What Does a Scattering Pattern Tell Us?

7th X-ray Scattering School

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Goal: See Atomic Scale Structures
Photography

Camera

Lights
Light

• Interaction of Light with Matter

  – Transparent
  – Scatters
  – Absorbs/re-emits (Resonance)
X-ray camera (microscope) at SSRL

BL 6-2

slit

Si(Li)

reflective Condenser

MZP

y

x

CCD

xradia
But not for atomic scale.

Why not?
What Does the Camera Do?

Light \rightarrow \text{Sample} \rightarrow \text{Angular Space} \rightarrow \text{Image Space} \rightarrow \text{Image}
Resolution of Full Field Camera

Full Field imaging is a “wave” phenomena - interference pattern $\rightarrow$ dark and light stops $\rightarrow$ image

Rayleigh’s Criteria

Image Resolution $\sim \frac{\lambda}{\sin(\theta)} +$ lens Aberrations

X-ray lens with resolution better than $\sim10$nm don’t exist
Can we create the image without a lens?

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

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

\[ A(\Delta K = (s-s_0)) = e^{i\omega t} \sum_{f_i} e^{2\pi i (r_i \sin(2\theta)/\lambda)} \]

Amplitude

\[ A(\Delta K) = \sum_{f_i} e^{i (r_i \cdot Q)} \]

Fourier Transform (\( r_i \))

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

Fourier Transform

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

Sample Space \rightarrow Angular Space
Fourier Transform Recap

- $1:\ FT\left(FT\left(S\right)\right) \sim S$
Lensless Imaging

Fourier Transform

Sample Space $\rightarrow$ Angular Space $\rightarrow$ Image Space

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

- 1: $\text{FT (FT (S))} \sim S$
- 2: $\text{FT (large)} \sim 1/\text{large} \rightarrow \text{small}$
Fourier Transform Recap

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

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

3: \( \text{FT (periodic fn)} \sim \text{periodic} \)
Fourier Transform Recap

1. $\text{FT}(\text{FT}(S)) \sim S$
2. $\text{FT}(\text{large}) \sim 1/\text{large} \Rightarrow \text{small}$
3. $\text{FT}(\text{periodic fn}) \sim \text{periodic}$
4. Convolution Theorem:
   - $\text{FT}(a \text{ multiply } b) =$
     - $\text{FT}(a) \text{ conv FT}(b)$
   - $\text{FT}(a \text{ conv } b) =$
     - $\text{FT}(a) \text{ multiply FT}(b)$
Multiplication vs Convolution

\[ \text{FT (a multiply b)} = \text{FT (a conv FT (b))} \]
\[ \text{FT (a conv b)} = \text{FT (a mult FT (b))} \]
Deconstructing the Sample space

Sample = S \times P \times M

- Sample size (S)
- Infinite Periodic Lattice (P)
- Motif (M)
FT(P)
\[ FT (S \times P) = FT(S) \ast FT(P) \]
FT(sample) = FT(S × P) × FT(M)

Along X direction
What does a diffraction pattern tell us?

- **Peak Shape & Width:**
  - Zero order peak
  - Higher order peaks
    - Crystallite size
    - Strain gradient

- **Peak Positions:**
  - Phase identification
  - Lattice symmetry
  - Lattice strain

- **Peak Intensity:**
  - Structure solution
  - Crystallite orientation

Small Angle Scattering & Reflectivity
Wide Angle Scattering
Questions?

1: FT (FT (S)) ~ S

2: Scattering Pattern (large) ~ 1/large \rightarrow small features

3: Scattering Pattern (periodic lattice) ~ periodic