Lecture 5 - Diffraction and Recip. Lat. - continued

**Solid State Physics 460- Lecture 5
Diffraction and the Reciprocal Lattice
Continued (Kittel Ch. 2)**

Ewald Construction

k_{out}
G
k_{in}
2θ

Recall from previous lectures

- **Definition of a crystal – Lattice + Basis**

- **Reciprocal lattice – Lattice in Fourier space (reciprocal space)**

- **Diffraction from crystals – Bragg Condition – 2d sin θ = n λ**

- Diffraction and the reciprocal lattice

- **Today:**
- Diffraction and the reciprocal lattice continued – **Ewald construction and the Brillouin Zone (BZ)**

Recall from Lecture 3 **Summary: Real and Reciprocal lattices**

- Crystal lattice of translations:
  $T(n_1,n_2,\ldots) = n_1\, a_1 + n_2\, a_2 + n_3\, a_3$ **Primitive vectors**
- Reciprocal lattice:
  $G(m_1,m_2,\ldots) = m_1\, b_1 + m_2\, b_2 + m_3\, b_3$,
  where
  $b_i \cdot a_j = 2\pi\, \delta_{ij}$, where $\delta_{ij} = 1$, $\delta_{ij} = 0$, $i \neq j$
- Any periodic function can be written
  $f(r) = \Sigma_G\, f_G \exp(\,i\, G \cdot r)$
- Information about the basis for the actual crystal is in the values of the Fourier coefficients

  $f_G = (1/V_{cell}) \int_{cell} d^3r\ f(r)\exp(-\,i\, G \cdot r)$

  Kittel Ch. 2

Recall from Lecture 3 **Bragg Scattering Law**

λ λ
θ θ
d
2 d sin θ

- Condition for constructive interference (Diffraction):
  2d sin θ = n λ
- **Maximum λ = 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
  λ < ~ 0.1 – 1 nm

Recall from Lecture 3 **Scattering and Fourier Analysis**

λ λ
k_{in} k_{out} $|k| = 2\pi/\lambda$
d

- 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:
  $\int_{space} dr\ n(r)\exp(i\,(k_{in} - k_{out})\cdot r)$

Recall from Lecture 3 **Scattering and Fourier Analysis**

Δk = G
λ λ
k_{in} k_{out} $|k| = 2\pi/\lambda$
d

- Define **Δk = k_in - k_out**
- Then we know from Fourier analysis that
  $(1/V_{cell}) \int_{cell} dr\ n(r)\exp(-\,i\, \Delta k \cdot r) = n_G$

  only if **Δk = G**, where **G** is a reciprocal lattice vector
- Otherwise the integral vanishes

Note: These statements are for a perfect crystal of size → infinity. See prob. Kittel 2.4 for a finite crystal where the scattering is peaked at Δk = G with a finite width.

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Elastic Scattering

$\Delta k = G$

k_{in} k_{out} $|k| = 2\pi/\lambda$

d

- 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)
  $2 k_{in} \cdot G = G^2$

  G Is any one of the recip. lattice vectors

- Equivalent to the Bragg condition – see next lecture

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Ewald Construction

G Is any one of the recip. lattice vectors

k_{out}

k_{in} G

2θ

- **Condition for diffraction:**

  $k_{out} = k_{in} + G$

  and

- $| 2 k_{in} \cdot G | = |G|^2 = 2 | k_{in} | | G | \sin \theta$

  $\Rightarrow$ $|G| = 2 | k_{in} | \sin \theta$

  (note sine function, not cosine)

  Why? Discussed in class

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Equivalent to Bragg Condition

k_{out}

k_{in} G

2θ

- **From last slide,**

  $| G | = 2 | k_{in} | \sin \theta$

- **But** $| k_{in} | = 2\pi/\lambda$, **and** $| G | = n (2\pi/d)$, **where d = spacing between planes (see homework, Kittel prob. 2-1)**

- $\Rightarrow$ **Bragg condition** $2d \sin \theta = n \lambda$

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Geometric Construction of Diffraction Conditions

b_2 $-k_{out}$ G

k_{in}

b_1

- **Recall** $k_{in} - k_{out} = G$ **and** $|k_{in}| = |k_{out}|$

- **Consequence of condition** $| 2 k_{in} \cdot G | = G^2$

- **The vector** k_{in} **(and** k_{out}**) lies along the perpendicular bisecting plane of a G vector**

- **One example is shown**

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Diffraction and the Brillouin Zone

- **Brillouin Zone - (BZ) - the Wigner-Seitz cell of the reciprocal lattice**

b_2 $-k_{out}$ G

k_{in}

b_1

Brillouin Zone

- **Formed by perpendicular bisectors of G vectors**

- **Special Role of Brillouin Zone**
  - **Diffraction occurs only for k on surface of Brillouin Zone**
  - **No diffraction occurs for any k inside the first Brillouin Zone**
  - **Important later in course**

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Comparison of diffraction from different lattices

- **The Bragg condition can also be written**
  $| G | = 2 | k_{in} | \sin \theta$
  $\Rightarrow \sin \theta = (\lambda /4\pi) | G |$

- **Thus the ratios of the sines of the angles for diffraction are given by:**
  $\sin \theta_1 / \sin \theta_2 = | G_1 | / | G_2 |$

- **Each type of lattice has characteristic ratios the positions of diffraction peaks as a function of sin θ**

- **Simple scaling with** λ

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Experimental Powder Pattern

- **Diffraction peaks at angles satisfying the Bragg condition**
- **Experimental example**

Differences for imperfect powder averages

Reciprocal Lattice units

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

Comparison of diffraction from different lattices

- **Ratios $\sin \theta_i / \sin \theta_0 = |G_i| / |G_0|$, where θ_0 is the lowest angle peak (smallest G)**
- **Easiest to give ratios of squares $G_i{}^2 / G_0{}^2$**

Simple Cubic lattice
(G in units of $2\pi/a$)

G_i	$G_i{}^2$	ratio
1,0,0	1	1
1,1,0	2	2
1,1,1	3	3
2,0,0	4	4
2,1,0	5	5

Comparison of diffraction from different lattices - continued

FCC real space lattice
(G in units of $2\pi/a$)

G_i	$G_i{}^2$	ratio
1,1,1	3	1
2,0,0	4	4/3
2,2,0	8	8/3
3,1,1	11	11/3
2,2,2	12	4
4,0,0	16	1/3

BCC real space lattice
(G in units of $2\pi/a$)

G_i	$G_i{}^2$	ratio
1,1,0	2	1
2,0,0	4	2
2,1,1	6	3
2,2,0	8	4
3,1,0	10	5
2,2,2	12	6

Same ratios as Simple cubic!

Example of KCl, KBr

- **See Kittel Fig. 17**

- **KCl and KBr have fcc structure – expect fcc "powder patterns"**

- **But KCl has a special feature**
  - **K+ and Cl- have the same number of electrons, they scatter x-rays almost the same ---- thus KCl has**
  - **a pattern like simple cubic**

  Why does this happen?

Comparison of diffraction from different lattices - continued

- **Lower symmetry lattices**
- **Example - Orthorhombic**
  $G = (n_1\, 2\pi/a_1,\ n_2\, 2\pi/a_2,\ n_3\, 2\pi/a_3\ )$
  - **Lengths of G's are in general not any special numbers since the a's can be in any ratios**

  - **Many lines in diffraction pattern because of many different values of |G|**

- **Hexagonal - length along c axis not related to lengths perpendicular to c axis**

Fourier Analysis of the basis

- **The intensity of the diffraction at each G is proportional to the square of the amplitude of the Fourier component**
  $n_G = (1/V_{cell}) \int_{cell} dr\ n(r)\ \exp(- i\, G \cdot r)$
- **It is also possible to regard the crystal density n(r) as a sum of atomic-like densities $n^{atom}(r - R_i)$, centered at point R_i**
  $n(r) = \sum_{all\ i} n^{atom\ i}(r - R_i)$
- **Then also**
  $n_G = \sum_{i\ in\ cell} \int_{space} dr\ n^{atom\ i}(r - R_i)\ \exp(- i\, G \cdot r)$

Cell

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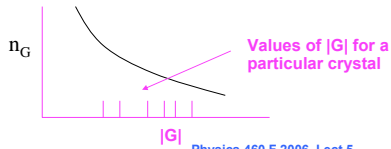# Lecture 5 - Diffraction and Recip. Lat. - continued

One atom per cell and Form Factor

- **Then one can set $R_i = 0$ and n_G is the Fourier transform of one atom density**

$$n_G = \int_{space} dr\ n^{atom}(r)\ exp(-\ i\ G \cdot r)$$

$$n^{atom}(r) \qquad |r|$$

- **Called Form Factor**
- **Example in Kittel**

$$n_G$$

Values of |G| for a particular crystal

$$|G|$$

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More than one atom per cell

- $n_G = \sum_{i\ in\ cell} \int_{space} dr\ n^{atom\ i}(r - R_i)\ exp(-\ i\ G \cdot r)$

$$= \sum_{i\ in\ cell} exp(-\ i\ G \cdot R_i)$$
$$\int_{space} dr\ n^{atom\ i}(r - R_i)\ exp(-\ i\ G \cdot (r - R_i))$$

$$= \sum_{i\ in\ cell} exp(-\ i\ G \cdot R_i)$$
$$\int_{space} dr\ n^{atom\ i}(r)\ exp(-\ i\ G \cdot r)$$

$$= \sum_{i\ in\ cell} exp(-\ i\ G \cdot R_i)\ n_G^{atom\ i}$$

- **Interpretation: Structure Factor = Form factor $n_G^{atom\ i}$ x phase factor $exp(-\ iG \cdot R_i)$ for each atom in unit cell**

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Structure factor

- **Often the basis contains more than one atom that is same element, e.g., diamond structure**
- **Then $n_G^{atom\ i} = n_G^{atom}$ is the same for each i and**

$$n_G = \sum_{i\ in\ cell} exp(-\ i\ G \cdot R_i)\ n_G^{atom\ i}$$

$$= n_G^{atom} \sum_{i\ in\ cell} exp(-\ i\ G \cdot R_i)$$

- **Define "pure" structure factor**

$$S_G^0 = (1/N_{cell}) \sum_{i\ in\ cell} exp(-\ i\ G \cdot R_i)$$
where N_{cell} = number of atoms in cell
- **Then $n_G = N^0\ S_G^0\ n_G^{atom}$**

NOTE - Kittel defines n_G to be the "structure factor"

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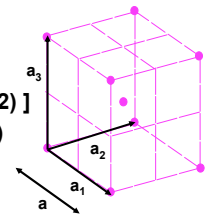## Body Centered Cubic viewed as Simple Cubic with 2 points per cell

$S_G^0 = (1/2) \sum_{i=1,2} exp(-\ i\ G \cdot R_i)$
$= (1/2)(1 + exp(-\ i\ G \cdot R_2)$
$= (1/2)\ exp(-\ i\ G \cdot R_2/2)$
$[exp(\ i\ G \cdot R_2/2) + exp(-\ i\ G \cdot R_2/2)]$
$= exp(-\ i\ G \cdot R_2/2)\ cos(G \cdot R_2/2)$

Result: If $G = (v_1\ v_2\ v_3)\ 2\pi/a$
$|S_G^0| = 1$ if sum of integers is even
$|S_G^0| = 0$ if sum is odd

Points at $R_1 = (0,0,0)$;
$R_2 = (1,1,1)\ a/2$

Same as we found before!
FCC reciprocal lattice

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Face Centered Cubic viewed as Simple Cubic with 4 points per cell
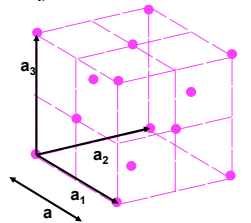
$S_G^0 = (1/4) \sum_{i=1,4} exp(-\ i\ G \cdot R_i)$

Result:

If $G = (v_1\ v_2\ v_3)\ 2\pi/a$ then

$S_G^0 = 1$ if all integers are odd or all are even

$S_G^0 = 0$ otherwise

Points at (0,0,0) ; (1,1,0) a/2 ;
(1,0,1) a/2 ; (0,1,1) a/2

Same as we found before!
BCC reciprocal lattice

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Structure factor for diamond

- **Example: diamond structure**

$$S_G^0 = (1/2) \sum_{i=1,2} exp(-\ i\ G \cdot R_i)$$

- **$R_1 = +\ (1/8, 1/8, 1/8)a$**
  $R_2 = -\ (1/8, 1/8, 1/8)a$

- **Homework problem**

- **Similar approach would apply to a graphite plane**
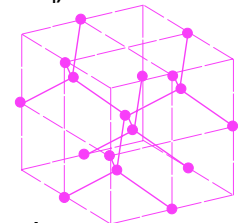
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Summary - Diffraction & Recip. Lattice

- Bragg Condition for diffraction
- Fourier Analysis and the Reciprocal Lattice
  $G(m_1, m_2, \ldots) = m_1 b_1 + m_2 b_2 + m_3 b_3$,
  where the b's are primitive vectors defined by
  $b_i \cdot a_j = 2\pi \delta_{ij}$, where $\delta_{ij} = 1$, $\delta_{ij} = 0$, $i \neq j$
- Examples of Reciprocal lattice: fcc, bcc, ...
- Ewald Construction
- Diffraction for k_{in}, k_{out} in planes - perp. bisectors of G's
- Defines Brillouin Zone - no diffraction in first BZ
- Information about the actual crystal is in the values of the Fourier coefficients f_G
  $f_G = (1/V_{cell}) \int_{cell} dr \, f(r) \exp(-i G \cdot r)$
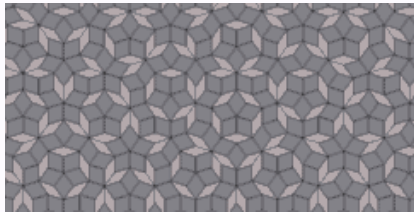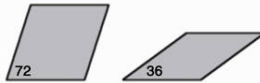- Form factor, "Pure" Structure factor

Quasicrystals

- **Not periodic in sense described before**

- **Example a crystal with periodicity a with a density wave that is a different period a´ with a´/a not a rational number**
  $n(x) = n_1 \cos(2\pi x/a) + n_2 \cos(2\pi x/a´)$
  never repeats!

- **Examples in higher dimensions
  Orientation order without translational order
  Penrose Tiles
  Five fold symmetry in x-ray patterns
  ….**

Penrose Tiles

- **Many examples
  Nice WWW sites**

  http://www.traipse.com/penrose_tiles/index.html

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  See this site for a Java program for Penrose tiles
  http://www.geocities.com/SiliconValley/Pines/1684/Penrose.html

Next Time

- **Crystal Binding (Chapter 3)**