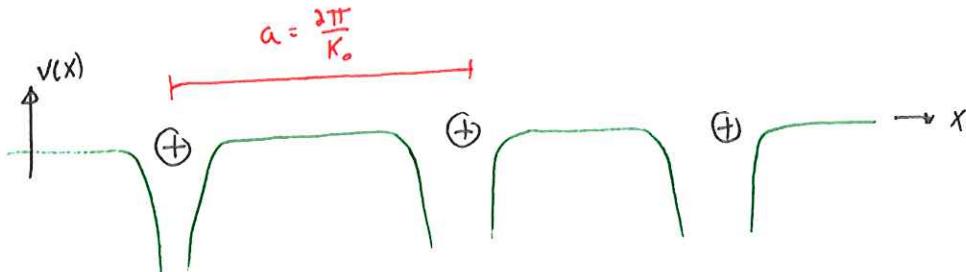


Physics 410/510 - Solid State Physics  
 Spring 2015  
Monday, Week 3 :

Review



The periodicity of crystal lends itself to many of the intrinsic properties of the crystal, such as  $V(x)$ ,  $n(x)$ , the lattice points themselves, etc.

$$\begin{aligned}
 V(x) &= \sum_{n=0}^{\infty} a_n \cos((k_0 n)x) + b_n \sin((k_0 n)x) \\
 &= \sum_{n=-\infty}^{\infty} A_n e^{i(k_0 n)x} \\
 &= \sum_{n=-\infty}^{\infty} A_n e^{i(\frac{2\pi}{a} n)x} = \boxed{\sum_{n=-\infty}^{\infty} A_n e^{i\frac{2\pi}{a} n x}}
 \end{aligned}$$

where the allowable wavevectors are the reciprocal lattice points  $\vec{G}_n$ ,

In 3D

$$V(\vec{r}) = \sum_{\vec{G}} A_{\vec{G}} \exp(i\vec{G} \cdot \vec{r}) \quad \vec{G} \in \text{reciprocal lattice}$$

Since  $V(\vec{r} + \vec{b}) = V(\vec{r})$

$\downarrow$   
 lattice vector

$$\begin{aligned}
 V(\vec{r} + \vec{b}) &= \sum_{\vec{G}} A_{\vec{G}} \exp(i\vec{G} \cdot (\vec{r} + \vec{b})) \\
 &= \sum_{\vec{G}} A_{\vec{G}} \exp(i\vec{G} \cdot \vec{r}) \exp(i\vec{G} \cdot \vec{b}) \\
 &= \sum_{\vec{G}} A_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})
 \end{aligned}$$

$\Rightarrow \exp(i\vec{G} \cdot \vec{b}) = 1$

why?

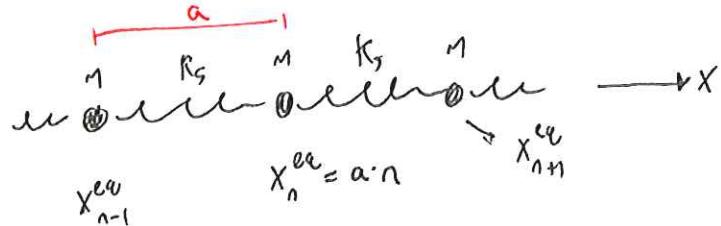
$$\vec{G} = \sum_i \vec{b}_i$$

$$\vec{b}_i = \frac{2\pi \vec{a}_i \times \vec{a}_K}{\vec{a}_i \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{a}_i \cdot \vec{b}_i = 2\pi \cdot \sum_i$$

So the reciprocal lattice arises naturally from spatially periodic functions, or periodicity in real space.

Another perspective of reciprocal space:



$$\begin{aligned} \delta x_n &= Ae^{i(Kx_n^{eq} - \omega t)} \\ &= Ae^{i(K(a \cdot n) - \omega t)} \end{aligned}$$

constant for given  $n$

where  $\omega(K)$  is dispersion relation.

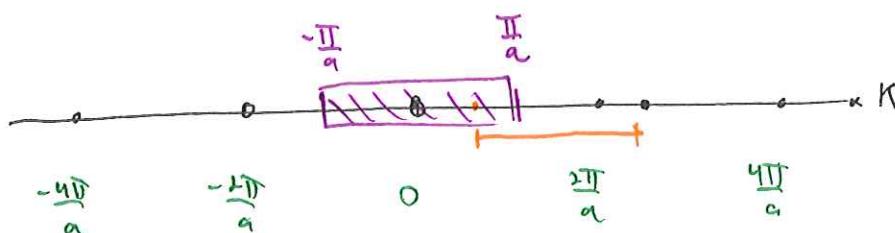
The overall motion of  $n^{\text{th}}$  mass will be periodic w/ free.  $\omega \notin \text{ap. A.}$

Since  $x_n^{eq} = a \cdot n \in [\text{Real Space Lattice}]$

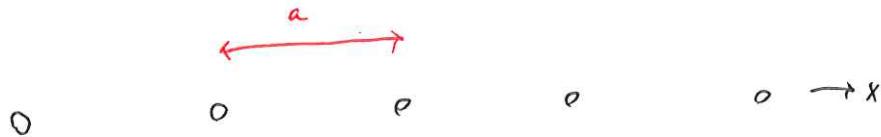
$$\delta x_n(K) = \delta x_n(K+g) \quad \text{where } g \in [\text{Reciprocal Lattice}]$$

So the vibrational motion of a mass in a crystal with wavevector  $K$  will be the same as  $K+g$ ,  $\omega(K+g) = \omega(K)$ .

So we only care about  $K \in [1^{\text{st}} \text{ Brillouin Zone}]$



The reciprocal lattice has further significance. It is the Fourier transform of the real space lattice:



The density of lattice points is:

$$g(x) = \sum_n \delta(x - a \cdot n) = \begin{cases} 0 & x \neq a \cdot n \\ \infty & x = a \cdot n \end{cases}$$

Then  $g(x) = \sum_n a e^{ik_n x}$

$$\begin{aligned} \text{where } A_m &= \frac{1}{a} \int g(x) e^{-imx} dx \\ &= \frac{1}{a} \sum_n \int \delta(x - a \cdot n) e^{-imx} dx \\ &= \frac{1}{a} \sum_n e^{-iK_m \cdot a \cdot n} \\ &= \frac{1}{a} \sum_n e^{-i\left(\frac{2\pi}{a} \cdot m\right) \cdot a \cdot n} \\ &= \frac{1}{a} \sum_n e^{-i g_m \cdot a \cdot n} \\ A(K) &= \frac{1}{a} \sum_m \delta(K - g_m) = \begin{cases} 0 & K \neq g_m \\ \infty & K = g_m = \frac{2\pi}{a} \cdot m \end{cases} \end{aligned}$$

Density  
of points  
in real  
space



So, the reciprocal lattice is the Fourier transform of the real space lattice.

Example Reciprocal lattice of bcc

$$\vec{a}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} a \quad \vec{a}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} a \quad \vec{a}_3 = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} a$$

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

$$\vec{a}_2 \times \vec{a}_3 = \frac{1}{a} \begin{vmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1/2 & 1/2 & 1/2 \end{vmatrix} = \left( \frac{1/2}{a^2} \right) \begin{pmatrix} 1/2 \\ 0 \\ -1/2 \end{pmatrix}$$

$$n_1 \cdot (\vec{a}_1 \times \vec{a}_3) = a \left( \frac{1}{2} \right) \cdot \left( \frac{1/2}{a^2} \right)^2 = \frac{1}{2} a^3$$

$$\vec{b}_1 = \frac{2\pi}{1/2 a^3} \begin{pmatrix} +1/2 \\ 0 \\ -1/2 \end{pmatrix}$$

$$= \boxed{\frac{4\pi}{a} \begin{pmatrix} 1/2 \\ 0 \\ -1/2 \end{pmatrix}}$$



$$\vec{b}_2 = \frac{2\pi \vec{a}_3 \times \vec{a}_1}{1/2 a^3}$$

$$= \boxed{\frac{4\pi}{a} \begin{pmatrix} 0 \\ 1/2 \\ -1/2 \end{pmatrix}}$$



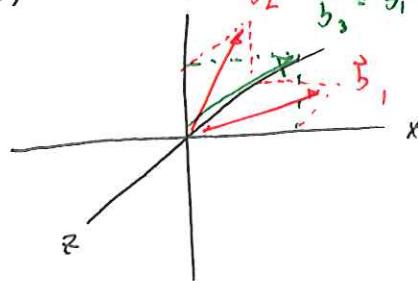
$$\vec{a}_3 \times \vec{a}_1 = \frac{1}{a} \begin{vmatrix} 1 & 1 & 1 \\ 1/2 & 1/2 & 1/2 \\ 1 & 0 & 0 \end{vmatrix} = \left( \frac{1}{a^2} \right) \begin{pmatrix} 0 \\ 1/2 \\ -1/2 \end{pmatrix}$$

$$\vec{b}_3 = \frac{2\pi \vec{a}_1 \times \vec{a}_2}{1/2 a^3}$$

$$= \frac{4\pi}{a} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\vec{a}_1 \times \vec{a}_2 = \frac{1}{a} \begin{vmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{vmatrix} = \left( \frac{1}{a^2} \right) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

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



The reciprocal lattice of the bcc lattice is the fcc lattice!

The " fcc  $\approx$  bcc

$\downarrow$  BZ is a truncated octahedron

$\downarrow$  1st Brillouin zone = rhombic dodecahedron

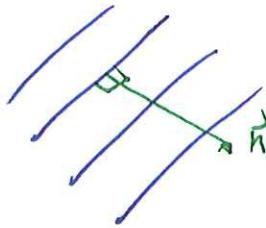
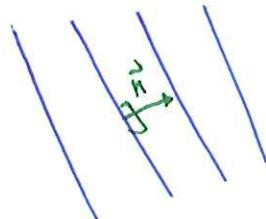
Reciprocal space also describes families of real space lattice planes:

recall

$$e^{i(\vec{k} \cdot \vec{r} - \omega t)}$$

describes a plane wave with

"fronts" perpendicular to  $\vec{k}$ :



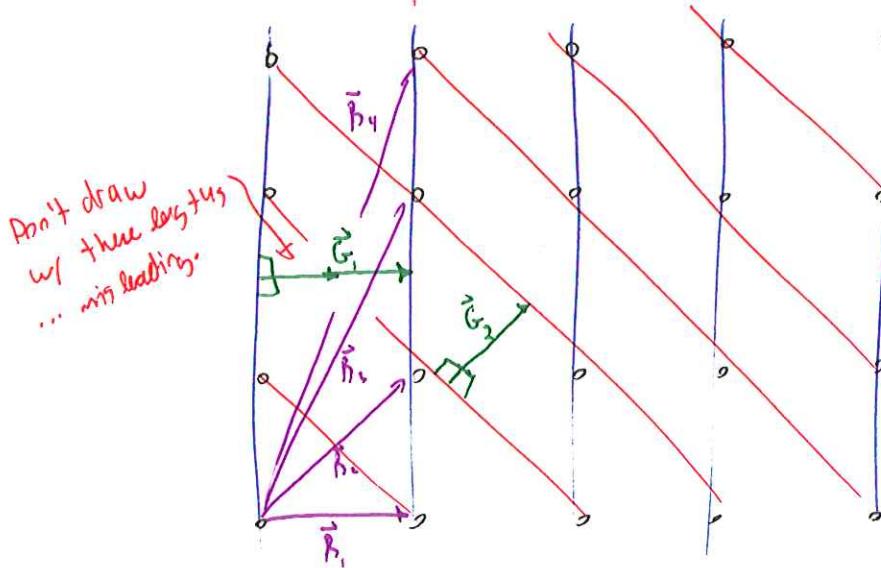
The condition for a reciprocal lattice vector representing the plane wave phase factor:  
(definition)

$$e^{i\vec{G} \cdot \vec{R}} = 1$$

$$\vec{R} = \vec{a}_1 n_1 + \cdots \vec{a}_3 n_3$$

is a real space lattice point.

$\rightarrow$  All  $\vec{R} \Rightarrow \vec{G} \cdot \vec{R} = 2\pi \cdot n$  for some fixed  $n$ .



are families of lattice planes.



Not

family!!

\* "wavefronts" are lattice planes  $\downarrow$ , they are perpendicular to  $\vec{G}$ :  $\vec{G} \cdot \vec{R} = 2\pi n$  for fixed  $n$ !

- A lattice plane (crystal plane) is a plane containing at least three non-collinear points of a lattice
- A family of lattice planes is an infinite set of equally separated parallel lattice planes which taken together contain all points of the lattice.

Claim: The families of lattice planes are in one-to-one correspondence ( $\text{mod } 1$ ) with the directions of possible reciprocal lattice vectors, to which they are normal.

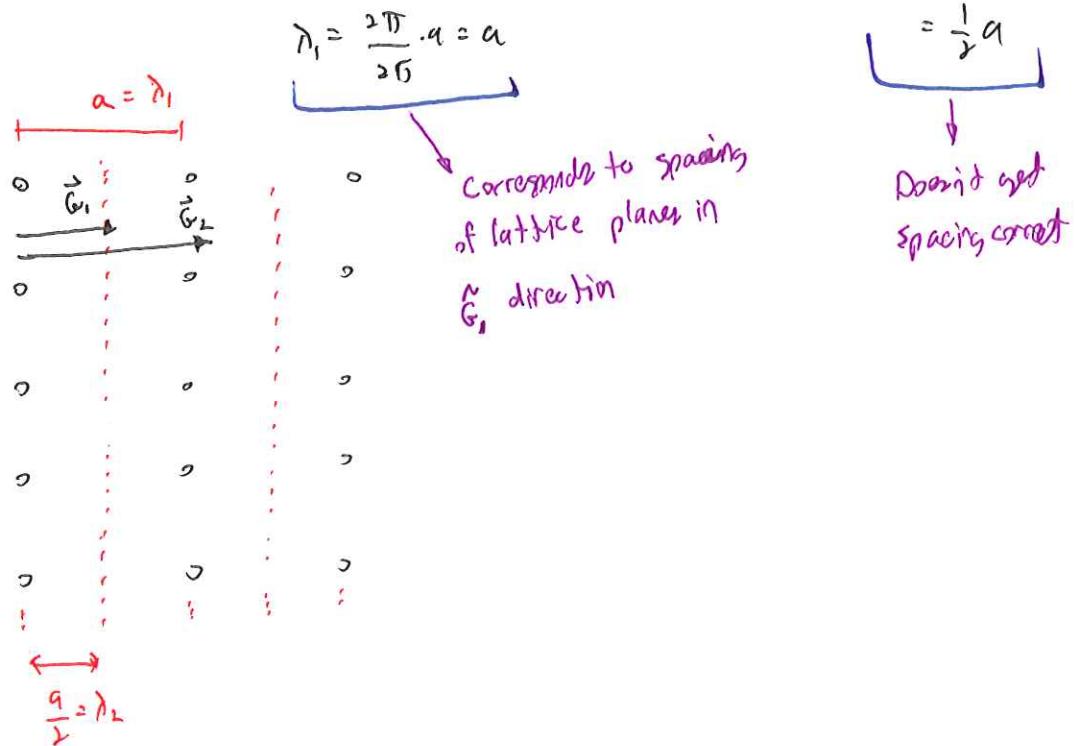
Also, Spacing between planes is

$$d = \frac{2\pi}{|\vec{G}_{\min}|}$$

Proof: Recall that  $\lambda = \frac{2\pi}{|G|}$  (for  $C^i(\vec{G} \cdot \vec{r} - \omega t)$ )

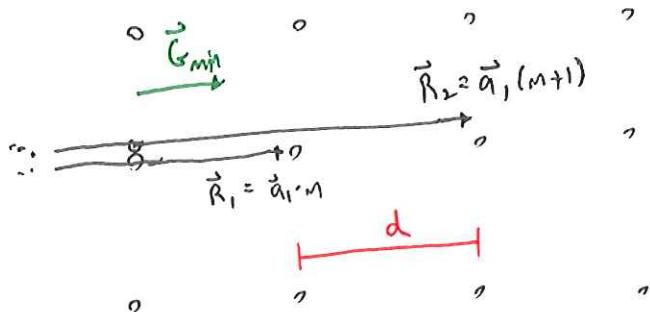
$$\text{so } \lambda_{||} \approx |\vec{G}| \ll 1 \quad \& \quad \lambda_{\perp} \approx |\vec{G}| > 1$$

Say we have smallest  $G_1 = \frac{2\pi}{a}$ , then  $G_2 = \frac{2\pi}{a} \cdot 2$  would give  $\lambda_2 = \frac{2\pi}{2 \cdot a}$



So smallest  $\vec{G}$  in a given direction defines family of lattice planes  $\perp$  to  $\vec{G}$ .

Now take  $\vec{G} = \vec{G}_{\min}$  in some direction, &  $\vec{R}_1, \vec{R}_2$  lattice points on neighboring planes



Then  $\vec{G}_{\min} \cdot \vec{R}_1 = 2\pi \cdot n \quad \text{for } n \in \mathbb{Z}$

$$\vec{G}_{\min} \cdot \vec{R}_2 = 2\pi(n+1)$$

$\therefore \vec{G}_{\min} \cdot (\vec{R}_2 - \vec{R}_1) = 2\pi$  chosen to be parallel, but they don't need to be.

$$|\vec{G}_{\min}| |\vec{R}_2 - \vec{R}_1| = 2\pi$$

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

Lattice Planes & Miller Indices:

Miller indices can be used to describe lattice planes or reciprocal lattice vectors:

1. Choose edge vectors  $\vec{a}_i$  for unit cell (not nec. primitive) in direct space
2. Build  $\vec{b}_i$ 's  $\rightarrow \vec{a}_i \cdot \vec{b}_i = 2\pi S_i$

Then

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

$$\text{Ex} \quad (1, -1, 1) = (1\bar{1}1)$$

- If  $\vec{a}_i$  are primitive,  $\vec{b}_i$  will also be primitive.

To represent a family of lattice planes, first choose the shortest  $\vec{G}$  in a given direction, so

$h, k, l$  have no common divisors

If  $(hkl)$  is not shortest  $\vec{G}$  in a given direction, then  $(hkl)$  represents a family of planes (not lattice planes).

- If  $\vec{a}_i$  are not primitive,  $\vec{b}_i$  will not be primitive, so shortest

$(hkl)$

does not necessarily define family of lattice planes.

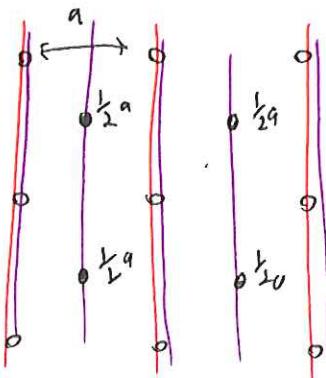
Ex) bcc is for lattices w/ conventional lattice vectors.

$$\text{Here, } \vec{a}_i = a\hat{e}_i$$

$$\vec{b}_i = \frac{2\pi}{a}\hat{e}_i$$

so  $\vec{b}_i$  are not primitive lattice vectors

bcc:



(100) plane

(family of planes)

(200) planes

(lattice planes)

Physics 410/510 - Solid State Physics  
 Spring 2015  
Wednesday, week 3

Review:

The reciprocal lattice comes up in a few different ways:

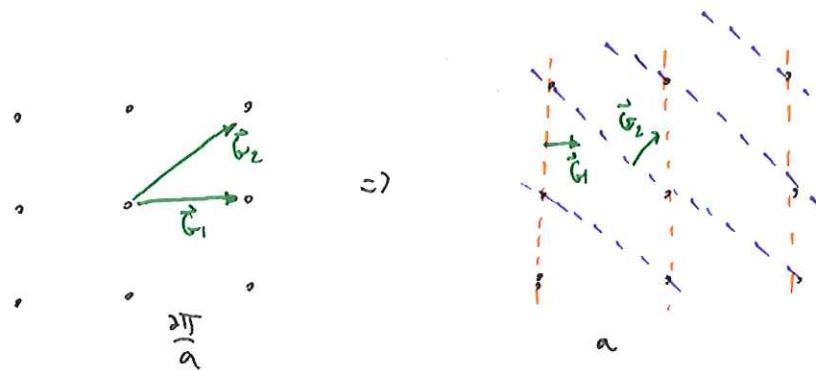
- $V(\vec{r}) = \sum_{\vec{G}} A_{\vec{G}} \exp(i\vec{G} \cdot \vec{r}) \quad \vec{G} \in [\text{Rec. Lattice}]$

- $S_{X_n} = A e^{i(\vec{K} \cdot \vec{R}_n - \omega t)} \quad \vec{R}_n \in [\text{Direct Lattice}]$

- $S_{X_n}(\vec{r}_1 + \vec{G}) = S_n(\vec{R}) \quad \text{Waves live in reciprocal space!}$

- Direct space lattice  $\xrightarrow[\text{Fourier Transform}]{}$  Reciprocal lattice

- $\vec{G}$  are in 1-1 correspondence with families of lattice plane



$$d = \frac{2\pi}{|\vec{G}_{min}|}$$

For a set of primitive  $\vec{G}_i$  & thus primitive  $\vec{b}_i$ , the smallest

$$G_{(h,k,l)} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 \quad \leftrightarrow (hkl)$$

defines family of lattice planes (otherwise, if  $\vec{b}_i$  is not primitive, defines family of planes)

- The spacing between adjacent planes of a family of planes:

$$d_{(n\text{ne})} = \frac{2\pi}{|\vec{c}|}$$

$$= \frac{2\pi}{\sqrt{h^2|\vec{b}_1|^2 + k^2|\vec{b}_2|^2 + l^2|\vec{b}_3|^2}}$$

If  $\vec{a}_i$  are  $\perp$ , then  $\vec{b}_i$  are  $\perp$ , so

$$|\vec{b}_i| = \frac{2\pi}{|\vec{a}_i|}$$

$$\frac{1}{|d_{(n\text{ne})}|^2} = \frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}$$

For a cubic lattice,

$$d_{(\text{cubic})} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Determining the Miller indices of a plane:

1. Find the intersection of a plane with the three coordinate axes,

\* PPT  
 $x_1, x_2, x_3$

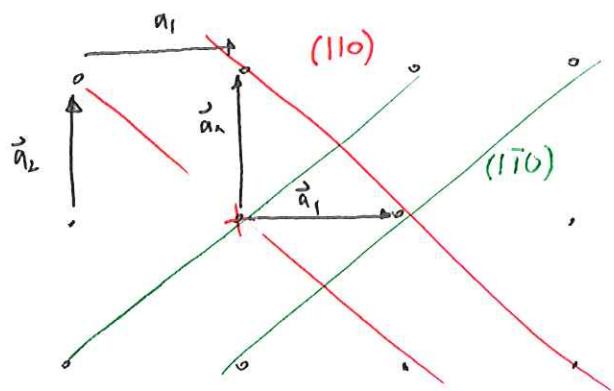
2. Take the reciprocal of  $x_i$ 's & reduce to three integers having the same radix; the integers will be  $(hkl)$ :

$$\frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3} = h : k : l$$

\* PPT of Examples.

②

Different lattice planes may be the same under a symmetry of the crystal :



In this case,  $\{hkl\}$  denotes planes equivalent by symmetry.

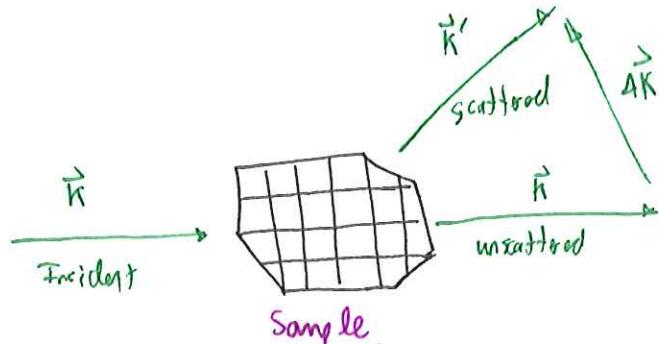
To summary,

$[uvw]$  direction in crystal  $\stackrel{\text{def}}{=}$  a direct lattice vector  
 $(hkl)$  in reciprocal lattice, a reciprocal lattice vector  
 $\{hkl\}$  family of lattice planes perpendicular to  $(hkl)$

$\{hkl\}$  Direct lattice planes equivalent by symmetry

## Scattering of waves by crystals - Diffraction:

Consider



Scattering experiments have illuminated nearly everything we know about the structure of matter: Thomson scattering, Rutherford scattering, HFR, PNR, etc.

where  $\vec{k}$  is the wavevector of an incident wave (X-ray, neutron, electron). The  $\lambda$  of the wave will have length  $\sim a$  of unit cell,

$$a \sim 1 \text{ nm} = 10^{-9} \text{ m}$$

$$\lambda = \frac{1240 \text{ eV}}{E(\text{eV})} = 1240 \text{ eV} !! \Rightarrow X\text{-rays}$$

How do we determine when scattering to  $\vec{k}'$  will occur?

• Born Approximation:

$$f(Q, \phi) \approx -\frac{M}{2\pi\hbar^2} \int e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}} V(\vec{r}) d^3 r$$

Kittel writes,

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

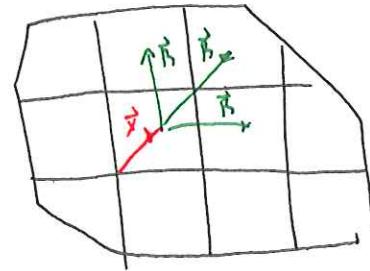
[Scattering Amplitude]

• Fermi's Golden Rule: The transition rate per unit time is

$$\Gamma(\vec{k}', \vec{k}) = \frac{2\pi}{\hbar} |\langle \vec{k}' | V | \vec{k} \rangle|^2 S(\vec{E}_{\vec{k}'} - \vec{E}_{\vec{k}})$$

True for any  $V(\vec{r})$

$$\begin{aligned}
 \langle \vec{k}' | V | \vec{k} \rangle &= \int_{\text{unit cell}} \frac{e^{-i\vec{k}' \cdot \vec{r}}}{V L^3} V(\vec{r}) \frac{e^{i\vec{k} \cdot \vec{r}}}{V L^3} d\vec{r} \\
 &= \frac{1}{L^3} \int e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}} V(\vec{r}) d\vec{r} \\
 &= \frac{1}{L^3} \sum_{\vec{R}} \int_{\text{unit cell}} e^{-i(\vec{k}' - \vec{k}) \cdot (\vec{x} + \vec{R})} V(\vec{x} + \vec{R}) d\vec{x} \\
 &\quad \vec{x} \in \text{Unit cell} \\
 &\quad \vec{R} \in \text{Direct Lattice} \\
 &= \frac{1}{L^3} \left[ \sum_{\vec{R}} e^{-i(\vec{k}' - \vec{k}) \cdot \vec{R}} \right] \int_{\text{unit cell}} e^{-i(\vec{k}' - \vec{k}) \cdot \vec{x}} V(\vec{x}) d\vec{x}
 \end{aligned}$$



$\vec{R} \in \text{direct lattice}$   
 $\vec{x} \in \text{Unit cell}$

Recall when we looked at the Fourier Transform of the direct lattice that

$$\sum_{\vec{R}} e^{-i(\vec{k}' - \vec{k}) \cdot \vec{R}} = 0$$

unless

$$\Delta \vec{k} = \vec{k}' - \vec{k} = \vec{G} \in [\text{Reciprocal Lattice}]$$

So scattering will happen when

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

For elastic scattering,

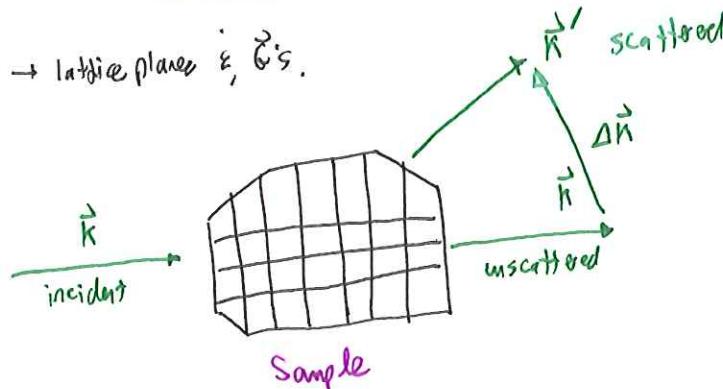
$$|\vec{k}'| = |\vec{k}|$$

1914 Nobel Prize, awarded  
in 1949 in West Hawk  
↑ Institute in Denmark,  
then received  
Lamme or K. remade  
Diffraction  
Condition  
after world war II

Physics 410/510 - Solid State Physics  
Spring 2015

Friday, Week 3 ?

Review:  $(h\bar{k}\ell) \rightarrow$  lattice planes &  $\vec{G}$ 's.



$$P(\vec{k}', \vec{k}) = \frac{2\pi}{\hbar} \underbrace{\left| \langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle \right|^2}_{\text{scattering amplitude}} \delta(E_{\vec{k}'} - E_{\vec{k}})$$

$\vec{k}$ 's actually discrete since wave bound to crystal; we'll see later that  $K_h = \frac{2\pi}{N \cdot a} n$   
 $= \frac{2\pi}{L} \cdot n$

$$= \int \frac{1}{V L^3} e^{-i \vec{k}' \cdot \vec{r}} V(\vec{r}) \frac{1}{V L^3} e^{i \vec{k} \cdot \vec{r}} d\vec{r}$$

$$= \frac{1}{L^3} \int_{x_{\text{full}}} V(\vec{r}) e^{-i (\vec{k}' - \vec{k}) \cdot \vec{r}} d\vec{r}$$

$$= \frac{1}{L^3} \sum_{\vec{R}} \int_{\text{unit cell}} e^{-i (\vec{k}' - \vec{k}) \cdot (\vec{x} + \vec{R})} V(\vec{x} + \vec{R}) d\vec{x}$$

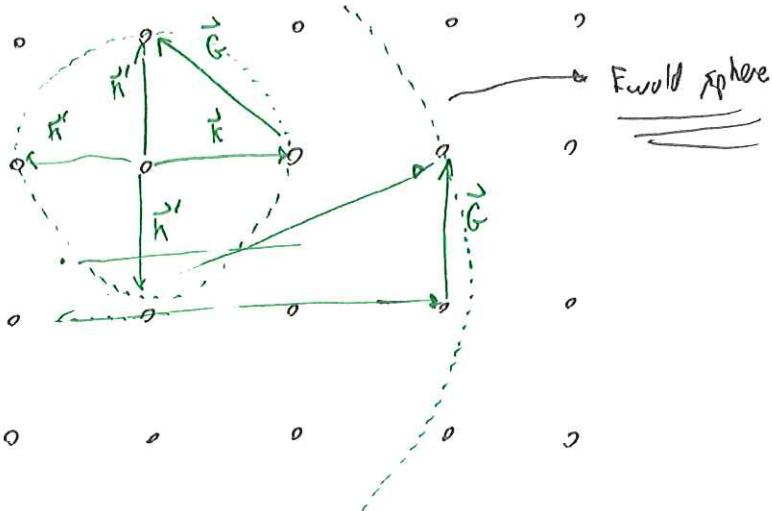
$$= \frac{1}{L^3} \left[ \sum_{\vec{R}} e^{-i (\vec{k}' - \vec{k}) \cdot \vec{R}} \right] \int_{\text{unit cell}} e^{-i (\vec{k}' - \vec{k}) \cdot \vec{x}} V(\vec{x}) d\vec{x}$$

$\vec{R} \in \text{Direct Lattice}$

$\vec{x} \in \text{Unit Cell}$

$$4\vec{R} = \vec{k}' - \vec{k} = \vec{G} \in [\text{Reciprocal Lattice}]$$

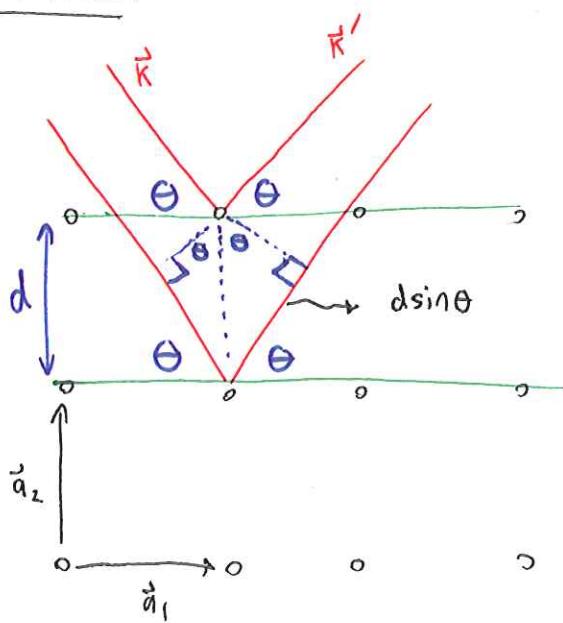
The condition tells us that given a  $\vec{R}$ ,  $\vec{R}' - \vec{R} = \vec{G}$ , where  $|\vec{R}'| = |\vec{R}|$



In X-ray diffraction, we must rotate sample or change  $\vec{R}$  in order to find diffraction directions. For a fixed  $\vec{R}$ , there may be only a few  $\vec{R}'$  or even none that lead to diffraction, i.e.,  $|\vec{R}'| \sim |\vec{G}|$ .

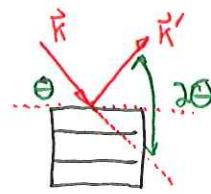
In e-beam diffraction,  $\lambda \sim \text{pm} \Rightarrow |\vec{R}| \sim 10^3 |\vec{G}|$ , so Ewald sphere has large radius & looks flat, so diffraction images come out blurry.

- Bragg Reflections:

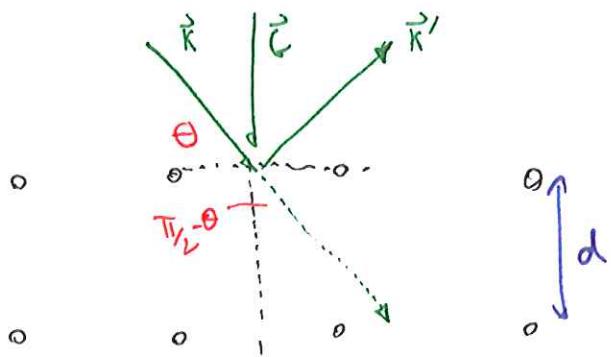


Constructive interference occurs when

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



## Equivalence of Laue & Bragg Conditions



$$\begin{aligned}\hat{\vec{K}} \cdot \hat{\vec{G}} &= \cos(\pi/2 - \theta) \\ &= \sin \theta \\ &= -\hat{\vec{K}'} \cdot \hat{\vec{G}}\end{aligned}$$

Thus by the Laue condition,

$$\frac{2\pi}{\lambda} (\hat{\vec{K}} - \hat{\vec{K}'}) = \hat{\vec{G}} \quad \text{where} \quad \hat{\vec{K}} = \frac{2\pi}{\lambda} \vec{K}$$

$$\hat{\vec{G}} \cdot \frac{2\pi}{\lambda} (\hat{\vec{K}} - \hat{\vec{K}'}) = \hat{\vec{G}} \cdot \hat{\vec{G}}$$

$$\frac{2\pi}{\lambda} \cdot 2 \sin \theta = |\vec{G}|$$

$$x \quad \frac{2\pi}{|\vec{G}|} \cdot 2 \sin \theta = \lambda$$

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

Using  $n\hat{\vec{G}}$ ,

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

Now suppose

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

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

$$|\vec{k}'|^2 = |\vec{k}|^2 + |\vec{G}|^2 + 2\vec{k} \cdot \vec{G}$$

$|\vec{k}'| = |\vec{k}|$  given,

$$2\vec{k} \cdot \vec{G} + \vec{G}^2 = 0$$

or

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

Since  $-\vec{G}$  is also a pd. solution  
to the Lame eq.,

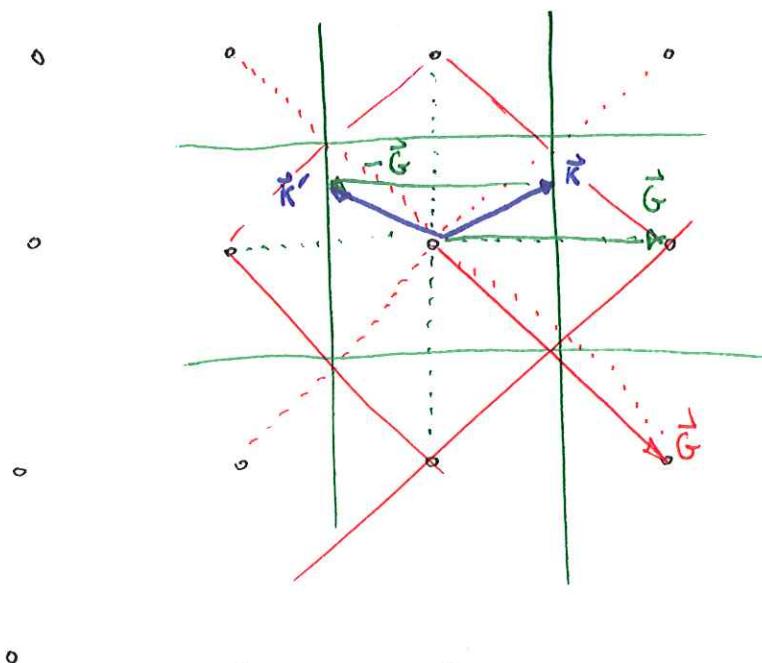
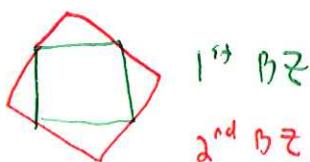
$$\vec{k}' - \vec{k} = -\frac{1}{2}\vec{G}$$

Thus, multiplying by  $\frac{1}{n}$ ,

$$\boxed{\vec{k} \cdot \left(\frac{1}{2}\vec{G}\right) = \left(\frac{1}{2}\vec{G}\right)^2}$$

$$\text{or } \boxed{\vec{k}' = \vec{k} - \vec{G}}$$

So diffraction will occur if  $\vec{k}$  is in a Brillouin Zone:



$\vec{k}$  can be in any direction  
but its length is constrained  
by coupling to its direction.

## Scattering Amplitude:

$$P(\vec{k}', \vec{k}) = \frac{2\pi}{\hbar} |\langle \vec{k}' | V | \vec{k} \rangle|^2 \delta(E_{\vec{k}'} - E_{\vec{k}})$$

{ for periodic  $V(\vec{r})$ :

$$\langle \vec{k}' | V | \vec{k} \rangle = \left[ \frac{1}{L^3} \sum_{\vec{R}} e^{-i(\vec{k}' - \vec{k}) \cdot \vec{R}} \right] \left[ \int e^{-i(\vec{k}' - \vec{k}) \cdot \vec{x}} V(\vec{x}) d\vec{x} \right]$$

\* This part ensures wave sees the lattice; picks out  $\vec{G}$

\* This part depends on the unit cell  $\vec{G}$ , determines the intensity of diffraction

Structure Factor

$$S(\vec{G}) = \int_{\text{unit cell}} V(\vec{x}) e^{i\vec{G} \cdot \vec{x}} d\vec{x}$$

Riffler written:

$$S(\vec{G}) = \int_{\text{unit cell}} n(\vec{r}) e^{i\vec{G} \cdot \vec{r}} dV$$

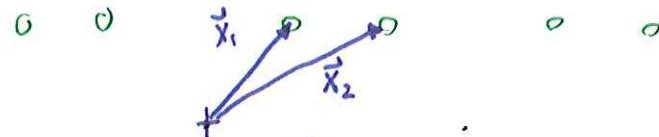
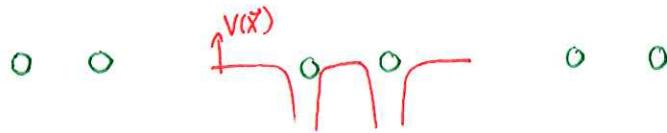
electron concentration

The scattering intensity is,

$$I_{\text{chiral}} \propto |S_{\text{chiral}}|^2$$

$\downarrow$   
Intensity of scattering off of (hkl) planes.

It's a good approximation to assume the scattering potential is a sum over scattering potentials of individual atoms in the unit cell.



$\vec{x}_i$  = position of  $i^{th}$  basis atom ;  $\vec{x} \in$  Unit cell

Then

$$V(\vec{x}) = \sum_{\text{atoms } j} V_j (\vec{x} - \vec{x}_j)$$

$$\vec{x} = \vec{x} - \vec{x}_j + \vec{x}_j$$

So

$$S(\vec{G}) = \sum_{\text{atoms } j} \int V_j (\vec{x} - \vec{x}_j) e^{i \vec{G} \cdot \vec{x}} d\vec{x}$$

$$= \sum_j e^{i \vec{G} \cdot \vec{x}_j} \int V_j (\vec{x} - \vec{x}_j) e^{i \vec{G} \cdot (\vec{x} - \vec{x}_j)} d\vec{x}$$

Atomic Form Factor (depends on type  
of wave body  
scattered; i.e. neutron,  
X-ray, electron,

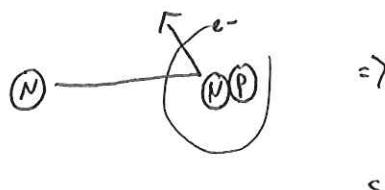
$$f_j(\vec{G})$$

Structure factor  
of the basis.

$\sum_j$   
the atoms of  
basis )

$$S(\vec{G}) = \sum_j f_j e^{i \vec{G} \cdot \vec{x}_j}$$

Neutrons: Scatter mostly from Nuclei



$$V_j(\vec{x} - \vec{x}_j) = b_j \delta(\vec{x} - \vec{x}_j)$$

$\Rightarrow$   
so

$$S(\vec{G}) = \sum_j b_j e^{i \vec{G} \cdot \vec{x}_j}$$

## X-Rays:

$$V_j(x - x_j) = Z_j \delta_j(x - x_j)$$

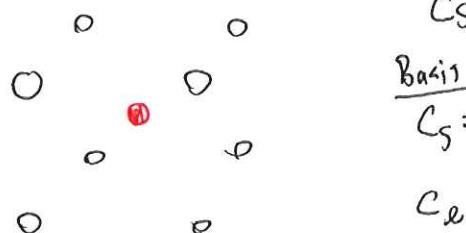
↓                    ↓  
 Atoms              short-range function  
 # of Atom

$$S(\vec{G}) = \sum_j h_j(\vec{G}) Z_j e^{i\vec{G} \cdot \vec{x}_j}$$

- N.B.
- X-Rays good for higher  $Z_j$
  - Cannot distinguish  $Z_j$ 's that are close

## Example of $S(\vec{G})$ :

• C<sub>g</sub> CL



C<sub>S</sub> CL

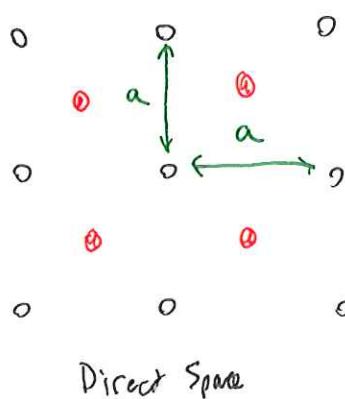
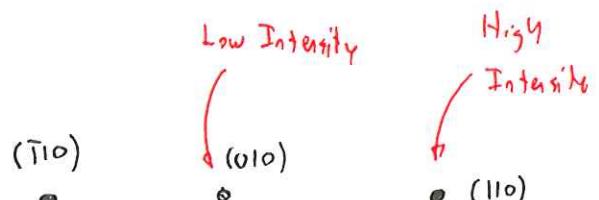
Basis:  
 $C_S = [0, 0, 0]$

$C_E = [1_1, 1_2, 1_3]$

$$S_{(hkl)} = f_{CE} e^{i\vec{G} \cdot \vec{0}} + f_{CS} e^{i\vec{G} \cdot (1_1, 1_2, 1_3)a} \rightarrow \frac{2\pi}{a} (h_1, k_1, l_1) \cdot (1_1, 1_2, 1_3)a$$

$$= f_{CE} + f_{CS} e^{i\pi(h+k+l)}$$

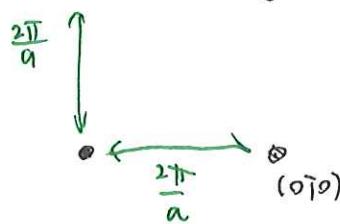
$$= f_{CE} + f_{CS} (-1)^{h+k+l}$$



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

$$\Rightarrow$$

printing out  
reciprocal  
lattice



(100)

(110)

(010)

⑦