Lecture 3

Diffraction from Crystals

“Shape Factor”

- Fultz & Howe, Chap. 5
- Williams & Carter, Chap. 17
- Reimer, Chap. 7
Shape Factor
“Crystal size effect”

- **Scattered wave:**
  \[ \psi(\Delta k) = \sum_{r_g} \frac{\nu}{lattice} F(\Delta k) \exp(-2\pi i \Delta k \cdot r_g) \]

- **Shape factor:**
  \[ S(\Delta k) = \sum_{r_g} \frac{\nu}{lattice} \exp(-2\pi i \Delta k \cdot r_g) \]

- Location of each unit cell:
  \[ r_g = n_x a \hat{x} + n_y b \hat{y} + n_z c \hat{z} \]

- \( \Delta k \) components:
  \[ \Delta k = \Delta k_x \hat{x} + \Delta k_y \hat{y} + \Delta k_z \hat{z} \]

\[
S(\Delta k) = \sum_{n_x=0}^{N_x-1} \sum_{n_y=0}^{N_y-1} \sum_{n_z=0}^{N_z-1} \exp\left[ -2\pi i \left( \Delta k_x a n_x + \Delta k_y b n_y + \Delta k_z c n_z \right) \right]
\]

\[
= \sum_{n_x=0}^{N_x-1} \exp\left( -2\pi i \Delta k_x a n_x \right) \sum_{n_y=0}^{N_y-1} \exp\left( -2\pi i \Delta k_y b n_y \right) \sum_{n_z=0}^{N_z-1} \exp\left( -2\pi i \Delta k_z c n_z \right)
\]
Shape Factor

\[ S(\Delta k) = \sum_{n_x=0}^{N_x-1} \exp(-2\pi i \Delta k_x a n_x) \sum_{n_y=0}^{N_y-1} \exp(-2\pi i \Delta k_y b n_y) \sum_{n_z=0}^{N_z-1} \exp(-2\pi i \Delta k_z c n_z) \]

- Each sum is a truncated geometric series of the form:

\[ S = 1 + r + r^2 + r^3 + r^4 + \ldots + r^{N-1} = \frac{(1 - r^N)}{1 - r} \]

where, e.g., \( r = \exp(-2\pi i \Delta k_x a) \)

\[ \sum_{n_x=0}^{N_x-1} \exp(-2\pi i \Delta k_x a)^{n_x} = \frac{1 - \exp(-2\pi i \Delta k_x a N_x)}{1 - \exp(-2\pi i \Delta k_x a)} \]

\[ S^* S(\Delta k_x) = \frac{1 - \exp(+2\pi i \Delta k_x a N_x)}{1 - \exp(+2\pi i \Delta k_x a)} \frac{1 - \exp(-2\pi i \Delta k_x a N_x)}{1 - \exp(-2\pi i \Delta k_x a)} \]

\[ S^* S(\Delta k_x) = \frac{\sin^2(\pi \Delta k_x a N_x)}{\sin^2(\pi \Delta k_x a)} \]
Shape Factor

- The denominator varies slowly with respect to the numerator, approximation leads to:

\[ S^*S(\Delta k_x) = \frac{\sin^2(\pi \Delta k_x a N_x)}{\sin^2(\pi \Delta k_x a)} \approx \frac{\sin^2(\pi \Delta k_x a N_x)}{(\pi \Delta k_x a)^2} \]

- The envelop function:

\[ E(\Delta k_x) \equiv \frac{1}{(\pi \Delta k_x a)^2} \]

- As N becomes large:
  - Height of main peak \( \uparrow \propto N^2 \)
  - Width of main peak \( \downarrow \propto (aN)^{-1} \)
  - Height of satellite peaks \( \downarrow \)
  - Satellite peaks get closer
Shape Factor
Thin foil effect – ‘Relrod’

- Reciprocal Lattice Rods (Relrod)

- Streaks may also occur along x or y direction if the dimension is small.
- Streaks are the reason why exact orientation of a crystal is not possible with spot diffraction pattern.
Shape Factor

\[ I(\Delta k) = |\psi(\Delta k)|^2 = |F(\Delta k)|^2 \frac{\sin^2(\pi \Delta k_x a N_x)}{\sin^2(\pi \Delta k_y a N_y)} \times \frac{\sin^2(\pi \Delta k_y b N_y)}{\sin^2(\pi \Delta k_y b)} \frac{\sin^2(\pi \Delta k_z c N_z)}{\sin^2(\pi \Delta k_z c)} \]
Shape Factor

- Example: Guinier-Preston (GP) zones - Al-4%Cu alloy

- Fe-2.9%Mo alloy

\[
\psi(\Delta k) = \left[ F_{Al-Cu}(\Delta k) - F_{Al}(\Delta k) \right] \sum_{r_g}^{disk} (-2\pi i \Delta k \cdot r_g) + F_{Al}(\Delta k) \sum_{r_g}^{whole} (-2\pi i \Delta k \cdot r_g)
\]
Deviation Vector

• Express $\Delta k$ as the difference of an exact reciprocal lattice vector, $g$, and a “deviation vector”, $s$:

$$\Delta k = g - s \quad \text{(*)}$$

$$g = \Delta k + s$$

$$s = s_x \bar{x} + s_y \bar{y} + s_z \bar{z}$$

• Effect on Shape Factor:

$$S(\Delta k) = \sum_{r_g}^{\text{lattice}} \exp(-2\pi i \Delta k \cdot r_g) = \sum_{r_g}^{\text{lattice}} \exp[-2\pi i (g - s) \cdot r_g] \quad (g \cdot r_g = \text{integer})$$

$$S(\Delta k) = \sum_{r_g}^{\text{lattice}} \exp(-2\pi i \times \text{integer}) \exp[+2\pi i s \cdot r_g] = \sum_{r_g}^{\text{lattice}} \exp[+2\pi i s \cdot r_g]$$

$$S(\Delta k) = S(-s)$$

• Effect on Structure Factor:

$$F(\Delta k) \approx F(g) \quad (s \cdot r_k \text{ is small})$$

* $\Delta k = g + s$, more general
Kinematical Intensity

\[ I(\Delta k) = |\psi(\Delta k)|^2 \]

\[ = |F(g)|^2 \frac{\sin^2(\pi s_x a N_x)}{\sin^2(\pi s_x a)} \times \]

\[ \frac{\sin^2(\pi s_y b N_y)}{\sin^2(\pi s_y b)} \times \frac{\sin^2(\pi s_z c N_z)}{\sin^2(\pi s_z c)} \]

- Shape factor, \( S(s) \), depends only on \( s \).
- Structure factor, \( F(g) \), depends only on \( g \).
Deviation from Exact Bragg Condition

- **Exact Bragg condition:** \( k - k_0 = g \)
- **Deviation, \( s \):** \( k - k_0 = g + s = S \)

\[
\psi(\Delta k) = F(\Delta k) \sum_{r_g} \exp\left[ -2\pi i (g - s) \cdot r_g \right] \quad \text{Since } g \cdot r_g \text{ is an integer}
\]

\[
\psi(s) = F(g) \sum_{r_g} \exp(2\pi i s \cdot r_g)
\]

- **Definition:**
  - if \( s < 0 \): reciprocal lattice point outside Ewald sphere
  - if \( s > 0 \): reciprocal lattice point inside Ewald sphere
Kikuchi Lines

\[ 2\theta = \beta - \alpha \]

Diffraction cone
Kikuchi Lines

Pair of a “bright” and “dark” line

\[ I_{K_1} = I_1(1 - c) + I_2c = I_1 - c(I_1 - I_2) \]
\[ I_{K_2} = I_2(1 - c) + I_1c = I_2 + c(I_1 - I_2) \]

Figure 3.37  Kikuchi line formation by inelastic scattering of electrons at point P in a single crystal. The lower diagram illustrates the intensity of light on the view screen, which is affected by the inelastic scattering at P.
Kikuchi Lines

- The dashed line right between the excess line and the deficient line marks the intersection of the reflecting planes with the plane of the diffraction pattern.

- The spacing $D_{hkl}$ of the two lines corresponds to $2\theta_B$, thus $D_{hkl} = 2L\theta_B = \lambda L/d_{hkl}$.
  \[ \Rightarrow D_{hkl} \text{ equals the spacing between the spot of the transmitted beam and the spot of the } (hkl) \text{ Bragg reflection} \]

- When the specimen is oriented exactly for Bragg reflection at the $(hkl)$ planes, the deficient Kikuchi line intersects the transmitted beam, while the excess Kikuchi line intersects the Bragg reflection.
Kikuchi Lines

• Pairs of parallel lines consisting of one bright and one dark lines in diffraction mode

• Electrons are scattered **elastically** (diffraction spots) or **inelastically** (diffuse in all directions, with maximum intensity along incident beam direction and decreasing intensity with increasing angle)

• The intensity decreases with increasing scattering angle.

• **Inelastically scattered electrons** (assumption: negligible energy-loss) act as a **new primary beam** which can undergo Bragg diffraction (in all three dimensions) causing diffraction cones

• Kikuchi lines exist only in thick samples

• Can be used for accurate determination of orientation (ca. 0.1 degree instead of typically 4 degrees in spot patterns)
Diffraction Condition

- **Exact Bragg**
  (strong “two-beam” condition)
  \[ s = 0 \]
  (dynamic theory required!)

- **Symmetric case**
  (Laue condition)
  \[ s < 0 \] with \( s = -\theta g \)
  (kinematic theory !)
Kinematical vs. Dynamical

**Kinematical theory**

\[ \psi(\Delta k) = F(\Delta k) \sum_{r_g} \exp(-2\pi i \Delta k \cdot r_g) \]

- \( I_d \ll I_0 \) (weak scattering)
- Thin samples
- Small deviation from exact Bragg condition (required):
  \( \Delta k = g + s \)
- Amplitude \( A \) of the diffracted beams are summed up taking phase shifts into account

**Dynamical theory**

\[ \psi(s) = F(g) \sum_{r_g} \exp(2\pi is \cdot r_g) \]

- \( I_d \approx I_0 \) (multiple scattering)
- Thick samples
- Exact Bragg condition
- Considers diffraction from beam diffracted back into the primary beam
- Uses Schrödinger equation (Howie-Whelan Eqn)
Home Work

- Due date: April 6th.