Today’s Outline - March 01, 2018

• Final presentation
• Ewald sphere (continued)
• Modulated Structures
• Crystal Truncation Rods
• Diffuse Scattering
• Debye-Waller factor

No class on Tuesday, March 06, 2018 or Thursday, March 08, 2018

Homework Assignment #04: Chapter 4: 2, 4, 6, 7, 10 due Tuesday, March 20, 2018

Homework Assignment #05: Chapter 5: 1, 3, 7, 9, 10 due Thursday, March 29, 2018
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Homework Assignment #05:
Chapter 5: 1, 3, 7, 9, 10
due Thursday, March 29, 2018
1. Choose paper for presentation
Final presentation

1. Choose paper for presentation

2. Clear it with me!
Final presentation

1. Choose paper for presentation

2. Clear it with me!

3. Do some background research on the technique
Final presentation

1. Choose paper for presentation

2. Clear it with me!

3. Do some background research on the technique

4. Prepare a 15 minute presentation
Final presentation

1. Choose paper for presentation
2. Clear it with me!
3. Do some background research on the technique
4. Prepare a 15 minute presentation
5. Be ready for questions!
The reciprocal lattice is defined by the unit vectors $\vec{a}_1^*$ and $\vec{a}_2^*$. 

As the crystal is rotated with respect to the incident beam, the reciprocal lattice also rotates. When the Ewald sphere intersects a reciprocal lattice point there will be a diffraction peak in the direction of the scattered x-rays. The diffraction vector, $\vec{Q}$, is thus a reciprocal lattice vector $\vec{G}_{hlk} = h\vec{a}_1^* + k\vec{a}_2^*$. 
The reciprocal lattice is defined by the unit vectors $\vec{a}_1^*$ and $\vec{a}_2^*$.

The key parameter is the relative orientation of the incident wave vector $\vec{k}$. When the Ewald sphere intersects a reciprocal lattice point there will be a diffraction peak in the direction of the scattered X-rays. The diffraction vector, $\vec{Q}$, is thus a reciprocal lattice vector $\vec{G}_{hlk} = h\vec{a}_1^* + k\vec{a}_2^*$. 

C. Segre (IIT)
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Ewald sphere & the reciprocal lattice

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$$\vec{G}_{h\ell k} = h\vec{a}_1^* + k\vec{a}_2^*$$
Ewald construction

It is often more convenient to visualize the Ewald sphere by keeping the reciprocal lattice fixed and “rotating” the incident beam to visualize the scattering geometry.
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In directions of \( \vec{k}' \) (detector position) where there is no reciprocal lattice point, there can be no diffraction peak.
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In directions of $\vec{k}'$ (detector position) where there is no reciprocal lattice point, there can be no diffraction peak.

If the crystal is rotated slightly with respect to the incident beam, $\vec{k}$, there may be no Bragg reflections possible at all.
Polychromatic radiation

If $\Delta \vec{k}$ is large enough, there may be more than one reflection lying on the Ewald sphere.
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With an area detector, there may then be multiple reflections appearing for a particular orientation (very common with protein crystals where the unit cell is very large).
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With an area detector, there may then be multiple reflections appearing for a particular orientation (very common with protein crystals where the unit cell is very large).

In protein crystallography, the area detector is in a fixed location with respect to the incident beam and the crystal is rotated on a spindle so that as Laue conditions are met, spots are produced on the detector at the diffraction angle.
Multiple scattering

If more than one reciprocal lattice point is on the Ewald sphere, scattering can occur internal to the crystal.
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The x-rays are first scattered along $\vec{k}_{int}$ then along the reciprocal lattice vector which connects the two points on the Ewald sphere, $\vec{G}$ and $\vec{k}'$, to the detector at $\vec{k}'$. This is the cause of monochromator glitches which sometimes remove intensity but can also add intensity to the reflection the detector is set to measure.
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Laue diffraction

The Laue diffraction technique uses a wide range of radiation from $\vec{k}_{\text{min}}$ to $\vec{k}_{\text{max}}$. These define two Ewald spheres and a volume between them such that any reciprocal lattice point which lies in the volume will meet the Laue condition for reflection.

This technique is useful for taking data on crystals which are changing or may degrade in the beam with a single shot of x-rays on a 2D detector.
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\[2 \ x, \ \overline{y}, \ \overline{z}\]
\[3 \ \overline{x}, \ y, \ \overline{z}\]
\[4 \ \overline{x}, \ \overline{y}, \ z\]
\[5 \ z, \ x, \ y\]
\[6 \ \overline{z}, \ x, \ y\]
\[7 \ z, \ \overline{x}, \ \overline{y}\]
\[8 \ \overline{z}, \ x, \ \overline{y}\]
\[9 \ y, \ z, \ x\]
\[10 \ \overline{y}, \ z, \ \overline{x}\]
\[11 \ \overline{y}, \ \overline{z}, \ x\]
\[12 \ y, \ \overline{z}, \ \overline{x}\]
## Wyckoff Positions of Group 195 (P23)

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<th>Coordinates</th>
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<tr>
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<td>8</td>
<td>a</td>
<td>-43m</td>
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Diffraction from a Truncated Surface

For an infinite sample, the diffraction spots are infinitesimally sharp.
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With finite sample size, these spots grow in extent and become more diffuse.
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If the sample is cleaved and left with flat surface, the diffraction will spread into rods perpendicular to the surface.
For an infinite sample, the diffraction spots are infinitesimally sharp.

With finite sample size, these spots grow in extent and become more diffuse.

If the sample is cleaved and left with flat surface, the diffraction will spread into rods perpendicular to the surface.

The scattering intensity can be obtained by treating the charge distribution as a convolution of an infinite sample with a step function in the z-direction.
CTR Scattering Factor

The scattering amplitude $F^{CTR}$ along a crystal truncation rod is given by summing an infinite stack of atomic layers, each with scattering amplitude $A(\vec{Q})$. 

$$F^{CTR} = \sum_{j=0}^{\infty} A(\vec{Q}) e^{iQz_j}$$

This sum has been discussed previously and gives

or, in terms of the momentum transfer along the z-axis, $Q_z = \frac{2\pi l}{a^3}$ since the intensity is the square of the scattering factor

$$I^{CTR} = |F^{CTR}|^2 = |A(\vec{Q})|^2 (1 - e^{i2\pi l/a^3}) (1 - e^{-i2\pi l/a^3})$$

$$= |A(\vec{Q})|^2 4 \sin^2 \left(\frac{\pi l}{a^3}\right)$$
The scattering amplitude $F^{CTR}$ along a crystal truncation rod is given by summing an infinite stack of atomic layers, each with scattering amplitude $A(\vec{Q})$.

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$$F^{CTR} = A(\vec{Q}) \sum_{j=0}^{\infty} e^{iQza_3j}$$

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$$\frac{1}{1 - e^{i2\pi l/a_3}} = \frac{\sin^2(\pi l/a_3)}{\sin^2(2\pi l/a_3)}$$
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$$F^{CTR} = A(\vec{Q}) \sum_{j=0}^{\infty} e^{iQza_3j}$$

$$= \frac{A(\vec{Q})}{1 - e^{iQza_3}}$$

this sum has been discussed previously and gives
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$$F^{CTR} = A(\vec{Q}) \sum_{j=0}^{\infty} e^{iQ_z a_3 j}$$

$$= \frac{A(\vec{Q})}{1 - e^{iQ_z a_3}} = \frac{A(\vec{Q})}{1 - e^{i2\pi l/a_3}}$$

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or, in terms of the momentum transfer along the z-axis,

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$$= \frac{A(\vec{Q})}{1 - e^{iQ_z a_3}} = \frac{A(\vec{Q})}{1 - e^{i2\pi l}}$$

since the intensity is the square of the scattering factor

$$I^{CTR} = \left| F^{CTR} \right|^2 = \frac{\left| A(\vec{Q}) \right|^2}{(1 - e^{i2\pi l})(1 - e^{-i2\pi l})}$$

this sum has been discussed previously and gives

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CTR Scattering Factor

The scattering amplitude $F^{CTR}$ along a crystal truncation rod is given by summing an infinite stack of atomic layers, each with scattering amplitude $A(\vec{Q})$.

$$F^{CTR} = A(\vec{Q}) \sum_{j=0}^{\infty} e^{iQ_z a_3 j}$$

$$= A(\vec{Q}) \frac{1 - e^{iQ_z a_3}}{1 - e^{i2\pi l}}$$

since the intensity is the square of the scattering factor

$$I^{CTR} = \left| F^{CTR} \right|^2 = \frac{\left| A(\vec{Q}) \right|^2}{(1 - e^{i2\pi l})(1 - e^{-i2\pi l})} = \frac{\left| A(\vec{Q}) \right|^2}{4 \sin^2 (\pi l)}$$

this sum has been discussed previously and gives

or, in terms of the momentum transfer along the z-axis,

$$Q_z = \frac{2\pi l}{a_3}$$
Dependence on Q

When \( l \) is an integer (meeting the Laue condition), the scattering factor is infinite but just off this value, the scattering factor can be computed by letting \( Q_z = q_z + 2\pi/a_3 \), with \( q_z \) small.
Dependence on $Q$

When $l$ is an integer (meeting the Laue condition), the scattering factor is infinite but just off this value, the scattering factor can be computed by letting $Q_z = q_z + 2\pi/a_3$, with $q_z$ small.

\[ I_{CTR} = \frac{|A(\vec{Q})|^2}{4 \sin^2 (Q_z a_3/2)} \]
Dependence on $Q$

When $l$ is an integer (meeting the Laue condition), the scattering factor is infinite but just off this value, the scattering factor can be computed by letting $Q_z = q_z + 2\pi/a_3$, with $q_z$ small.

\[
I^{CTR} = \frac{|A(\mathbf{Q})|^2}{4 \sin^2 (Q_z a_3/2)} = \frac{|A(\mathbf{Q})|^2}{4 \sin^2 (\pi l + q_z a_3/2)}
\]
Dependence on Q

When \( I \) is an integer (meeting the Laue condition), the scattering factor is infinite but just off this value, the scattering factor can be computed by letting \( Q_z = q_z + 2\pi/a_3 \), with \( q_z \) small.

\[
I^{CTR} = \frac{|A(\vec{Q})|^2}{4 \sin^2 (Q_z a_3 / 2)}
= \frac{|A(\vec{Q})|^2}{4 \sin^2 (\pi l + q_z a_3 / 2)}
= \frac{|A(\vec{Q})|^2}{4 \sin^2 (q_z a_3 / 2)}
\]
Dependence on $Q$

When $l$ is an integer (meeting the Laue condition), the scattering factor is infinite but just off this value, the scattering factor can be computed by letting $Q_z = q_z + 2\pi/a_3$, with $q_z$ small.

\[
I_{CTR} = \frac{|A(\vec{Q})|^2}{4 \sin^2 (Q_z a_3 / 2)} \approx \frac{|A(\vec{Q})|^2}{4(q_z a_3 / 2)^2}
\]
Dependence on Q

When \( l \) is an integer (meeting the Laue condition), the scattering factor is infinite but just off this value, the scattering factor can be computed by letting \( Q_z = q_z + 2\pi/a_3 \), with \( q_z \) small.

\[
I_{CTR}^{Q_z} = \frac{|A(\vec{Q})|^2}{4 \sin^2 (Q_z a_3/2)}
\]

\[
= \frac{|A(\vec{Q})|^2}{4 \sin^2 (\pi l + q_z a_3/2)}
\]

\[
= \frac{|A(\vec{Q})|^2}{4 \sin^2 (q_z a_3/2)}
\]

\[
\approx \frac{|A(\vec{Q})|^2}{4(q_z a_3/2)^2} = \frac{|A(\vec{Q})|^2}{q_z^2 a_3^2}
\]
Dependence on Q

When \( l \) is an integer (meeting the Laue condition), the scattering factor is infinite but just off this value, the scattering factor can be computed by letting \( Q_z = q_z + 2\pi/a_3 \), with \( q_z \) small.

\[
I^{CTR} = \frac{|A(\vec{Q})|^2}{4 \sin^2 (Q_z a_3 / 2)}
\]

\[
= \frac{|A(\vec{Q})|^2}{4 \sin^2 (\pi l + q_z a_3 / 2)}
\]

\[
= \frac{|A(\vec{Q})|^2}{4 \sin^2 (q_z a_3 / 2)}
\]

\[
\approx \frac{|A(\vec{Q})|^2}{4(q_z a_3 / 2)^2} = \frac{|A(\vec{Q})|^2}{q_z^2 a_3^2}
\]
Absorption Effect

Absorption effects can be included as well by adding a term for each layer penetrated

\[ F_{CTR} = A(\mathbf{Q}) \sum_{j=0}^{\infty} e^{iQz_a} e^{-\beta_j} = A(\mathbf{Q}) \frac{1}{1-e^{iQz_a} e^{-\beta}} \]

This removes the infinity and increases the scattering profile of the crystal truncation rod.
Absorption Effect

Absorption effects can be included as well by adding a term for each layer penetrated

\[ F^{CTR} = A(Q) \sum_{j=0}^{\infty} e^{iQz a_3 j} \]
Absorption effects can be included as well by adding a term for each layer penetrated

\[ F^{CTR} = A(\vec{Q}) \sum_{j=0}^{\infty} e^{iQz_3j} e^{-\beta j} \]
Absorption Effect

Absorption effects can be included as well by adding a term for each layer penetrated.

\[ F^{CTR} = A(\vec{Q}) \sum_{j=0}^{\infty} e^{iQ_z a_3 j} e^{-\beta j} \]

\[ = \frac{A(\vec{Q})}{1 - e^{iQ_z a_3} e^{-\beta}} \]
Absorption Effect

Absorption effects can be included as well by adding a term for each layer penetrated.

\[
F^{CTR} = A(\vec{Q}) \sum_{j=0}^{\infty} e^{iQ_z a_3 j} e^{-\beta j} = \frac{A(\vec{Q})}{1 - e^{iQ_z a_3} e^{-\beta}}
\]

\[
\beta = 0.2
\]
Absorption Effect

Absorption effects can be included as well by adding a term for each layer penetrated

\[ F^{CTR} = A(\vec{Q}) \sum_{j=0}^{\infty} e^{iQ_z a_3 j} e^{-\beta j} \]

\[ = \frac{A(\vec{Q})}{1 - e^{iQ_z a_3} e^{-\beta}} \]

This removes the infinity and increases the scattering profile of the crystal truncation rod.
Density Effect

The CTR profile is sensitive to the termination of the surface. This makes it an ideal probe of electron density of adsorbed species or single atom overlayers.

\[ F_{\text{total}} = F_{\text{CTR}} + F_{\text{top layer}} = A(\vec{Q})^1 - e^{i2\pi l} + A(\vec{Q})e^{-i2\pi(1+z_0)}l \]

where \( z_0 \) is the relative displacement of the top layer from the bulk lattice spacing. This effect gets larger for larger momentum transfers.
Density Effect

The CTR profile is sensitive to the termination of the surface. This makes it an ideal probe of electron density of adsorbed species or single atom overlayers.

\[ F_{\text{total}} = F^{CTR} + F^{\text{top layer}} \]
Density Effect

The CTR profile is sensitive to the termination of the surface. This makes it an ideal probe of electron density of adsorbed species or single atom overlayers.

\[ F_{total} = F_{CTR} + F_{top\ layer} = \frac{A(\vec{Q})}{1 - e^{i2\pi l}} \]
Density Effect

The CTR profile is sensitive to the termination of the surface. This makes it an ideal probe of electron density of adsorbed species or single atom overlayers.

\[ F^{\text{total}} = F^{CTR} + F^{\text{top layer}} \]
\[ = \frac{A(\vec{Q})}{1 - e^{i2\pi l}} \]
\[ + A(\vec{Q})e^{-i2\pi(1+z_0)l} \]
Density Effect

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\[
F_{\text{total}} = F_{\text{CTR}} + F_{\text{top layer}}
\]

\[
= \frac{A(Q)}{1 - e^{i2\pi l}} + A(Q)e^{-i2\pi(1+z_0)/l}
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