Introduction to Reciprocal Space

7th X-ray Scattering School

Apurva Mehta
Can we create the image without a lens?

$$Q = \frac{4\pi \sin(\theta)}{\lambda}$$
Lensless Imaging

Sample Space → Angular Space

Scattering Pattern

light sample
Elastic Scattering → |Ki| = |Ks|

\[ \Delta K = Q = \text{momentum transfer} \]

\[ \Delta K = Q = 2*K_i \times \sin(\theta) \]

\[ K_i = 2\pi/\lambda \]

\[ Q = 4\pi \sin(\theta)/\lambda \]
Lensless Imaging

Sample Space → Scattering Space

Measured in
\[ Q = \frac{4\pi \sin(\theta)}{\lambda} \]
Bragg's Law
Bragg’s Law

Proposed in 1912-1913
Nobel Price in Physics - 1915

\[ 2d \sin(\theta) = \lambda \]

\[ Q = \frac{4\pi \sin(\theta)}{\lambda} \]

\[ Q = \frac{4\pi \sin(\theta)}{\lambda} = \frac{2\pi}{d} \]

\[ |Q| = \frac{2\pi}{d} \]

2014 - International year of Crystallography
Bragg’s Law Tells Us

• About the Position of the scattering peaks
• But not the Direction
• And not its Intensity
• Nor its Width

Need to go beyond Bragg’s Law
Bragg Planes
Bragg Planes

\[ |Q| = \frac{2\pi}{d} \]
Bragg Planes

\[ |Q| = \frac{2\pi}{d} \]
Reciprocal Lattice

$|Q| = \frac{2\pi}{d}$
Scattering Physics

Sample

Space

Sample

Space

Measured in

$Q = \frac{4\pi \sin(\theta)}{\lambda}$

Scattering Pattern

Measured in

$Q = \frac{4\pi \sin(\theta)}{\lambda}$

Real Space Lattice

Reciprocal (Space) Lattice
Scattering Physics

- Reciprocal Lattice Points
  - Have Position
  - Direction
  - Intensity
  - Width

Measured in
\[ Q = 4\pi \sin(\theta) / \lambda \]
Scattering Physics

Fourier Transform

Real Space Lattice

Reciprocal (Space) Lattice

light
Recap

1: \( \text{FT} \left( \text{FT} \left( S \right) \right) \sim S \)

2: FT (large) \( \sim \frac{1}{\text{large}} \Rightarrow \text{small} \)
   - Rec Sp (large) \( \Rightarrow \text{small} \)

3: FT (periodic fn) \( \sim \text{periodic} \)
   - Rec Sp (periodic Real Sp) \( \sim \text{periodic} \)
Sailing Through Reciprocal Space
Scattering from a Single Crystal

Elastic Scattering

Reciprocal Lattice

Ewald’s Sphere
Multi-circle diffractometer

- Need at least
  - 2 angles for the sample
  - 1 for the detector

- But often more for ease, polarization control, environmental chambers

- New Diffractometer @7-2
  - 4 angles for the sample
  - 2 for the detector
Scattering Pattern and Ewald’s Sphere

Ewald’s Sphere
2D detectors and Ewald Sphere

Elastic Scattering

Reciprocal Lattice

Ewald’s Sphere
Scattering from Many Crystallites: polycrystal or powder
Powder Diffraction Pattern

Ewald Sphere

Q

Q_D

Q_0

Nested Reciprocal Sphere
Powder Diffractometer with an Area Detector
Condition for Polycrystalline/powder Diffraction

• Just 1 angle (detector)

• If large area detector → 0 angles
• Nothing moves
  – Very useful for fast/time dependent measurements
Texture

Oriented Polycrystals

Ewald’s sphere

Reciprocal Sphere

Partial diffraction ring

Diffraction pattern
Deformation of Reciprocal sphere

\[ u_i = \epsilon_{ij} k_{0j} \]

Strain Ellipsoid
Strain Ellipsoid

- small strain
- continuous strain
Coordinate transformation
Measuring Full Strain Tensor
Elastic Strain Tensors for Fe

\[ E_m = 211 \text{ GPa} \]

\[ E_m = 167 \text{ GPa} \]

\[ E_m = 218 \text{ GPa} \]
Resolution

Area Detector

Point Detector
Questions?

- Think in Q space
  - (yardstick of reciprocal space)
  - $Q = \frac{4\pi \sin(\theta)}{\lambda}$
Effect of Beam Divergence
Effect of Energy Width