Interpreting Reciprocal Space-peaks

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Physics of Diffraction

X-ray Lens not very good

Mathematically

Intersection of Ewald sphere with Reci Lattice
Diffraction Pattern:

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

\[ A(\Delta K = (s-s_0)) = e^{iwt} \sum f_i e^{2\pi i \left( r_i \sin(2\theta)/\lambda \right)} \]

amplitude
Diffraction Physics

\[ K_0 = \frac{2\pi}{\lambda} \]

\[ K_i = \frac{2\pi}{\lambda} \]

\[ \Delta K = 2\sin(\theta) \times \frac{2\pi}{\lambda} \]

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

\[ s-s0 = Q/2\pi \]

\[ A(\Delta K) = \sum f_i e^{2\pi i \left( r_i \sin(2\theta) / \lambda \right)} \]

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

\[ A(Q) = \text{Fourier Transform (} r_i \text{)} \]
Diffraction Physics

Sample Space $\rightarrow$ Scattering Space

Fourier Transform
Reciprocal Space

Real Space

X-ray Diffraction
Momentum Transfer Space

Real Space Lattice

Reciprocal Lattice
Real Space Lattice

Reciprocal Lattice

Fourier Transform

Intensity (Reciprocal) \sim \{ \text{FT}(f_n(\text{sample})) \} \{ \text{FT}(f_n(\text{sample})) \}

f_n(\text{sample}) = \sum f_i \text{ atom}_i

X-ray Diffraction
Momentum Transfer Space

Real Space

Reciprocal Space
Fourier Transform Recap

- FT (large) \sim 1/large \rightarrow \text{small}
  
alarge \text{structures in real space} \rightarrow \text{small in reciprocal space}

- FT (periodic fn) \sim \text{periodic}

- FT (FT (S)) \sim S
  
FT (real space) \rightarrow \text{reciprocal space: FT (rec. space)} \rightarrow \text{image of real space}

- Convolution Theorem:
  
- FT (a multiply b) = FT (a) \text{ conv } FT (b)
  
- FT (a conv b) = FT (a) \text{ mult } FT (b)
**Multiplication vs Convolution**

\[
\text{FT (a multiply b)} = \text{FT (a)} \text{ conv } \text{FT (b)}
\]

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

Sample = S x P * M

Sample size (S) = Infinite Periodic Lattice (P) * Motif (M)
Reciprocal Space Peaks

\[ I(Q) = \text{FT(sample)} \times \text{FT(sample)} \]

\[ = \text{FT} (S \times P \ast M) \times \text{FT} (S \times P \ast M) \]

\[ = \{\text{FT}(S \times P) \times \text{FT}(M)\} \{\text{......}\} \]

\[ = \{\text{FT}(S) \ast \text{FT}(P) \times \text{FT}(M)\} \{\text{......}\} \]
$FT(S)$
FT(P)
FT (S x P) = FT(S) * FT(P)
FT(sample) = FT(S x P) x FT(M)

Along X direction
Scattering from a Single crystal

Ewald’s Sphere

$Q_D$, $Q_1$, $Q_0$
Diffraction for Polycrystals

Ewald Sphere

Reciprocal Sphere
Polycrystalline Diffraction

Ewald Sphere

Reciprocal Sphere

$Q$

$Q_D$

$Q_0$
What does a diffraction pattern tell us?

- **Peak Shape & Width:**
  - crystallite size
  - Strain gradient

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

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