Thinking in Reciprocal Space

Apurva Mehta
Introduction to Reciprocal Space

Reciprocal Space may at first appear strange.
- Examples → thinking in reciprocal space makes interpreting scattering experiments easier.
Why X-ray Scattering?

- Structure of Materials
  - 10s of nm to A
Scattering Physics

X-ray lens with resolution better than ~10nm don’t exist.

X-ray Scattering/diffraction is about probing the structure without a lens.
Sample to Scattering Space

Transformation of distance into angle

Diffraction Pattern:
Contains all the contrast relevant information at the resolution of $\lambda/2\sin(\theta)$

Fourier Transform: sample space $\rightarrow$ scattering space
Scattering Physics: Bragg's Law

2dsin(\theta) = \lambda

1/2d = \text{sin}(\theta)/\lambda

1. Distance $\leftrightarrow$ Angle
   "Reciprocal" relation

2. Fundamental unit is not $\theta$ but $\text{sin}(\theta)/\lambda$
Fundamental Units for scattering

- $s = \frac{\sin(\theta)}{\lambda}$

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

- Think in $Q$

- Or provide both $\theta$ and $\lambda$
  
  - $\lambda = \frac{hc}{E}$ – synchrotron units are $E$
Scattering Physics

Elastic Scattering

Momentum $K_0 = 2\pi/\lambda$

$K_f = 2\pi/\lambda$

$\Delta K = Q = 4\pi \sin(\theta) / \lambda$

Momentum change
Reciprocal Space

Ordered Lattice can only provide discrete momentum kicks: Bloch

- Elastic Scattering
- X-ray Diffraction
- Momentum Transfer Space

Real Space Lattice  Reciprocal Lattice
Graphical Solution: Single crystal

Ewald’s Sphere

$Q_D$, $Q_0$, $Q_1$
Conditions for Single Crystal Diffraction

Bragg’s law provides condition for only the detector

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

Necessary but not sufficient

Ewald’s Sphere

Detector AND the crystal at desired location/angles.
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
Diffraction from Polycrystals

Ewald Sphere

Reciprocal Sphere

\[ Q_1 \]
Diffraction from Polycrystals

Ewald Sphere

Q_0

Q

Q_D

Reciprocal Sphere

Diffraction Cone
Diffraction from Polycrystals

Ewald’s sphere

Nested Reciprocal Spheres

Diffraction Pattern
Condition for Polycrystalline/powder Diffraction

- Just 1 angle (detector)
- Bragg’s law sufficient
- If large area detector $\rightarrow$ 0 angles
  - Very useful for fast/time dependent measurements
Powder Diffractometer with an Area Detector
Powder Average and Rocking

Ewald’s sphere

Oscillate while collecting data
Texture

Oriented Polycrystals

Ewald’s sphere

Reciprocal Sphere

Diffraction pattern

Partial diffraction ring
\[ \varepsilon = \frac{d_f - d_0}{d_0} \]
Strain in Polycrystals

\[ \vec{u}_i = \epsilon_{ij} k_{0j} \]

Reciprocal Sphere

Strain Ellipsoid
Coordinate Transformation
Strain Relaxation

![Image of strain relaxation experiment](image)

Load vs. Displacement graph showing load increasing and then unloading.

Graphs showing strain relaxation for different orientations:
- 110
- 200
- 211

Equations:
- $Q (nm^{-1})$
- $\chi$

TMS 2008
Elastic Strain Tensor: bcc Fe

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

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

\[ E_z = 218 \text{ GPa} \]

\[ v_{xy} = v_{xz} = v_{yz} = 0.3 \]

Stress (MPa)

\[ \varepsilon_{yy} \]

\[ \varepsilon_{zz} \]

\[ \varepsilon_{xx} \]

% Strain

Poisson's Ratio

Load

Displacement

Zurich 2008
X-ray lens with resolution better than ~10nm don’t exist

X-ray Scattering/diffraction is about probing the structure without a lens
Reciprocal Space is the map of diffraction pattern

Think in Q space

(yardstick of reciprocal space)

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