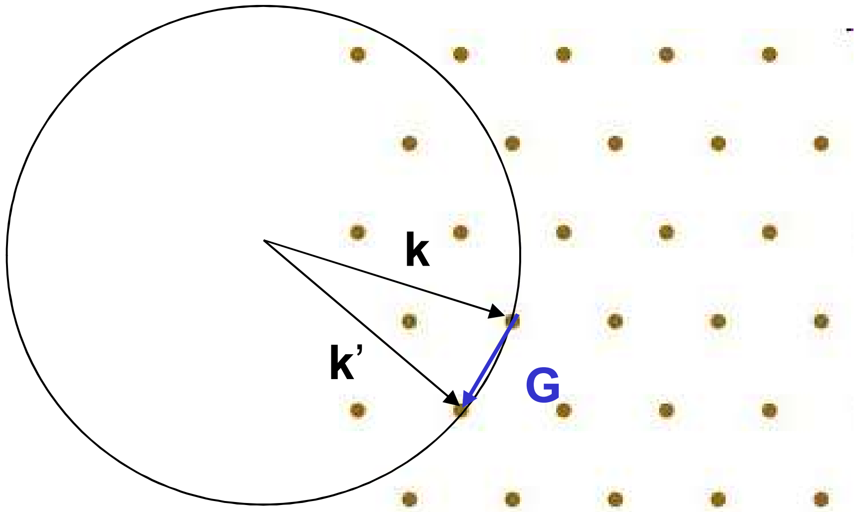
Ewald construction (Ewald 構圖法)

Laue's diffraction condition: $\mathbf{k}' = \mathbf{k} + \mathbf{G}_{hkl}$

- Given an incident **k**, want to find a **k**' that satisfies this condition

(under the constraint $|\mathbf{k}'|=|\mathbf{k}|$)

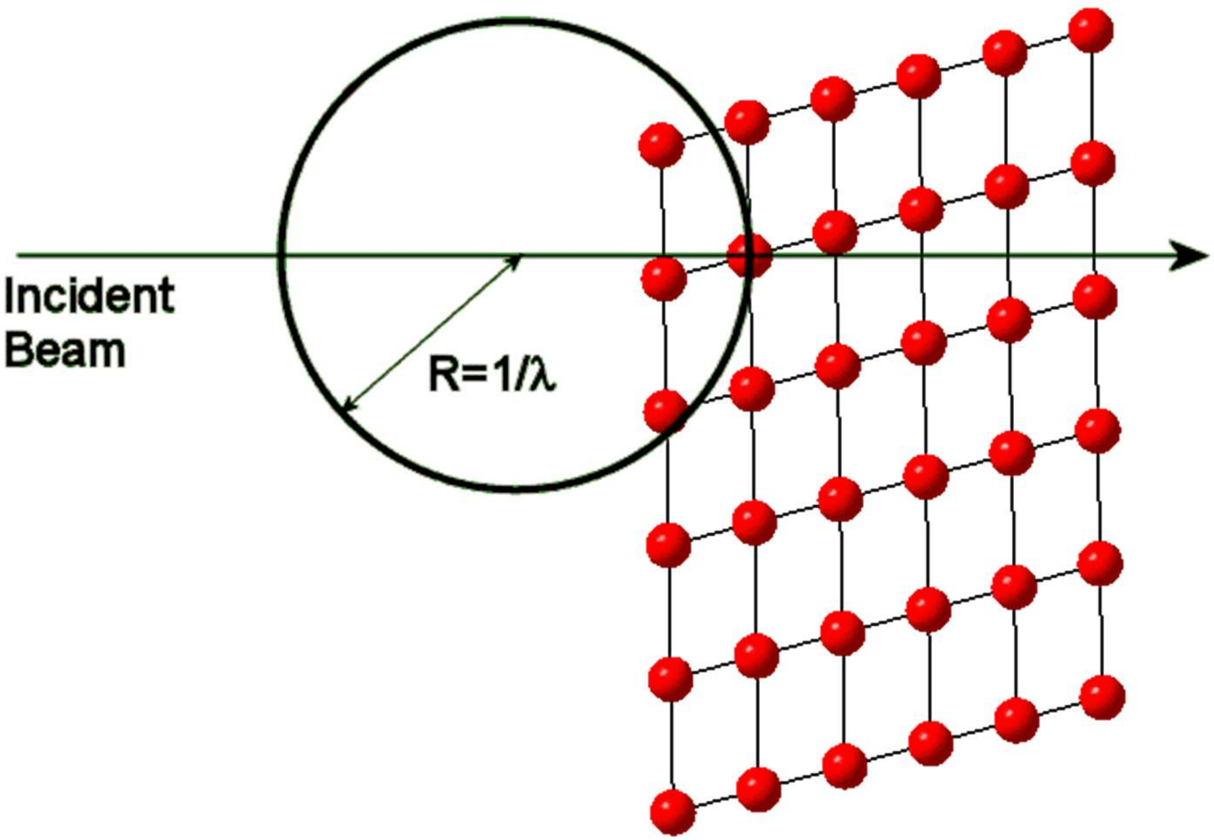
- One problem: there are infinitely many $\mathbf{G}_{hkl}$'s.
- It's convenient to solve it graphically using the Ewald construction



Reciprocal lattice

More than one (or none) solutions may be found.

When you rotate a crystal, its reciprocal lattice rotates the same amount as well.



http://capsicum.me.utexas.edu/ChE386K/docs/28_The_Laue_Experiment.ppt

- Braggs' theory of diffraction
- Reciprocal lattice
- Laue's theory of diffraction
- Bragg theory = Laue theory

Geometrical relation between $\boldsymbol{G}_{hkl}$ vector and (hkl) planes

$$(h,k,l) \text{ planes} \perp \vec{G}_{hkl} \equiv h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

(Prob.2)

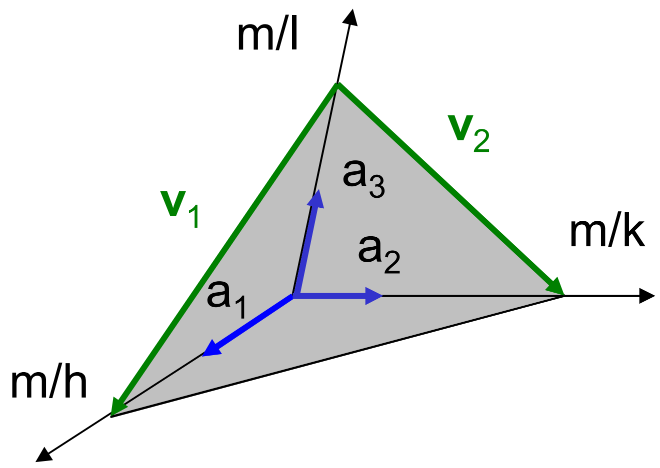
Pf:

$$(h,k,l) = m\left(\frac{1}{x},\frac{1}{y},\frac{1}{z}\right)$$

$$\begin{cases} \vec{v}_1 = \dfrac{m}{h}\vec{a}_1 - \dfrac{m}{l}\vec{a}_3 \\ \vec{v}_2 = \dfrac{m}{k}\vec{a}_2 - \dfrac{m}{l}\vec{a}_3 \end{cases}$$

$$\Rightarrow \begin{matrix} \vec{G}_{hkl}\cdot\vec{v}_1 = 0 \\ \vec{G}_{hkl}\cdot\vec{v}_2 = 0 \end{matrix}$$

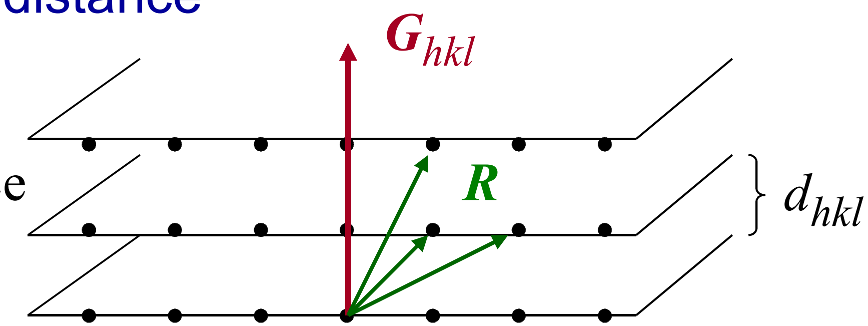
$$\therefore\ \vec{G}_{hkl} \perp (h,k,l)\text{-plane}$$



$$Cf:\quad [h,k,l] = h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$$

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

Inter-plane distance



$$\vec{G}_{hkl} \cdot \vec{R} = 2\pi n \quad (n \text{ could be any integer})$$

$$\Rightarrow \quad \hat{G}_{hkl} \cdot \vec{R} = 2\pi n / |\vec{G}_{hkl}|$$

$\therefore$ inter-plane distance $d_{hkl} = 2\pi / |\vec{G}_{hkl}|$

For a cubic lattice

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

$$= \frac{2\pi}{a}\left(h\hat{x} + k\hat{y} + l\hat{z}\right)$$

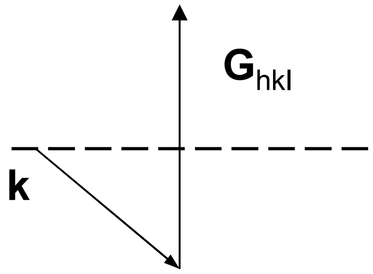
$$\therefore \quad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \qquad \text{(Prob.1)}$$

- In general, planes with higher index have smaller inter-plane distance

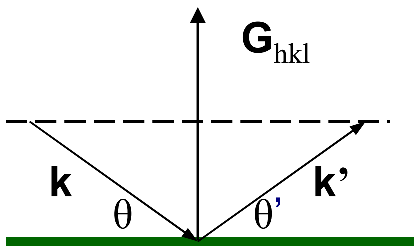
Laue condition = Bragg condition

- From the Laue condition, we have

$$\boxed{\vec{k}\cdot\hat{G}_{hkl} = -\frac{G_{hkl}}{2}}$$



- Given k and $\mathbf{G}_{hkl}$, we can find the diffracted wave vector **k**'



a (*hkl*)-lattice plane

- It's easy to see that θ = θ' because |**k**|=|**k**'|.

By using $2k\sin\theta = G_{hkl} = \frac{2\pi}{d_{hkl}}(\times n)$

If $\boldsymbol{G}_{hkl}$ exists, then $n\boldsymbol{G}_{hkl}$ also exists

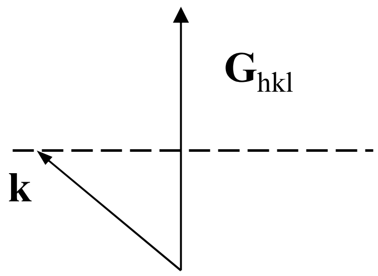
and $k = \frac{2\pi}{\lambda}$,

$$\Rightarrow \boxed{2d_{hkl}\sin\theta = n\lambda.}$$

Bragg diffraction condition

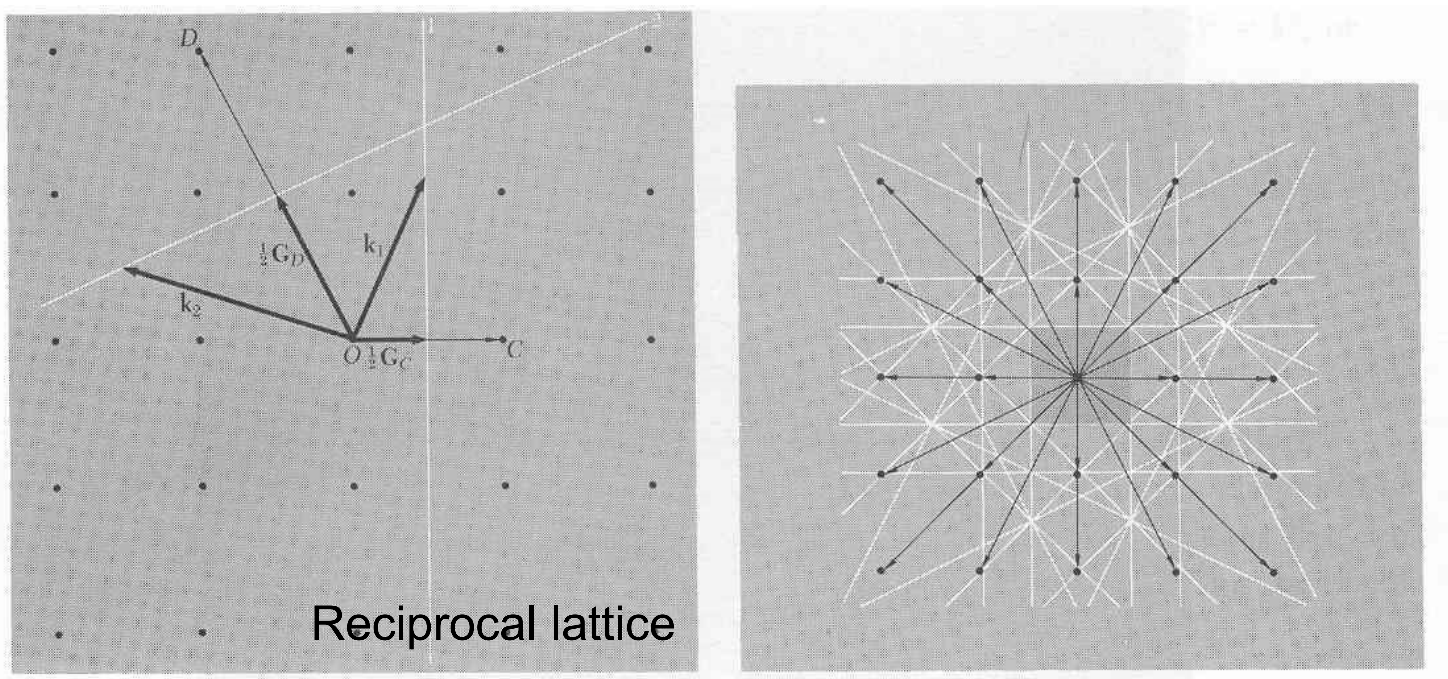
Another view of the Laue condition

$$\vec{k} \cdot \hat{G}_{hkl} = \pm \frac{G_{hkl}}{2}$$



(If $\boldsymbol{G}_{hkl}$ exists, then $-\boldsymbol{G}_{hkl}$ also exists)

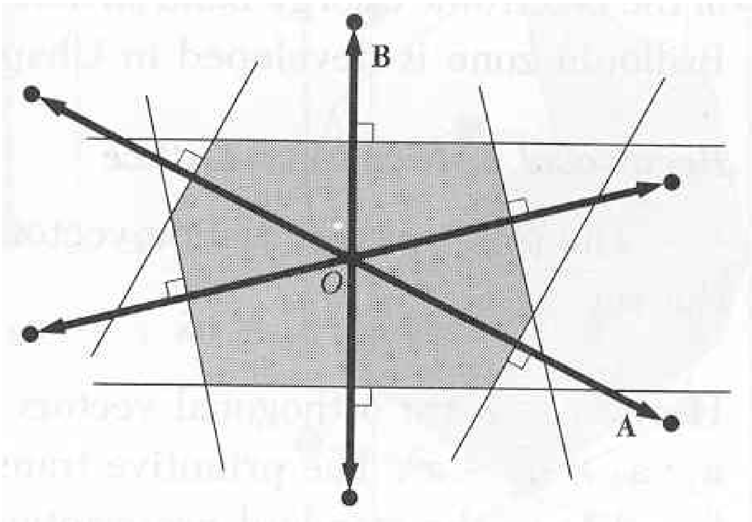
∴ The **k** vector that points to the plane bi-secting a $\mathbf{G}_{hkl}$ vector will be diffracted.



important

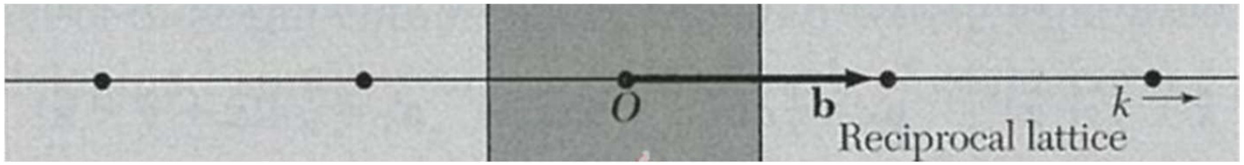
First Brillouin zone (later, there will be higher BZs)

Def: It is the Wigner-Seitz cell of the reciprocal lattice



1-dim

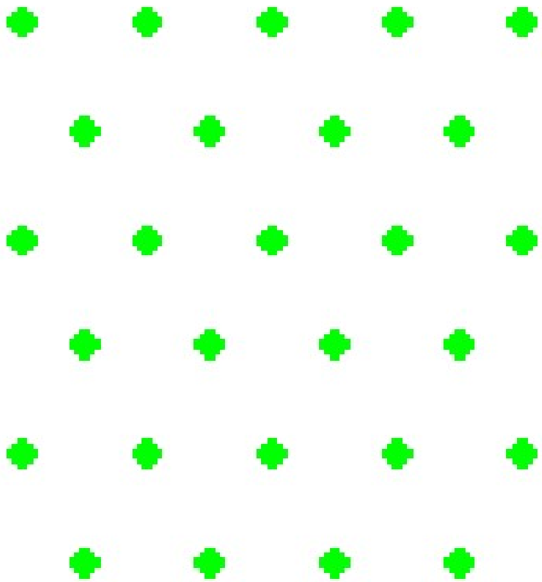
1st BZ



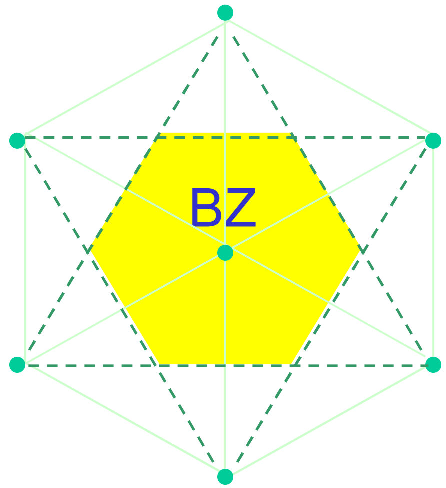
2-dim

Triangle lattice

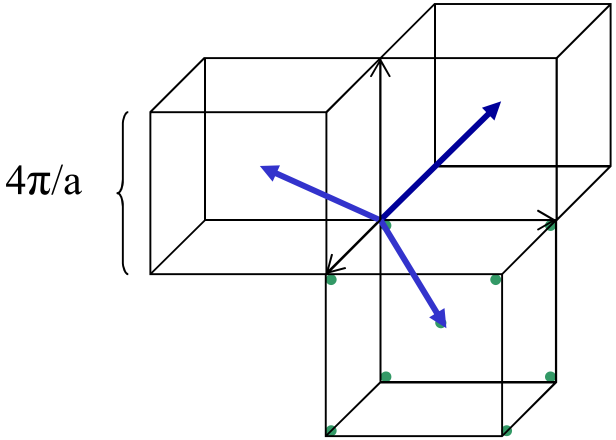
direct lattice

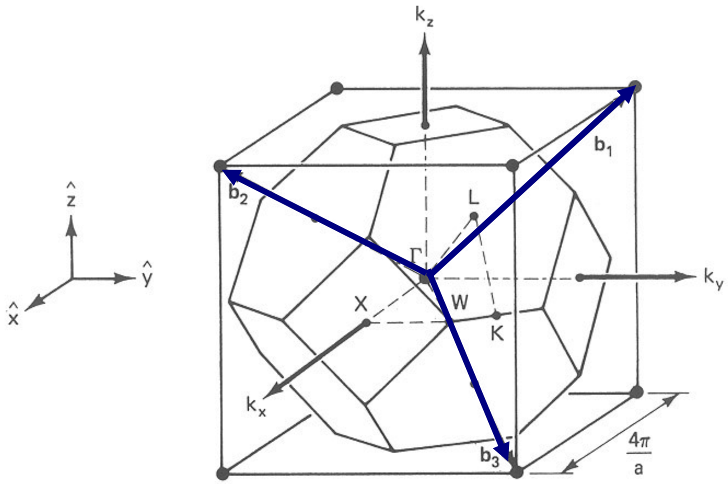


reciprocal lattice



3-dim The first BZ of fcc lattice (its reciprocal lattice is bcc lattice)





- The first BZ of bcc lattice (its reciprocal lattice is fcc lattice)