
Model of helical domains in myoglobin. Image courtesy of Magnus Manske
Homework for Wed Nov 23

• Prof Wuensch Lecture Notes
• http://capsicum.me.utexas.edu/ChE386K/ for many details (Lect 19 onwards, but note different $2\pi$ convention)
• Buy turkey
Last time:

1. X-rays generation: undulators and wigglers in synchrotrons, bremsstrahlung and core excitations (e.g. \(K_\alpha\)) in X-ray tubes
2. Reciprocal lattice
3. Diffraction gratings – Huygens construction
4. Laue diffraction from periodic arrays in 1-d, 2-d, 3-d
Reciprocal lattice (IV)

\[ \mathbf{G} = h\mathbf{b}_1 + i\mathbf{b}_2 + j\mathbf{b}_3 \]  with  \( h, i, j \) integers,

\[ \mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \quad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \quad \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \]

\[ \mathbf{G} = (h, i, j) \]  are the reciprocal-lattice vectors

\( d^*_\text{hkl} \) is distance between two planes of Miller indices \( h k l \)

in the reciprocal lattice  \( d^*_\text{hkl} = \frac{2\pi}{\mathbf{d}_\text{hkl}} \)
First and second Laue conditions

\[ \vec{a} \cdot \vec{S} = a \cos \alpha_n \]

\[ \vec{a} \cdot \vec{S}_0 = a \cos \alpha_0 \]

\[ a (\cos \alpha_n - \cos \alpha_0) = \vec{a} \cdot (\vec{S} - \vec{S}_0) = n_x \lambda \]
All three Laue conditions

\[ \vec{a}_1 \cdot (\vec{S} - \vec{S}_0) = \text{integer multiple of } \lambda \]

\[ \vec{a}_2 \cdot (\vec{S} - \vec{S}_0) = \text{integer multiple of } \lambda \]

\[ \vec{a}_3 \cdot (\vec{S} - \vec{S}_0) = \text{integer multiple of } \lambda \]
Ewald construction

\[ \Delta S \overset{\varphi}{\underset{\lambda}{\longrightarrow}} 2\pi \in \text{RECIP LATT.} \]

Figure by MIT OCW.
Laue condition needs “white” spectrum
Alternate geometrical view
Bragg Law

\[ n\lambda = d_{hkl} \cdot 2\sin \theta \]
Equivalence to Laue condition

\[ d_{hkl}^* = \frac{2\pi}{\lambda} (S - S_0) \]

where

- \( d_{hkl}^* \) is the reciprocal lattice constant
- \( \lambda \) is the wavelength
- \( S - S_0 \) is the difference in momentum transfer

The figure illustrates the relationship between the incident beam, diffracted beam, and reciprocal lattice origin. The Ewald sphere is a key component in understanding this relationship.
Powder diffraction (I)

Figure by MIT OCW.
Powder diffraction (II)

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Powder diffraction (III)

Diagrams of the Powder Method removed for copyright reasons.
See the images at http://www.matter.org.uk/diffraction/x-ray/powder_method.htm
X-ray filters

Image removed for copyright reasons.
Please see the graph at http://capsicum.me.utexas.edu/ChE386K/html/absorption_edge.htm.

Image removed for copyright reasons.
Please see the diagrams at http://capsicum.me.utexas.edu/ChE386K/html/filter.htm.
Debye-Scherrer camera

Photographs of a Debye-Scherrer camera removed for copyright reasons.

Figure by MIT OCW.
Interplanar spacings

Cubic: \[ \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \]

Tetragonal: \[ \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2 + c^2} \]

Hexagonal: \[ \frac{1}{d^2} = \frac{4}{3} \left( \frac{h^2 + k^2 + l^2}{a^2} \right) \]

Monoclinic: \[ \frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left( \frac{h^2 + k^2 \sin^2 \beta + l^2}{a^2 + b^2 - \frac{2hl \cos \beta}{ac}} \right) \]

Triclinic: \[ \frac{1}{d^2} = \frac{1}{V^2} (S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl) \]

In the equation for triclinic crystals

\[ V = abc \sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma} \]

- \[ S_{11} = b^2 c^2 \sin^2 \alpha, \]
- \[ S_{22} = a^2 c^2 \sin^2 \beta, \]
- \[ S_{33} = a^2 b^2 \sin^2 \gamma, \]
- \[ S_{12} = abc (\cos \alpha \cos \beta - \cos \gamma), \]
- \[ S_{23} = ab^2 c (\cos \beta \cos \gamma - \cos \alpha), \]
- \[ S_{13} = abc^2 (\cos \gamma \cos \alpha - \cos \beta). \]

Cubic: \[ d_{hkl}^2 = \frac{a^2}{h^2 + k^2 + l^2} \]

3.012 Fundamentals of Materials Science: Bonding - Nicola Marzari (MIT, Fall 2005)
Debye-Scherrer camera

\[ \lambda = d_{hkl} 2\sin \theta \]

Cubic: \[ d_{hkl}^2 = \frac{a^2}{h^2 + k^2 + l^2} \]

\[ 2\theta = \frac{S_1}{2W} \text{ RADIANS} \]

\[ \sin \theta = \frac{\lambda}{2d_{hkl}} \]

\[ \sin^2 \theta = \frac{\frac{\lambda^2}{a^2} h^2 + k^2 + l^2}{4} \]
Tables removed for copyright reasons. See http://www.matter.org.uk/diffraction/x-ray/indexing_powder_pattern.htm
Systematic absences

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Please see the table at http://capsicum.me.utexas.edu/ChE386K/html/systematic_absences.htm.
Effects of symmetry on diffraction

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Please see the images at http://capsicum.me.utexas.edu/ChE386K/html/diffraction_symmetry1.htm.
Structure Factor

\[ F(hkl) = \sum_{n=1}^{N} f_n e^{2\pi i (hx_n + ky_n + lz_n)} \]

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Please see the graph at http://capsicum.me.utexas.edu/ChE386K/html/scattering_factor_curve.htm.

\[ ||F||^2 = \text{INTENSITY} \]
Friedel’s law

\[ F(hk\ell) = F^*(-h,-k,-\ell) \]

\[ \| F(hk\ell) \|^2 = \| F^*(-h,-k,-\ell) \|^2 \]

• The diffraction pattern is always centrosymmetric, even if the crystal is not centrosymmetric
Point symmetry + inversion = Laue

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Please see the table at http://capsicum.me.utexas.edu/ChE386K/html/diffraction_symmetry2.htm.
Back-reflection and transmission Laue