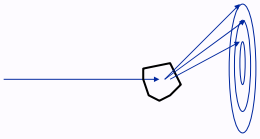
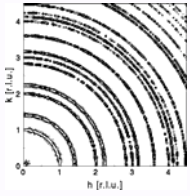
Solid State Physics 460 - Lecture 3
Diffraction and the Reciprocal Lattice
(Kittel Ch. 2)

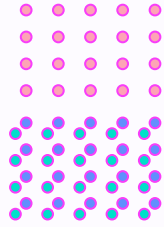




Diffraction (Bragg Scattering) from a powder of crystallites - real example of image at right from
http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/pow.html

From Previous Lectures Crystals

- A crystal is a repeated array of atoms
- Crystal ⇔ Lattice + Basis



Crystal

Lattice of points (Bravais Lattice)

Basis of atoms

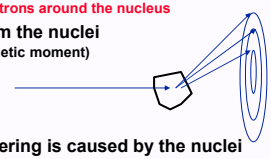
How can we study crystal structure?

- 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?

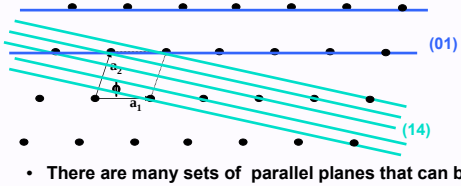
- X-rays scatter from the electrons
  - intensity proportional to the density n(r)
  - Mainly the core electrons around the nucleus
- High energy electrons
  - Also mainly core electrons around the nucleus
- Neutrons scatter from the nuclei
  (and electron magnetic moment)



- 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

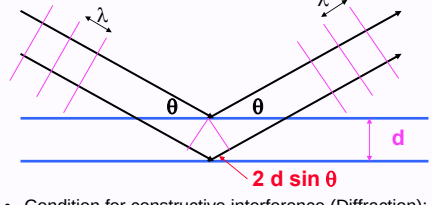
The crystal can be viewed as made up of planes of atoms

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 λ smaller than 2d can satisfy the Bragg scattering law for diffraction
- For a typical crystal the maximum d ~ 0.1 – 1 nm, so that
  $\lambda < \sim 0.1 – 1$ nm

What energy x-rays, neutrons… are required?

- **What energy waves (particles) can satisfy the Bragg scattering law for a typical crystal?**
  $\lambda < 0.1 - 1$ nm

From Homework 0:	λ=0.1 nm	λ=1.0 nm
X-rays	E= 1.24 10^4 *eV*	E= 1.24 10^3 *eV*
Neutron	E= 8.16 10^{-2} *eV*	E= 8.16 10^{-4} *eV*
Electron	E= 1.50 10^2 *eV*	E= 1.50 *eV*

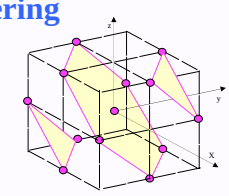
See Fig. 1, Ch. 2 of Kittel for plot of E vs. λ

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

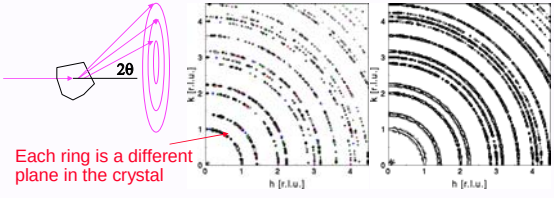
Example of scattering

- Aluminum (Al) is fcc with a = 0.405 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 λ is 2d = 2 a /$\sqrt{3}$ = 0.468 nm
- Using E = hν = hc/λ , (hc = 1.24 x 10^{-6} m = 1.24 10^3 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?

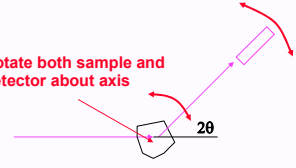


Each ring is a different plane in the crystal

- For fixed λ, Bragg condition satisfied only for certain angles θ
- 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)

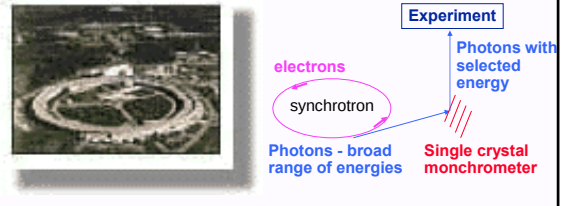
http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/pow.html

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 θ , vary the energy (i.e., λ) 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 monochrometer 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:

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

- Easier expression:

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

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

- Expression for Fourier Components:

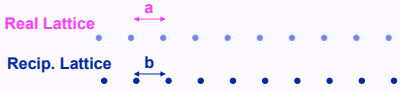
$$n_m = \int_0^a dx\, n(x) \exp(-i 2\pi m x/a)$$

Reciprocal Lattice and Fourier Analysis in 1D

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

$$f(x) = \Sigma_m f_m \exp(i\, 2\pi\, m\, x/a)$$
$$= \Sigma_m f_m \exp(i\, m\, b\, x),\ m = \text{integer}$$

- The set of all integers $\times$ 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**

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

where the **G**'s are vectors, i.e.,

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

- **A periodic function satisfies**

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

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

- **Thus**

$$f(\mathbf{r}+\mathbf{T}) = \Sigma_{\mathbf{G}} f_{\mathbf{G}} \exp(i\,\mathbf{G}\cdot\mathbf{r})\exp(i\,\mathbf{G}\cdot\mathbf{T}) = f(\mathbf{r})$$
$$\Rightarrow \exp(i\,\mathbf{G}\cdot\mathbf{T}) = 1 \Rightarrow \mathbf{G}\cdot\mathbf{T} = 2\pi \times \text{integer}$$

Reciprocal Lattice

- **Reciprocal lattice is defined by the vectors** $\mathbf{G}(m_1,m_2,\ldots) = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$, 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 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_G in the Fourier analysis**

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

- **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(**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

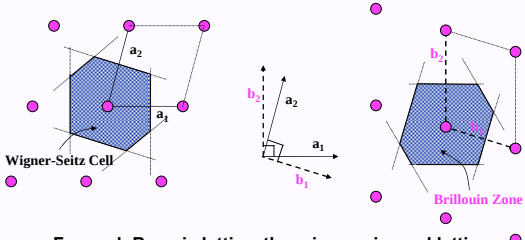
•For a periodic crystal the only non-zero Fourier components are for $\mathbf{k} = \mathbf{G}$

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

•**Real lattice: Set of translations** $\mathbf{T}(n_1,n_2,\ldots) = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$

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
- $\mathbf{b}_1$ perpendicular to $\mathbf{a}_2$ -- $\mathbf{b}_2$ perpendicular to $\mathbf{a}_1$
- Wigner-Seitz Cell of Reciprocal lattice called the "First Brillouin Zone" or simply "Brillouin Zone"

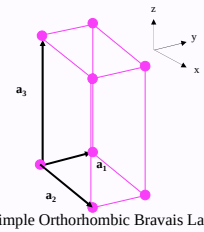
Reciprocal Lattice in 3D

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

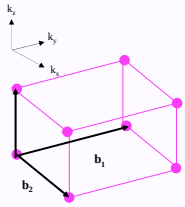
$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\,\delta_{ij},\ \text{where}\ \delta_{ij} = 1,\ \delta_{ij} = 0,\ i \neq j$$

- **How to find the 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



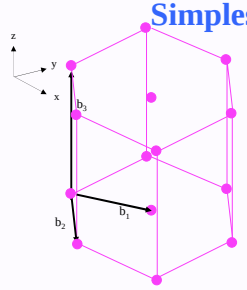
Simple Orthorhombic Bravais Lattice
with $a_3 > a_2 > a_1$



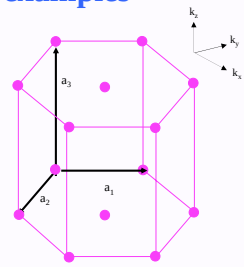
Reciprocal Lattice
Note: $b_1 > b_2 > b_3$

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

Three Dimensional Lattices
Simplest examples



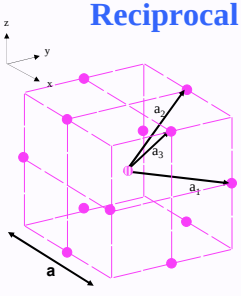
Reciprocal Lattice



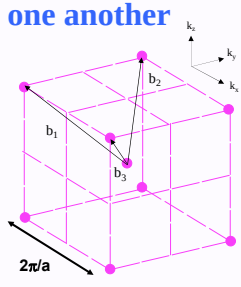
Hexagonal Bravais Lattice

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

Face Centered - Body Centered Cubic
Reciprocal to one another

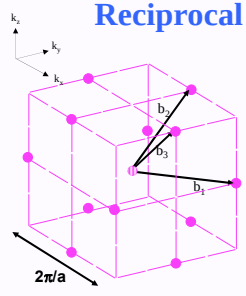


Primitive vectors and the conventional cell of fcc lattice

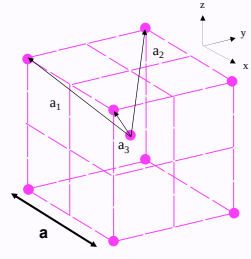


Reciprocal lattice is Body Centered Cubic

Face Centered - Body Centered Cubic
Reciprocal to one another

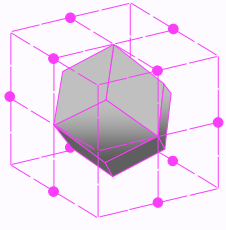


Reciprocal lattice is Face Centered Cubic

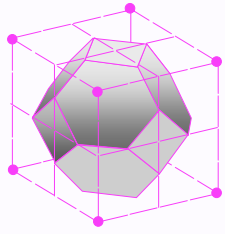


Primitive vectors and the conventional cell of bcc lattice

Face Centered Cubic

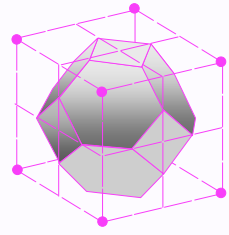


Wigner-Seitz Cell for Face Centered Cubic Lattice

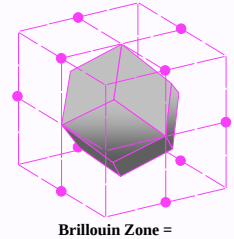


Brillouin Zone = Wigner-Seitz Cell for Reciprocal Lattice

Body Centered Cubic

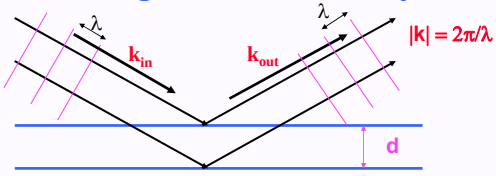


Wigner-Seitz Cell for Body Centered Cubic Lattice



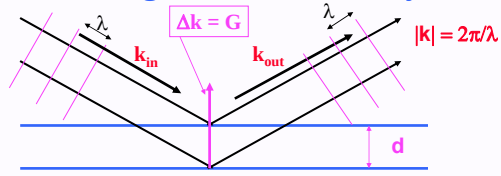
Brillouin Zone = Wigner-Seitz Cell for Reciprocal Lattice

Scattering and Fourier Analysis



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

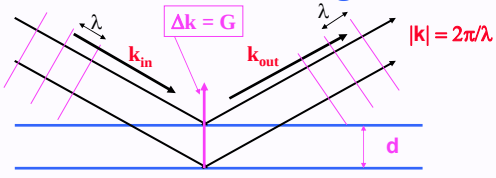
Scattering and Fourier Analysis



- Define $\Delta k = k_{in} - k_{out}$
- Then we know from Fourier analysis that
  $\int_{space} dr\, n(r) \exp(- i\, \Delta k \cdot r) = N_{cell}\, n_G$

  only if $\Delta k = G$, where **G** is a reciprocal lattice vector
- Otherwise the integral vanishes

Elastic Scattering



- For elastic scattering (energy the same for in and out waves)
  $|k_{in}| = |k_{out}|$, or $k_{in}^2 = k_{out}^2 = |k_{in} + G|^2$
- Then one arrives at the condition for diffraction: (using -**G** in expression above)
  $2\, k_{in} \cdot G = G^2$
- 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
- $G(m_1,m_2,\ldots) = m_1 b_1 + m_2 b_2 + m_3 b_3$, where the b's are primitive vectors defined by
  $b_i \cdot a_j = 2\pi\, \delta_{ij}$, where $\delta_{ij} = 1$, $\delta_{ij} = 0$, $i \neq j$
- Any periodic function can be written
  $f(r) = \Sigma_G f_G \exp(i\, G \cdot r)$
- 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 f_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**