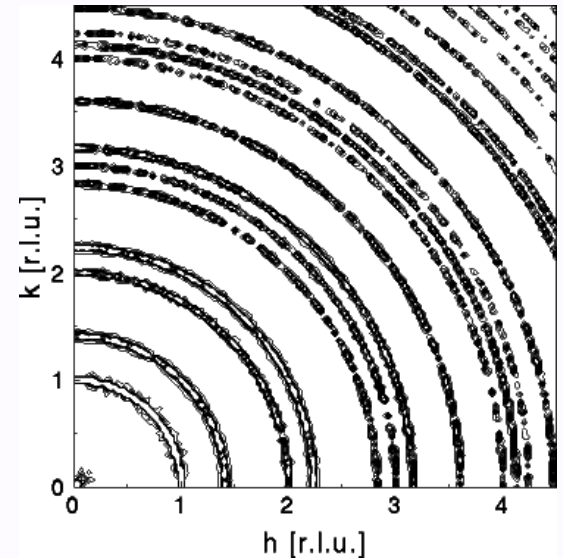
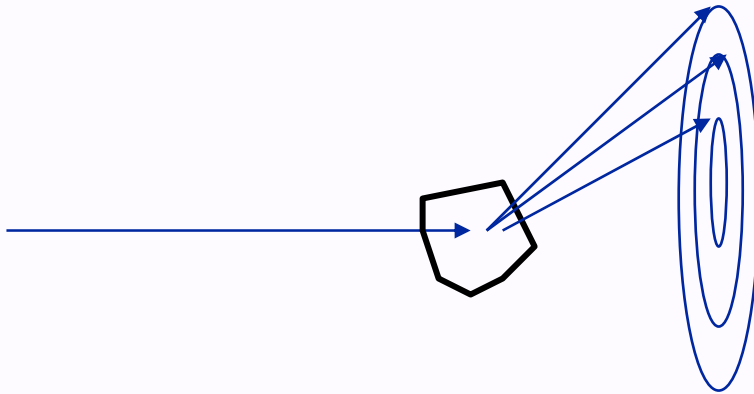


# Solid State Physics 460 - Lecture 3

## Diffraction and the Reciprocal Lattice (Kittel Ch. 2)



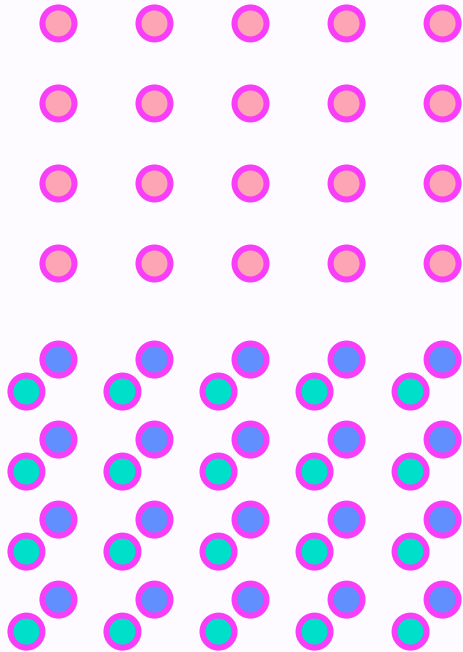
**Diffraction (Bragg Scattering) from a powder of crystallites - real example of image at right from**

<http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/pow.html>

# Crystals

- A crystal is a repeated array of atoms

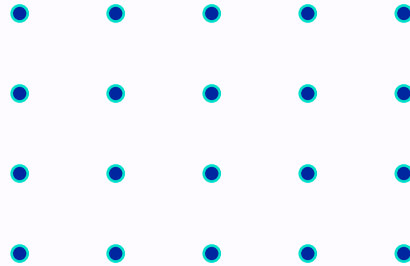
- **Crystal**  $\Leftrightarrow$  **Lattice** + **Basis**



**Crystal**



**Lattice**



**Lattice of points  
(Bravais Lattice)**

**+**

**Basis**



**Basis of atoms**

# How can we study crystal structure?

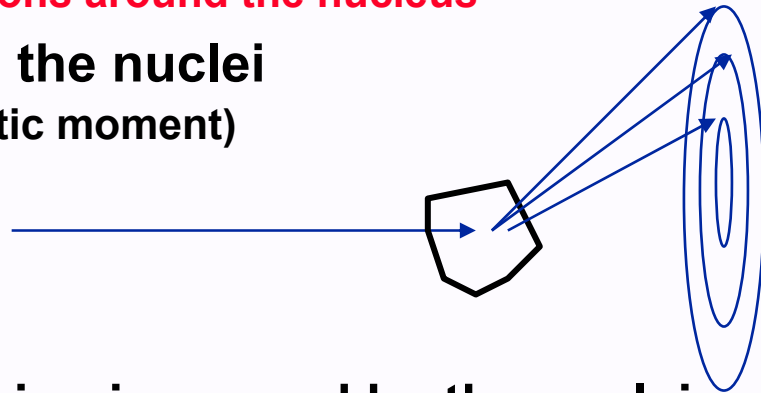
- Need probe that can penetrate into crystal
- X-rays, neutrons, (high energy electrons)



- X-rays discovered by Roentgen in 1895 - instant sensation round the world - view of his wife's hand
- Neutrons (discovered in 1932) penetrate with almost no interaction with most materials

# How can we study crystal structure?

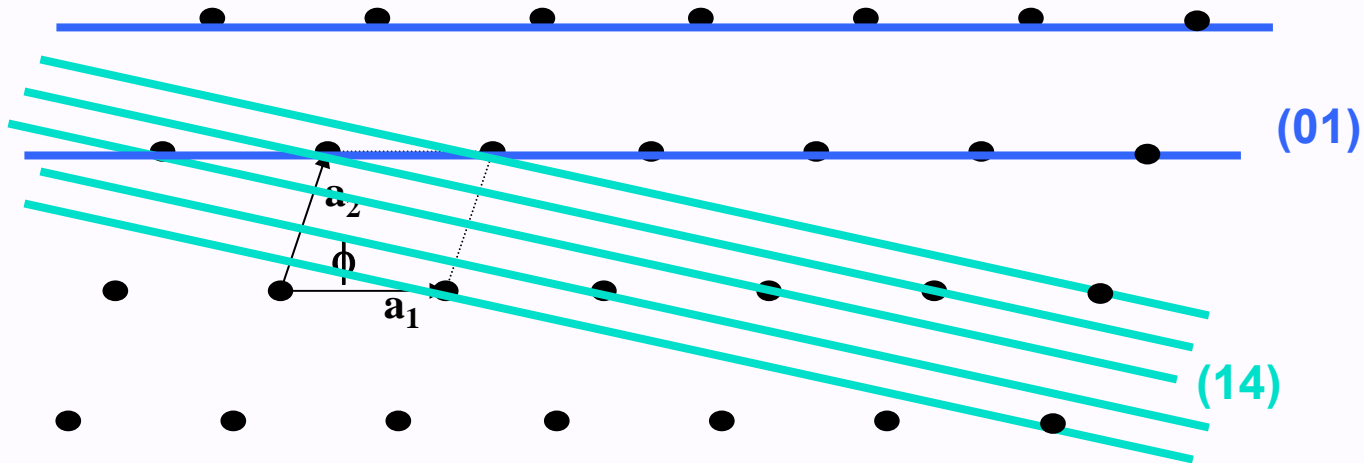
- **X-rays** scatter from the electrons
  - intensity proportional to the density  $n(r)$
  - **Mainly the core electrons around the nucleus**
- **High energy electrons**
  - **Also mainly core electrons around the nucleus**
- **Neutrons** scatter from the nuclei  
(and electron magnetic moment)



- In all cases the scattering is caused by the nuclei or the core electrons near the nuclei
- The scattering amplitude is periodic - the same in each cell of the crystal
- **Diffraction is the constructive interference of the scattering from the very large number of cells of the crystal**

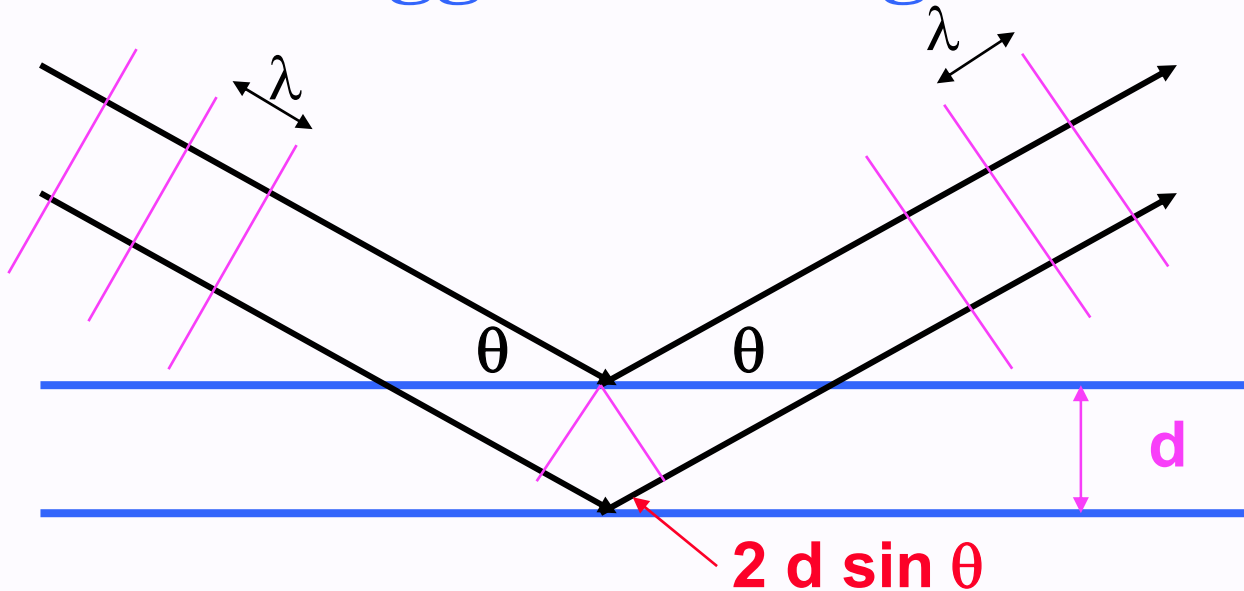
# The crystal can be viewed as made up of planes of atoms

## Lattice



- There are many sets of parallel planes that can be drawn through the crystal
- Low index planes: more dense, more widely spaced
- High index planes: less dense, more closely spaced

# Bragg Scattering Law



- Condition for constructive interference (Diffraction):  
 **$2d \sin \theta = n \lambda$**
- **Maximum  $\lambda = 2d$**
- Only waves with  $\lambda$  smaller than  $2d$  can satisfy the Bragg scattering law for diffraction
- For a typical crystal the maximum  $d \sim 0.1 - 1 \text{ nm}$ , so that  
 **$\lambda < \sim 0.1 - 1 \text{ nm}$**

# What energy x-rays, neutrons... are required?

- **What energy waves (particles) can satisfy the Bragg scattering law for a typical crystal?**

$$\lambda < 0.1 - 1 \text{ nm}$$

From Homework 0:	$\lambda=0.1 \text{ nm}$	$\lambda=1.0 \text{ nm}$
X-rays	$E= 1.24 \cdot 10^4 \text{ eV}$	$E= 1.24 \cdot 10^3 \text{ eV}$
Neutron	$E= 8.16 \cdot 10^{-2} \text{ eV}$	$E= 8.16 \cdot 10^{-4} \text{ eV}$
Electron	$E= 1.50 \cdot 10^2 \text{ eV}$	$E= 1.50 \text{ eV}$

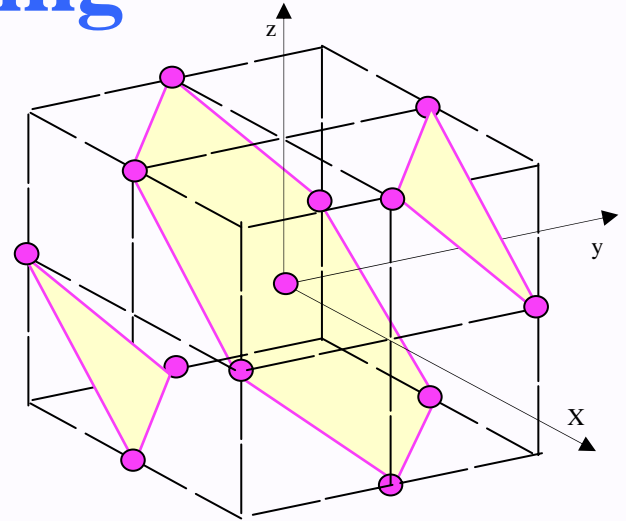
See Fig. 1, Ch. 2 of Kittel for plot of E vs.  $\lambda$

**X-rays** and **neutrons** at these energies penetrate solids and are useful for studies of the bulk material

**Electrons** of these energies scatter very strongly – they do not penetrate far and they can be used to study surfaces

# Example of scattering

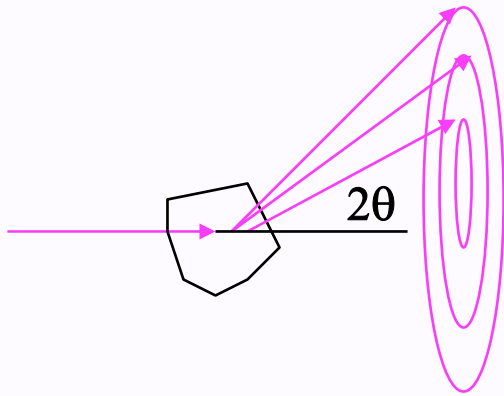
- Aluminum (Al) is fcc with  $a = 0.405 \text{ nm}$
- What is minimum energy x-ray that can satisfy the Bragg condition?



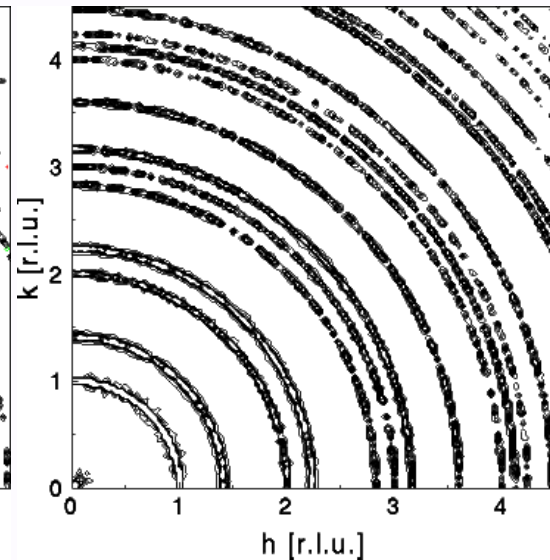
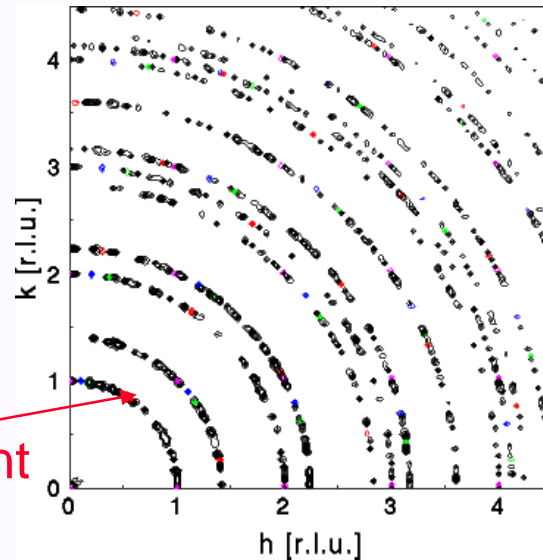
- The largest distance between planes is for 111 planes:  
 $d = (a \sqrt{3})/3 = a / \sqrt{3}$
- Maximum  $\lambda$  is  $2d = 2 a / \sqrt{3} = 0.468 \text{ nm}$
- Using  $E = h\nu = hc/\lambda$ , ( $hc = 1.24 \times 10^{-6} \text{ m} = 1.24 \times 10^3 \text{ nm}$ ), the minimum energy x-ray for Bragg scattering is 2.65 keV.
- Higher energy x-rays are needed for diffraction from all other planes in the crystal



# Why is a powder “better” than a single crystal for x-ray diffraction?



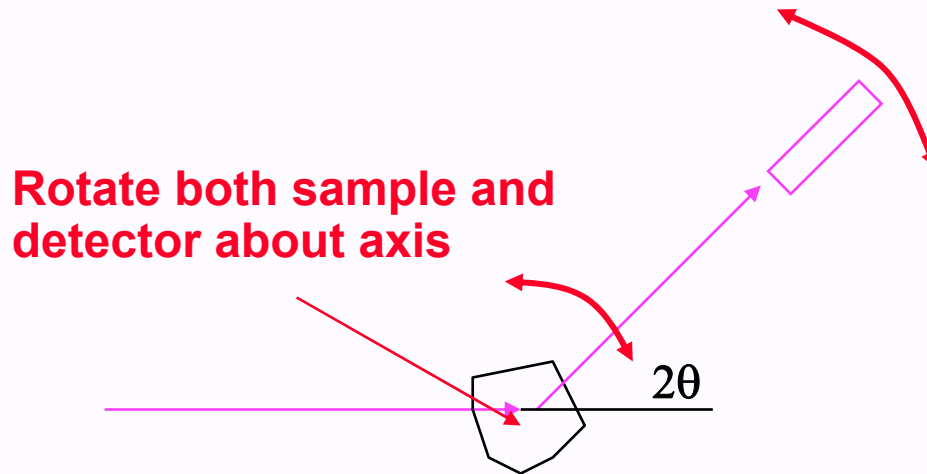
Each ring is a different plane in the crystal



- For fixed  $\lambda$ , Bragg condition satisfied only for certain angles  $\theta$
- Random powder automatically averages over all angles
- Diffraction (Bragg Scattering) from a powder of crystallites
- Example of too few crystallites (left) and better sample (right)

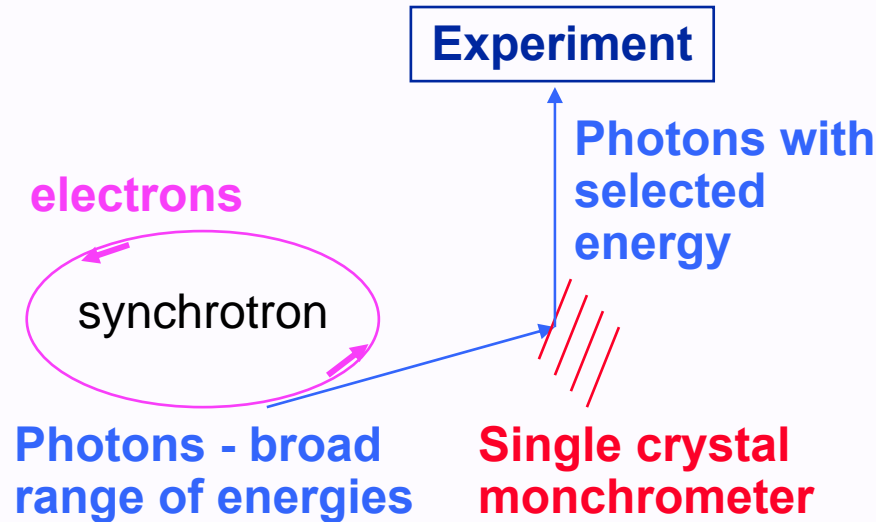
<http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/pow.html>

# Single crystal diffraction



- Crystal must be oriented in all directions in 3D space using “Gonier Spectrometer”
- Observe scattering only at Bragg angles for a fixed wavelength x-ray or neutrons or .....

# Alternative approach - energy dispersive diffraction



- For fixed angle  $\theta$ , vary the energy (i.e.,  $\lambda$ ) to satisfy Bragg condition for a sample (the “experiment”)
- X-rays over broad energy range now available at synchrotrons like the Advanced Photon Source at Argonne
- Note that diffraction from a single crystallite is also used at the **monochromator** to select X-rays with desired wavelength
- See <http://www.aps.anl.gov/>

# Periodic Functions and Fourier Analysis

- **Any periodic function can be expressed in terms of its periodic Fourier components (harmonics).**
- Example of density  $n(x)$  in 1 D crystal:

$$n(x) = n_0 + \sum_{m>0} [C_m \cos (2\pi m x/a) + S_m \sin (2\pi m x/a)]$$

- Easier expression:

$$n(x) = \sum_m n_m \exp( i 2\pi p x/a)$$

(easier because  $\exp( a + b ) = \exp( a ) \exp( b )$  )

- Expression for Fourier Components:

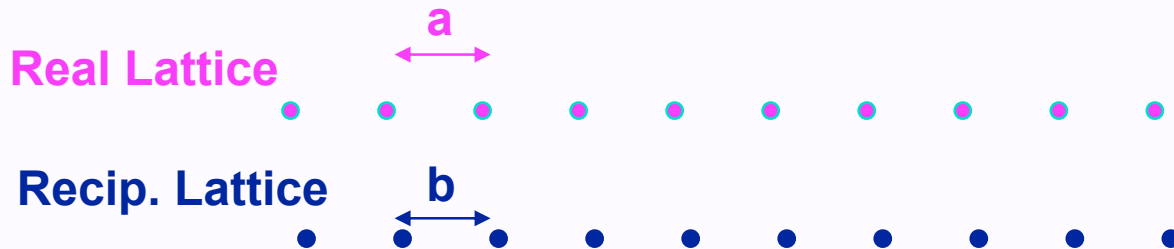
$$n_m = \int_0^a dx n(x) \exp( - i 2\pi m x/a)$$

# Reciprocal Lattice and Fourier Analysis in 1D

- In 1D,  $b = 2 \pi / a$
- Periodic function  $f(x)$ :

$$\begin{aligned} f(x) &= \sum_m f_m \exp(i 2\pi m x/a) \\ &= \sum_m f_m \exp(i m b x), \quad m = \text{integer} \end{aligned}$$

- The set of all integers  $x \cdot b$  are the **reciprocal lattice**



# Fourier Analysis in 3 dimensions

- Define vector position  $\mathbf{r} = (x,y,z)$  [  $\mathbf{r} = (x,y)$  (2D) ]

- **Fourier analysis**

$$f(\mathbf{r}) = \sum_{\mathbf{G}} f_{\mathbf{G}} \exp(i \mathbf{G} \cdot \mathbf{r})$$

where the  $\mathbf{G}$ 's are vectors, i.e.,

$$\begin{aligned} \exp(i \mathbf{G} \cdot \mathbf{r}) &= \exp(i (G_x x + G_y y + G_z z) ) \\ &= \exp(i G_x x) \exp(i G_y y) \exp(i G_z z) \end{aligned}$$

- **A periodic function satisfies**

$f(\mathbf{r}) = f(\mathbf{r} + \mathbf{T})$  where  $\mathbf{T}$  is any translation vector

$$\mathbf{T}(n_1, n_2, \dots) = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3, \text{ integer } n\text{'s}$$

- **Thus**

$$f(\mathbf{r} + \mathbf{T}) = \sum_{\mathbf{G}} f_{\mathbf{G}} \exp(i \mathbf{G} \cdot \mathbf{r}) \exp(i \mathbf{G} \cdot \mathbf{T}) = f(\mathbf{r})$$

$$\Rightarrow \exp(i \mathbf{G} \cdot \mathbf{T}) = 1 \Rightarrow \mathbf{G} \cdot \mathbf{T} = 2\pi \times \text{integer}$$

# Reciprocal Lattice

- **Reciprocal lattice is defined by the vectors**

$$\mathbf{G}(m_1, m_2, \dots) = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3,$$

where the  $m$ 's are integers and

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}, \text{ where } \delta_{ij} = 1, \delta_{ij} = 0, i \neq j$$

- **The reciprocal lattice is a set of  $\mathbf{G}$  vectors that is determined by the real space Bravais lattice**
- **The **only** information about the actual basis of atoms is in the quantitative values of the Fourier components  $f_{\mathbf{G}}$  in the Fourier analysis**

$$f(\mathbf{r}) = \sum_{\mathbf{G}} f_{\mathbf{G}} \exp(i \mathbf{G} \cdot \mathbf{r})$$

- **Inversion formula:**

$$f_{\mathbf{G}} = \int_{\text{cell}} d\mathbf{r} f(\mathbf{r}) \exp(-i \mathbf{G} \cdot \mathbf{r})$$

# Reciprocal Space

- **Reciprocal space is the space of Fourier components**

- The Fourier transform of a general function  $g(\mathbf{r})$ :

$$g(\mathbf{r}) = \int_{\text{all } \mathbf{k}} d\mathbf{k} g(\mathbf{k}) \exp(i \mathbf{k} \cdot \mathbf{r}),$$

$$g(\mathbf{k}) = (1/2\pi) \int_{\text{all } \mathbf{r}} d\mathbf{r} g(\mathbf{r}) \exp(-i \mathbf{k} \cdot \mathbf{r}),$$

where  $\mathbf{k} = (k_x, k_y, k_z)$  where  $k_x, k_y, k_z$  are continuous variables that can have any values.

- $\mathbf{k} = (k_x, k_y, k_z)$  is a **vector in reciprocal space**
- **Reciprocal space is defined independent of any crystal!**

- The reciprocal lattice is the set of Fourier components

$\mathbf{G}(m_1, m_2, m_3) = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3,$   
which are vectors that form a lattice in reciprocal space

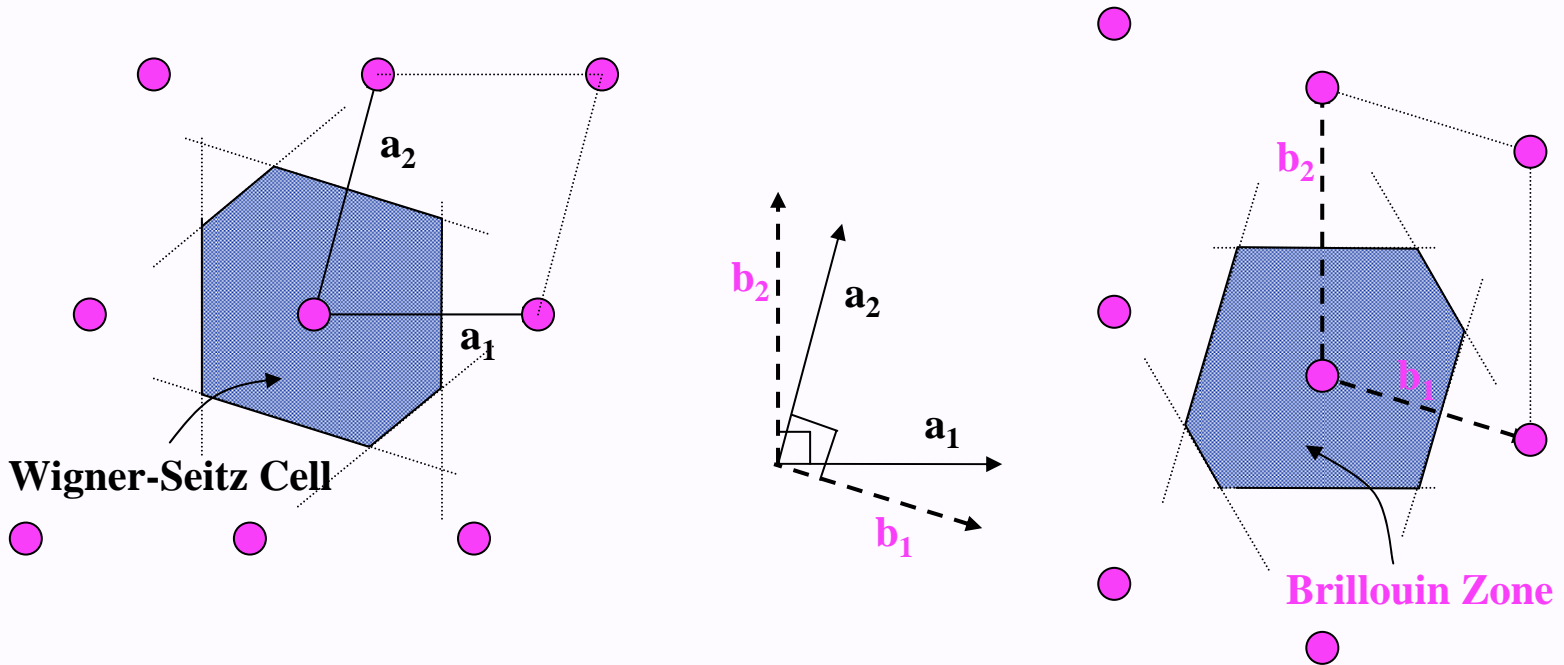
- For a periodic crystal the only non-zero Fourier components are for  $\mathbf{k} = \mathbf{G}$

• **For each Bravais lattice in “real space” there is a unique reciprocal lattice in reciprocal space.**

• **Real lattice: Set of translations**  $\mathbf{T}(n_1, n_2, \dots) = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$   
**Reciprocal lattice: Set of**  $\mathbf{G}(m_1, m_2, m_3) = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3$



# Real & Reciprocal lattices in 2 D



- For each Bravais lattice, there is a reciprocal lattice
- $b_1$  perpendicular to  $a_2$  --  $b_2$  perpendicular to  $a_1$
- Wigner-Seitz Cell of Reciprocal lattice called the “First Brillouin Zone” or simply “Brillouin Zone”

# Reciprocal Lattice in 3D

- The primitive vectors of the reciprocal lattice are defined by the vectors  $\mathbf{b}_i$  that satisfy

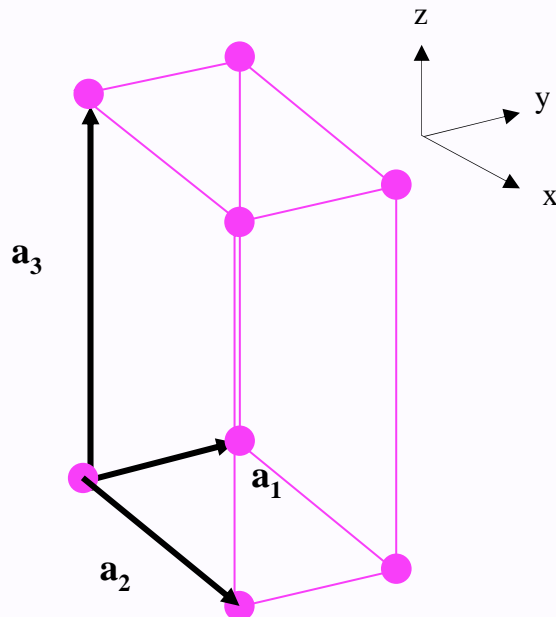
$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}, \text{ where } \delta_{ij} = 1, \delta_{ij} = 0, i \neq j$$

- How to find the  $\mathbf{b}$ 's?

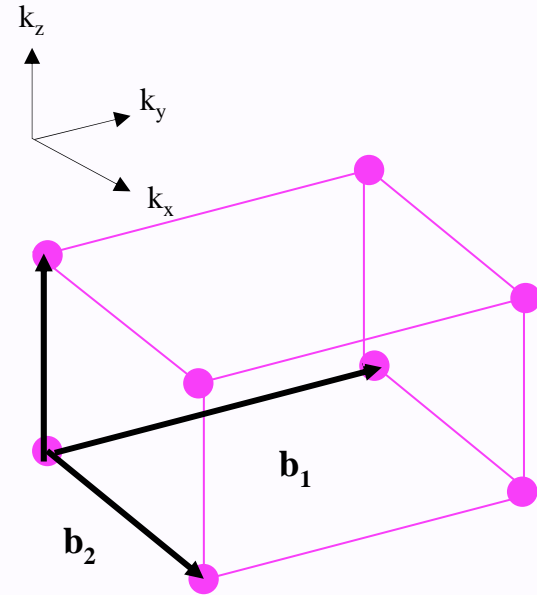
- Note:  $\mathbf{b}_1$  is orthogonal to  $\mathbf{a}_2$  and  $\mathbf{a}_3$ , etc.
- In 3D, this is found by noting that  $(\mathbf{a}_2 \times \mathbf{a}_3)$  is orthogonal to  $\mathbf{a}_2$  and  $\mathbf{a}_3$
- Also volume of primitive cell  $V = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$
- Then  $\mathbf{b}_i = (2\pi / V) (\mathbf{a}_j \times \mathbf{a}_k)$ , where  $i \neq j \neq k$

# Three Dimensional Lattices

## Simplest examples



Simple Orthorhombic Bravais Lattice  
with  $a_3 > a_2 > a_1$

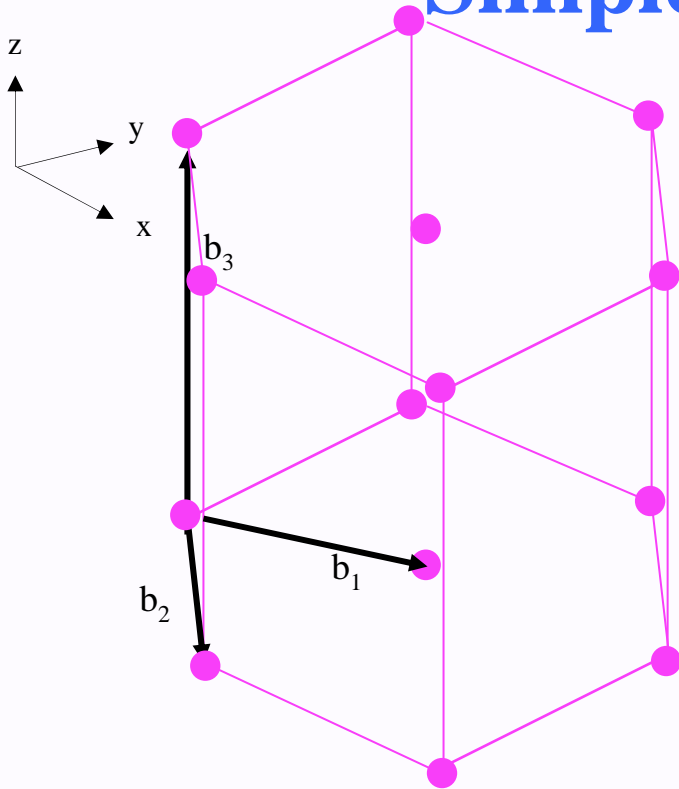


Reciprocal Lattice  
Note:  $b_1 > b_2 > b_3$

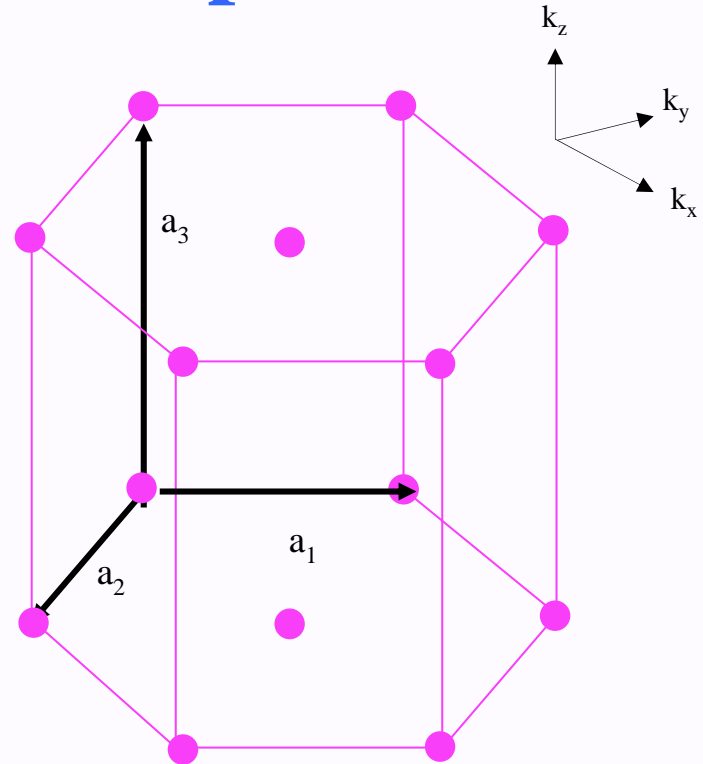
- **Long lengths in real space imply short lengths in reciprocal space and vice versa**

# Three Dimensional Lattices

## Simplest examples



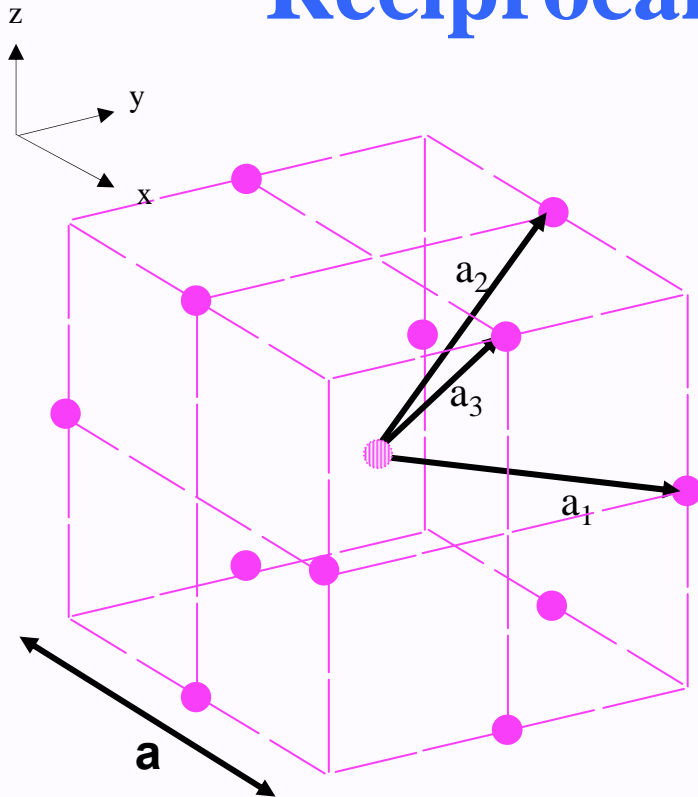
Reciprocal Lattice



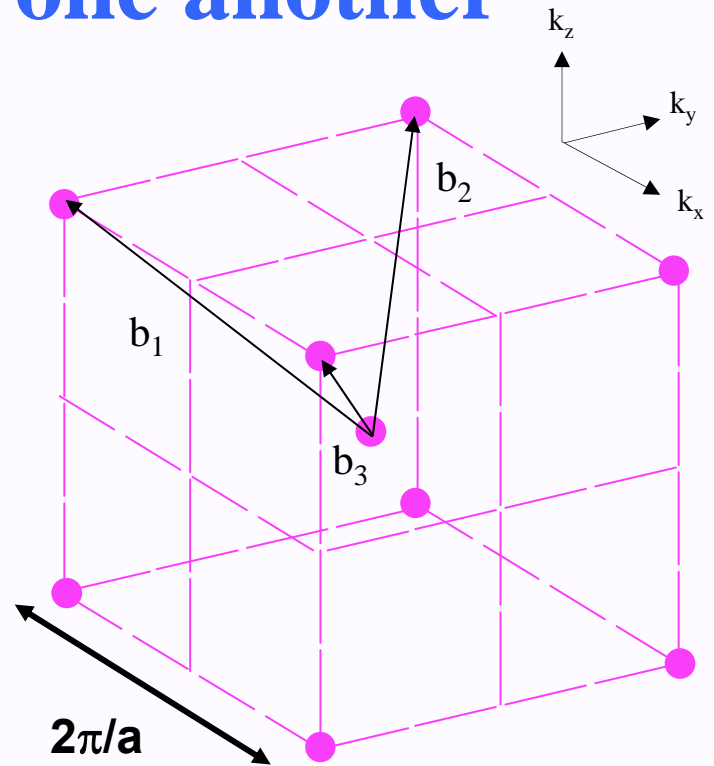
Hexagonal Bravais Lattice

- **Reciprocal lattice is also hexagonal, but rotated**
- **See homework problem in Kittel**

# Face Centered - Body Centered Cubic Reciprocal to one another

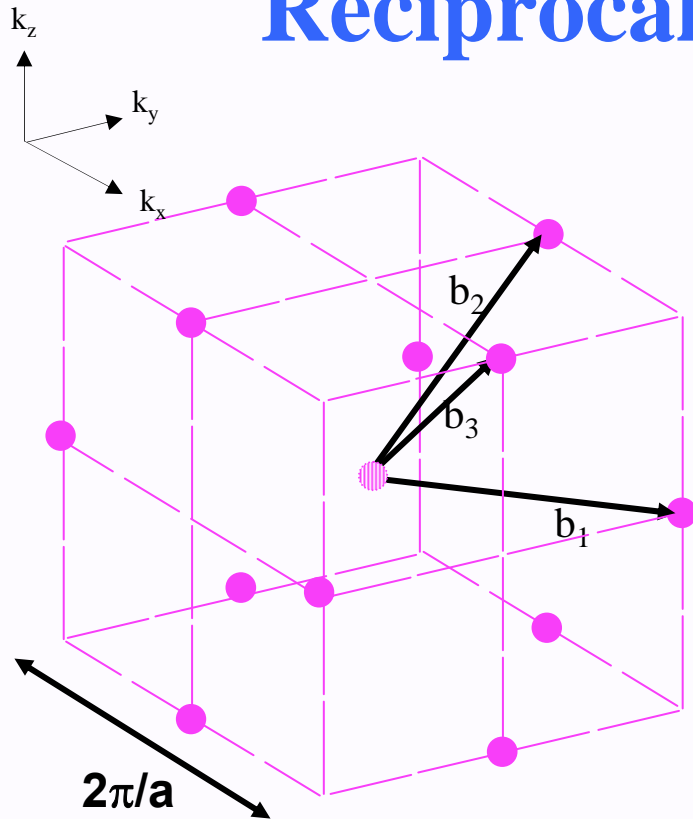


Primitive vectors and the  
conventional cell of fcc lattice

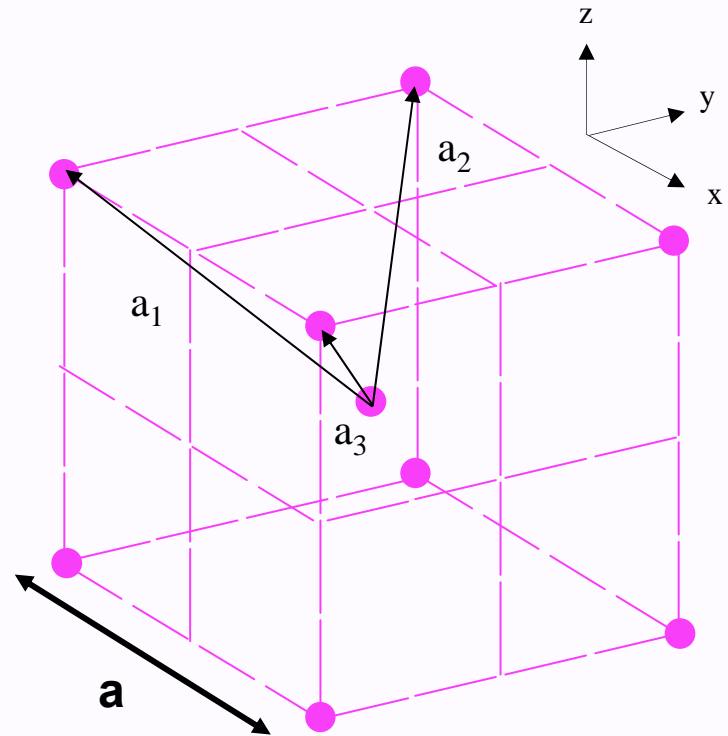


Reciprocal lattice is  
Body Centered Cubic

# Face Centered - Body Centered Cubic Reciprocal to one another

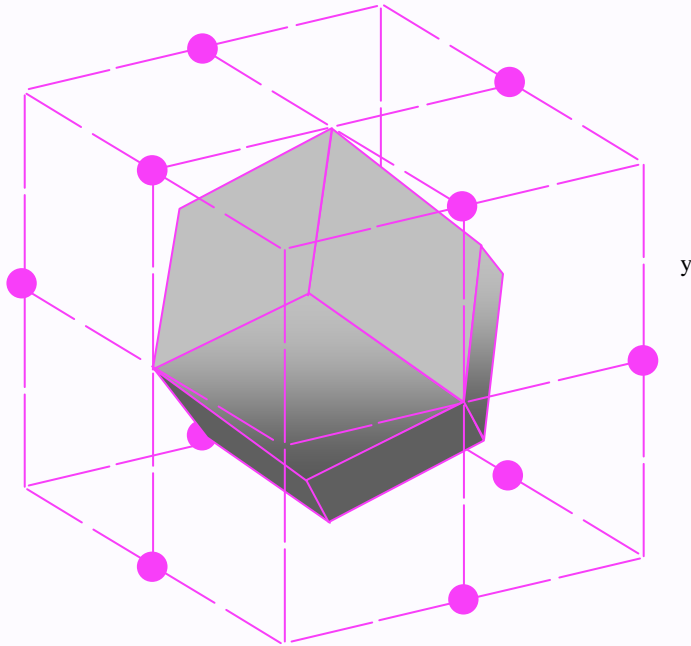


**Reciprocal lattice is  
Face Centered Cubic**

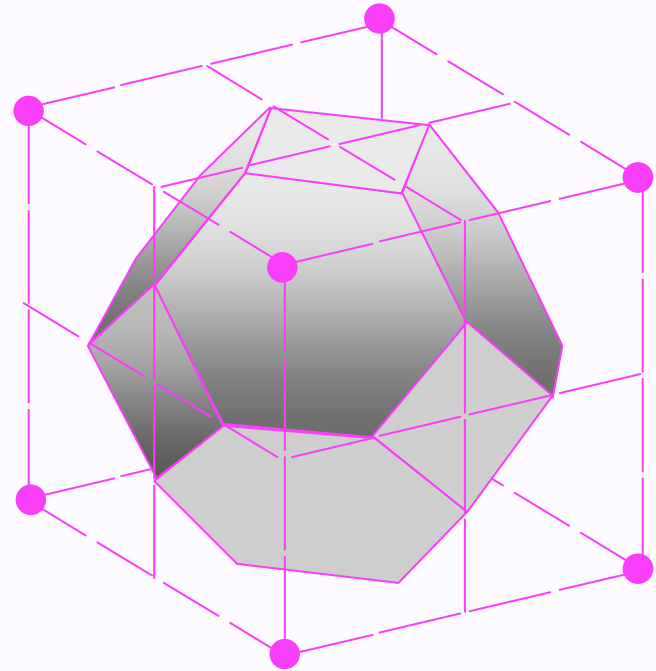


**Primitive vectors and the  
conventional cell of bcc lattice**

# Face Centered Cubic

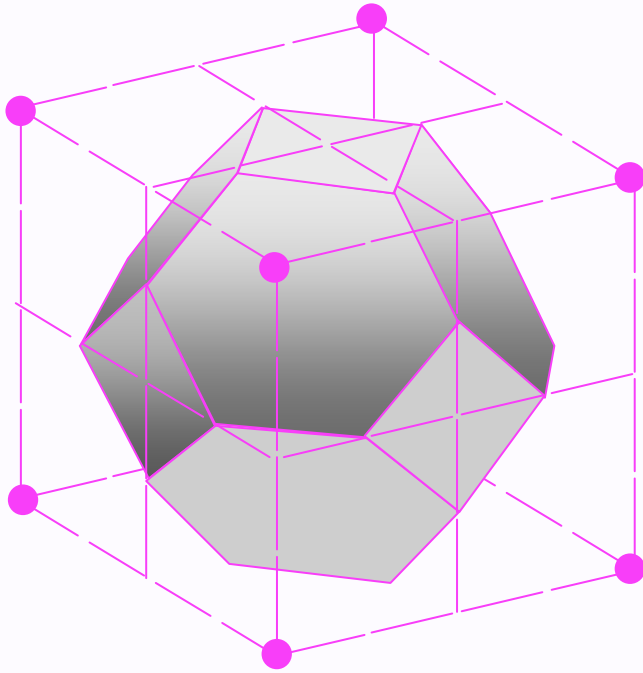


**Wigner-Seitz Cell for  
Face Centered Cubic Lattice**

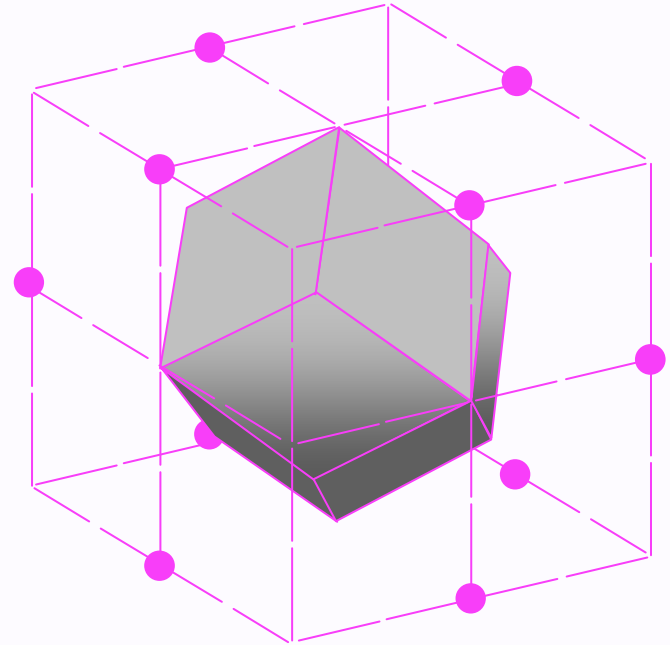


**Brillouin Zone =  
Wigner-Seitz Cell for  
Reciprocal Lattice**

# Body Centered Cubic



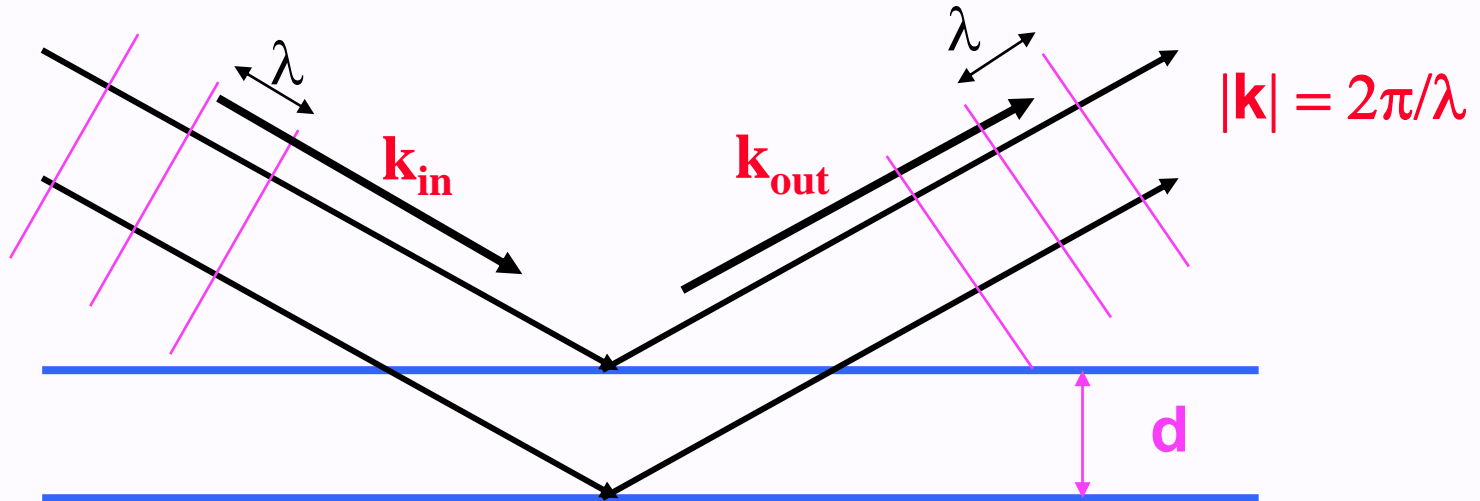
**Wigner-Seitz Cell for  
Body Centered Cubic Lattice**



**Brillouin Zone =  
Wigner-Seitz Cell for  
Reciprocal Lattice**



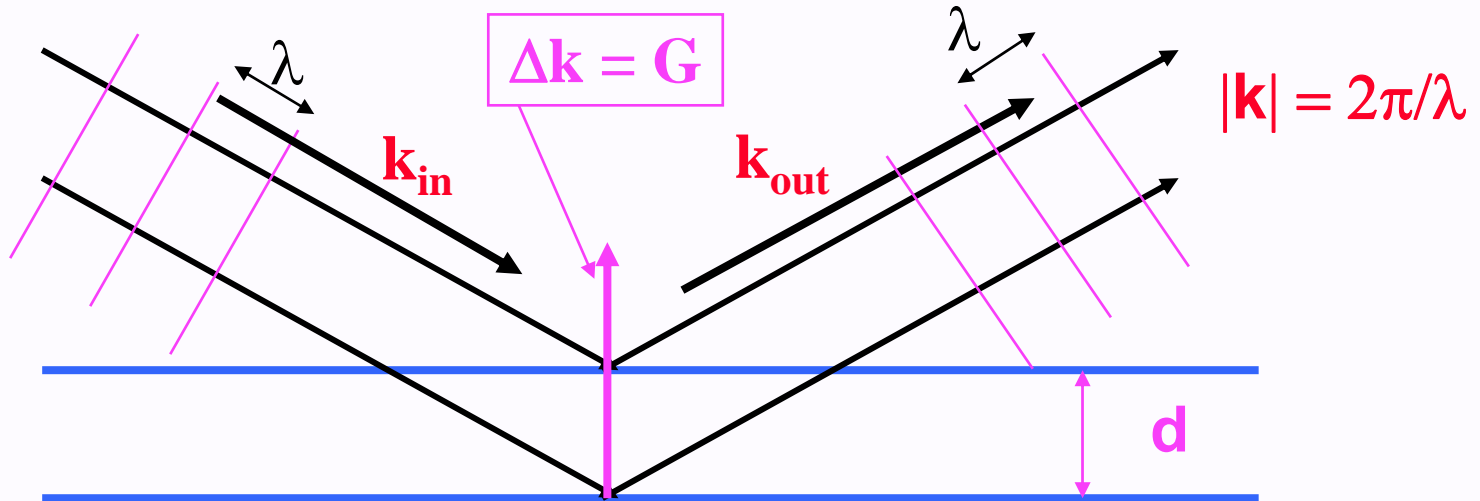
# Scattering and Fourier Analysis



- Note that  $\mathbf{k}$  is a vector in reciprocal space with  $|\mathbf{k}| = 2\pi/\lambda$
- The in and out waves have the form:  
 $\exp(i \mathbf{k}_{in} \cdot \mathbf{r} - i \omega t)$  and  $\exp(i \mathbf{k}_{out} \cdot \mathbf{r} - i \omega t)$
- If the incoming wave drives the electron density, which then radiates waves, the **amplitude** of the outgoing wave is proportional to:

$$\int_{\text{space}} d\mathbf{r} n(\mathbf{r}) \exp(i (\mathbf{k}_{in} - \mathbf{k}_{out}) \cdot \mathbf{r})$$

# Scattering and Fourier Analysis



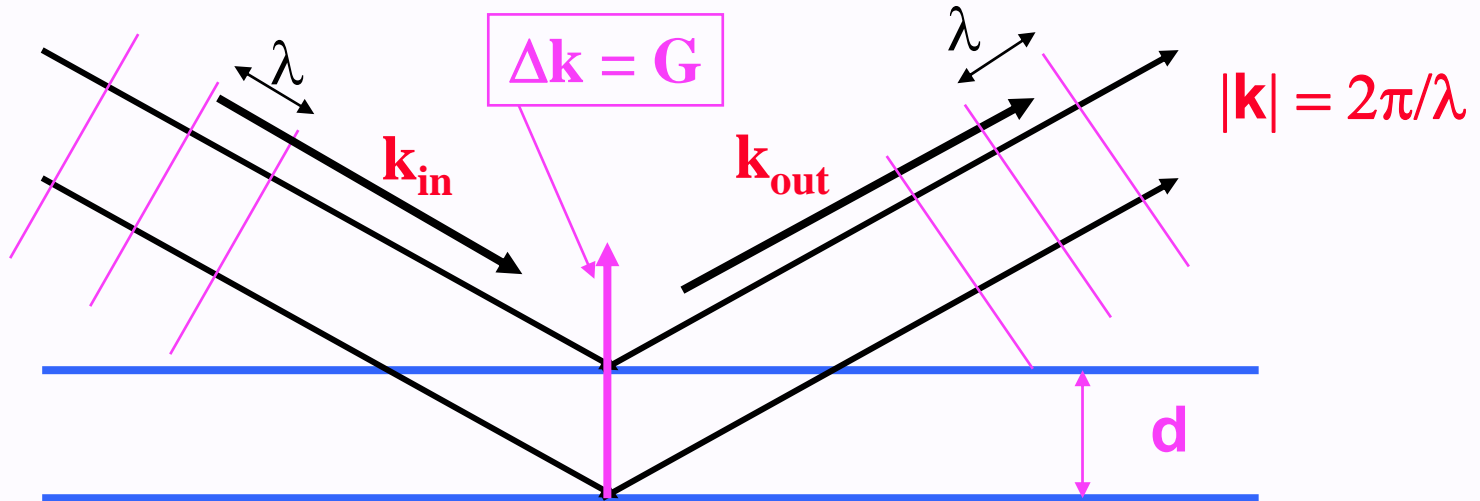
- Define  $\Delta \mathbf{k} = \mathbf{k}_{in} - \mathbf{k}_{out}$
- Then we know from Fourier analysis that

$$\int_{\text{space}} d\mathbf{r} n(\mathbf{r}) \exp(-i \Delta \mathbf{k} \cdot \mathbf{r}) = N_{\text{cell}} \mathbf{n}_{\mathbf{G}}$$

only if  $\Delta \mathbf{k} = \mathbf{G}$ , where  $\mathbf{G}$  is a reciprocal lattice vector

- Otherwise the integral vanishes

# Elastic Scattering



- For elastic scattering (energy the same for in and out waves)  
 $|\mathbf{k}_{in}| = |\mathbf{k}_{out}|$ , or  $k_{in}^2 = k_{out}^2 = |\mathbf{k}_{in} + \mathbf{G}|^2$
- Then one arrives at the condition for diffraction: (using  $\mathbf{G}$  in expression above)

$$2 \mathbf{k}_{in} \cdot \mathbf{G} = G^2$$

- Equivalent to the Bragg condition – see next lecture

# Summary on Reciprocal lattice

- All Crystals have a lattice of translations in real space, and a lattice of Fourier components in Reciprocal space
- Reciprocal lattice defined as
- $\mathbf{G}(m_1, m_2, \dots) = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3$ ,  
where the  $\mathbf{b}$ 's are primitive vectors defined by  
 $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}$ , where  $\delta_{ij} = 1$ ,  $\delta_{ij} = 0$ ,  $i \neq j$
- Any periodic function can be written  
$$\mathbf{f}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{f}_{\mathbf{G}} \exp(\mathbf{i} \mathbf{G} \cdot \mathbf{r})$$
- The reciprocal lattice is defined strictly by translations (it is a Bravais lattice in reciprocal space)
- Information about the basis for the actual crystal is in the values of the Fourier coefficients  $\mathbf{f}_{\mathbf{G}}$

# Next Lecture

- **More on use of reciprocal lattice**
- **Diffraction from crystals – Ewald construction**
- **Continue reading Kittel Ch 2**
- **Start Crystal Binding (Chapter 3) if there is time**