LECTURE 4: Diffraction

by

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This Lecture

2. Diffraction

1. Diffraction by a lattice in the kinematic approximation
2. Direct lattice and reciprocal lattice
3. Effect of lattice vibrations, absorption, and instrument resolution
4. Single-crystal compared with powder diffraction
5. Use of monochromatic beams and time-of-flight to measure powder diffraction
6. Rietveld refinement of powder patterns
7. Examples of science with powder diffraction
   • Refinement of structures of new materials
   • Materials texture
   • Strain measurements
   • Protein crystallography
   • Pair distribution functions (PDF)
From Previous Lecture:

\[
\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered through angle } 2\theta \text{ per second into } d\Omega}{\text{number of incident neutrons per square cm per second}}
\]

\[
\left( \frac{d\sigma}{d\Omega} \right)_{coh} = \sum_{i,j} b_i^{coh} b_j^{coh} e^{i(k_0 - k')(\vec{R}_i - \vec{R}_j)} = \sum_{i,j} b_i^{coh} b_j^{coh} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)}
\]

where the wavevector transfer \(\vec{Q}\) is defined by \(\vec{Q} = \vec{k}' - \vec{k}_0\)

For elastic scattering \(k_0 = k' = k\):
\[
Q = 2k \sin \theta
\]
\[
Q = 4\pi \sin \theta/\lambda
\]
Neutron Diffraction

- Neutron diffraction is used to measure the differential cross section, \( \frac{d\sigma}{d\Omega} \) in the static approximation i.e. integrated over \( k' \) – measures \( G(r,0) \)
  - Crystalline solids (elastic scattering – \( G(r,\infty) \))
    - Unit cell size; crystal symmetry; atomic arrangement and thermal motions (ellipsoids)
  - Liquids and amorphous materials
  - Large scale structures

- Depending on the scattering angle, structure on different length scales, \( d \), is measured:
  
  \[
  \frac{2\pi}{Q} = d = \frac{\lambda}{2\sin(\theta)}
  \]

- For crystalline solids & liquids, use wide angle diffraction. For large structures, e.g. polymers, colloids, micelles, etc. use small-angle neutron scattering
The Kinematical Approximation

• Note that the approximation we have just seen ignores
  – Depletion of the incident beam by scattering or absorption
  – Multiple scattering
  i.e. energy is not conserved

• This so-called “kinematic approximation” is OK for weak scattering, very small crystals or “bad” crystals

• It is usually used for interpreting diffraction experiments, though “extinction corrections” are often needed with single crystals
  – If it’s not adequate, use dynamical theory (see H. Kaiser’s lecture)

• In addition, we have so-far ignored thermal motion of atoms
Diffraction by a Lattice of Atoms

\[ S(\vec{Q}) = \frac{1}{N} \left< \sum_{i,j} e^{-i\vec{Q} \cdot (\vec{R}_i - \vec{R}_j)} \right> \quad \text{with} \quad \vec{R}_i = \vec{i} + \vec{u}_i \quad \text{where} \vec{i} \quad \text{is the equilibrium position of atom} \ i \ \text{and} \ \vec{u}_i \ \text{is any displacement (e.g. thermal)} \ \text{from the equilibrium position.} \]

Ignoring thermal vibrations, \( S(Q) \) is only non-zero for \( Q \)'s such that \( \vec{Q} \cdot (\vec{i} - \vec{j}) = 2M\pi \).

In a Bravais lattice, we can write \( \vec{i} = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3 \) where \( \vec{a}_1, \vec{a}_2, \vec{a}_3 \) are the primitive translation vectors of the unit cell.

Define \( \vec{a}_i^* = \frac{2\pi}{V_0} \vec{a}_2 \wedge \vec{a}_3 \) and cyclic permutations.

Then \( \vec{a}_i^* \cdot \vec{a}_j = 2\pi \delta_{ij} \).

If \( \vec{Q} = \vec{G}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^* \) then \( \vec{Q} \cdot (\vec{i} - \vec{j}) = 2M\pi \).

So scattering from a (frozen) lattice only occurs when the scattering wavevector, \( Q \), is equal to a reciprocal lattice vector, \( \vec{G}_{hkl} \).
Direct and Reciprocal Lattices

In a Bravais lattice, we can write \( \mathbf{R}_i = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3 \) where \( \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \) are the primitive translation vectors of the unit cell (see previous viewgraph).

Let's define \( \mathbf{a}_1^* = \frac{2\pi}{V_0} \mathbf{a}_2 \times \mathbf{a}_3; \quad \mathbf{a}_2^* = \frac{2\pi}{V_0} \mathbf{a}_3 \times \mathbf{a}_1; \quad \mathbf{a}_3^* = \frac{2\pi}{V_0} \mathbf{a}_1 \times \mathbf{a}_2 \)

where \( V_0 = \mathbf{a}_1 . (\mathbf{a}_2 \times \mathbf{a}_3) \) is the volume of the unit cell.

The \( \mathbf{a}_i^* \) have the dimensions of (length)\(^{-1}\) and the property that \( \mathbf{a}_i^* . \mathbf{a}_j = 2\pi \delta_{ij} \), i.e. \( \mathbf{a}_1^* \) is perpendicular to the plane defined by \( \mathbf{a}_2 \) and \( \mathbf{a}_3 \) etc.

If we choose a vector \( \mathbf{G}_{hkl} \) defined by \( \mathbf{G}_{hkl} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^* \) then \( \mathbf{G}_{hkl} . (\mathbf{R}_i - \mathbf{R}_j) = 2M\pi \).

i.e. \( \mathbf{G}_{hkl} \) is normal to sets of planes of atoms spaced \( 2\pi / G_{hkl} \) apart

Scattering from a lattice of atoms occurs only when \( \mathbf{Q} = \mathbf{G}_{hkl} \)

The vectors \( \mathbf{G}_{hkl} \) define a lattice of points called the **reciprocal lattice**

Homework: verify that Bragg’s (\( \lambda = 2 \) d sin\( \theta \)) follows from the above
Reciprocal Space – An Array of Points \((hkl)\) that is Precisely Related to the Crystal Lattice

\[ (hkl) = (260) \]

\[ a^* = 2\pi(b \times c)/V_0, \text{ etc.} \]

A single crystal has to be aligned precisely to record Bragg scattering
Notation

- $\mathbf{G}_{hkl}$ is called a reciprocal lattice vector (node denoted hkl)

- $h$, $k$ and $l$ are called Miller indices

- (hkl) describes a set of planes perpendicular to $\mathbf{G}_{hkl}$, separated by $2\pi/G_{hkl}$

- $\{hkl\}$ represents a set of symmetry-related lattice planes

- [hkl] describes a crystallographic direction

- $<hkl>$ describes a set of symmetry equivalent crystallographic directions
For Periodic Arrays of Nuclei, Coherent Scattering Is Reinforced Only in Specific Directions Corresponding to the Bragg Condition:

\[ \lambda = 2 d_{hkl} \sin(\theta) \text{ or } 2 k \sin(\theta) = G_{hkl} \]
Atomic Vibrations

- The formalism on the previous slide works fine if the atoms are stationary: in reality, they are not.

- Remember, from the last lecture that

\[ S(Q) = \frac{1}{N} \left \langle \sum_{i,j} e^{-i\vec{Q} \cdot (\vec{R}_i - \vec{R}_j)} \right \rangle \text{ensemble} \]

- We average over the (fluctuating) atomic positions by introducing a probability that an atom will be at given position. Instead of the Fourier Transform of \( \delta \) functions, this gives the FT of the \( \delta \) functions \textit{convolved} with a spread function. The result is that \( S(Q) \) is \textit{multiplied} by the FT of the spread function i.e. by \( \exp -Q^2 \left \langle \sigma^2 \right \rangle / 3 \) if we use a Gaussian spread function.

- Atomic vibrations cause a decrease in the intensity of Bragg scattering. The “missing” scattering appears between Bragg peaks and results in inelastic scattering.
Key Points about Diffraction

• A monochromatic (single $\lambda$) neutron beam is diffracted by a single crystal only if specific geometrical conditions are fulfilled.

• These conditions can be expressed in several ways:
  – Laue’s conditions: $\vec{Q}.\vec{a}_1 = h; \vec{Q}.\vec{a}_2 = k; \vec{Q}.\vec{a}_3 = l$ with $h$, $k$, and $l$ as integers.
  – Bragg’s Law: $2d_{hkl} \sin \theta = \lambda$.
  – Ewald’s construction.
    see http://www.matter.org.uk/diffraction/geometry/default.htm

• Diffraction tells us about:
  – The dimensions of the unit cell.
  – The symmetry of the crystal.
  – The positions of atoms within the unit cell.
  – The extent of thermal vibrations of atoms in various directions.
Bragg Scattering from Crystals

Working through the math (see, for example, Squires' book), we find:

\[
\left( \frac{d\sigma}{d\Omega} \right)_{\text{Bragg}} = N \frac{(2\pi)^3}{V_0} \sum_{hkl} \delta(\vec{Q} - \vec{G}_{hkl}) |F_{hkl}(\vec{Q})|^2
\]

where the unit-cell structure factor is given by

\[
F_{hkl}(\vec{Q}) = \sum_d \bar{b}_d e^{i\vec{Q}.\vec{d}} e^{-W_d}
\]

and \(W_d\) is the Debye-Waller factor that accounts for thermal motions of atoms

- Using either single crystals or powders, neutron diffraction can be used to measure \(F^2\) (which is proportional to the intensity of a Bragg peak) for various values of \(hkl\).
- Direct Fourier inversion of diffraction data to yield crystal structures is not possible because we only measure the magnitude of \(F\), and not its phase => models must be fit to the data.
- Neutron powder diffraction has been particularly successful at determining structures of new materials, e.g. high \(T_c\) materials.
The Structure Factor

- The intensity of scattering at reciprocal lattice points is given by the square of the structure factor:
  \[ F_{hkl}(Q) = \sum_d \overrightarrow{b}_d e^{i\overrightarrow{Q} \cdot \overrightarrow{d}} e^{-W_d} \]

- Crystallography attempts to deduce atomic positions and thermal motions from measurements of a large number of such “reflections”:
  - (Reciprocal) distance between diffraction “spots” \( \Rightarrow \) size of unit cell
  - Systematic absences and symmetry of reciprocal lattices \( \Rightarrow \) crystal symmetry (e.g. bcc \( h+k+l=2n \))
  - Intensities of “spots” \( \Rightarrow \) atomic positions and thermal motions

Laue diffraction pattern showing crystal symmetry
Resolution and Integrated Intensity

- Neutron beam is not perfectly collimated or monochromatic

- At a CW source, measure intensities of Bragg peaks either by rocking the crystal through the Ewald sphere or scanning 2θ.  
  - Width of rocking curve reflects instrumental resolution and (perhaps) crystallite size

- Integrated intensity of rocking curve is proportional to structure factor.  
  Constant of proportionality depends on resolution function – called the Lorentz factor
Useful Web Sites

• The following sites provide tutorials on diffraction. It is a good idea to go through them and try the examples.

• http://www.matter.org.uk/diffraction/introduction/default.htm

• http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/teaching.html
If we could measure the complex quantity $F_{hkl}$ we could figure out the positions of all atoms. But we only measure $|F_{hkl}|^2$. In fact, we would be better off if diffraction measured phase of scattering rather than amplitude! Unfortunately, nature did not oblige us.

The Phase Problem
Powder – A Polycrystalline Mass

All orientations of crystallites possible

Typical Sample: 1cc powder of 10μm crystallites - $10^9$ particles
if 1μm crystallites - $10^{12}$ particles

Single crystal reciprocal lattice
- smeared into spherical shells
Incident beam
x-rays or neutrons

Bragg’s Law \( \lambda = 2dsin\Theta \)

Powder pattern – scan \(2\Theta\) or \(\lambda\)

Sample

Powder Diffraction gives Scattering on Debye-Scherrer Cones

(111)
(200)
(220)
Measuring Neutron Diffraction Patterns with a Monochromatic Neutron Beam

Since we know the neutron wavevector, $k$, the scattering angle gives $G_{hkl}$ directly:

$$G_{hkl} = 2k \sin \theta$$

Use a continuous beam of mono-energetic neutrons.
Neutron Powder Diffraction using Time-of-Flight

L₀ = 9-100m

Pulsed source

Sample

Detector bank

L₁ ~ 1-2m

Θ - fixed

2Θ - fixed

Φ

λ = 2dsinΘ

Measure scattering as a function of time-of-flight t = const*λ
Time-of-Flight Powder Diffraction

Use a pulsed beam with a broad spectrum of neutron energies and separate different energies (velocities) by time of flight.
Compare X-ray & Neutron Powder Patterns

X-ray Diffraction - CuKa
Phillips PW1710
• Higher resolution
• Intensity fall-off at small d spacings
• Better at resolving small lattice distortions

Neutron Diffraction - D1a, ILL
λ=1.909 Å
• Lower resolution
• Much higher intensity at small d-spacings
• Better atomic positions/thermal parameters
There’s more than meets the eye in a powder pattern*

Rietveld Model \( I_c = I_b + \Sigma Y_p \)

*Discussion of Rietveld method adapted from viewgraphs by R. Vondreele (LANSCE)
The Rietveld Model for Refining Powder Patterns

\[ I_c = I_o \left\{ \sum k_h F^2_h m_h L_h P(\Delta_h) + I_b \right\} \]

- $I_o$ - incident intensity - variable for fixed $2\Theta$
- $k_h$ - scale factor for particular phase
- $F^2_h$ - structure factor for particular reflection
- $m_h$ - reflection multiplicity
- $L_h$ - correction factors on intensity - texture, etc.
- $P(\Delta_h)$ - peak shape function – includes instrumental resolution, crystallite size, microstrain, etc.
How good is this function?

Protein Rietveld refinement - Very low angle fit
1.0-4.0° peaks - strong asymmetry
“perfect” fit to shape
What do Neutron Powder Diffractometers look like?

Note: relatively massive shielding; long flight paths for time-of-flight spectrometers; many or multi-detectors on modern instruments.
Examples of Science using Neutron Diffraction

• Refinement of structures of new materials
• Materials texture
• Strain measurements
• Laue instruments for neutron protein crystallography
• Pair distribution functions (PDF)
High-resolution Neutron Powder Diffraction in CMR manganates*

• In Sr$_2$LaMn$_2$O$_7$ – synchrotron data indicated two phases at low temperature. Simultaneous refinement of neutron powder data at 2 $\lambda$’s allowed two almost-isostructural phases (one FM the other AFM) to be refined. Only neutrons see the magnetic reflections.

• High resolution powder diffraction with Nd$_{0.7}$Ca$_{0.3}$MnO$_3$ showed splitting of (202) peak due to a transition to a previously unknown monoclinic phase. The data showed the existence of 2 Mn sites with different Mn-O distances. The different sites are likely occupied by Mn$^{3+}$ and Mn$^{4+}$ respectively.

* E. Suard & P. G. Radaelli (ILL)
Texture: “Interesting Preferred Orientation”

Random powder - all crystallite orientations equally probable - flat pole figure

Pole figure - stereographic projection of a crystal axis down some sample direction

Loose powder

Metal wire

(100) random texture   (100) wire texture
Crystallites oriented along wire axis - pole figure peaked in center and at the rim (100’s are 90° apart)

Orientation Distribution Function - probability function for texture
Texture Measurement by Diffraction

Non-random crystallite orientations in sample

Incident beam
x-rays or neutrons

Sample

Debye-Scherrer cones
• uneven intensity due to texture
• different pattern of unevenness for different hkl’s
• intensity pattern changes as sample is turned
Texture Determination of Titanium Wire Plate
(Wright-Patterson AFB/LANSCE Collaboration)

Possible “pseudo-single crystal” turbine blade material

Ti Wire - (100) texture

Ti Wire Plate - does it still have wire texture?

- Bulk measurement
- Neutron time-of-flight data
- Rietveld refinement of texture
- Spherical harmonics to $L_{\text{max}} = 16$
- Very strong wire texture in plate

reconstructed (100) pole figure
Definitions of Stress and Strain

- **Macroscopic strain** – total strain measured by an extensometer
- **Elastic lattice strain** – response of lattice planes to applied stress, measured by diffraction
  \[ \varepsilon_{hkl} = \frac{d_{hkl} - d_0}{d_0} \]
- **Intergranular strain** – deviation of elastic lattice strain from linear behavior
  \[ \varepsilon_I = \varepsilon_{hkl} - \frac{\sigma_{\text{applied}}}{E_{hkl}} \]
- **Residual strains** – internal strains present with no applied force
- **Thermal residual strains** – strains that develop on cooling from processing temperature due to anisotropic coefficients of thermal expansion
Neutron Diffraction Measurements of Lattice Strain*

Neutron measurements: -
- Non destructive, bulk, phase sensitive
- Time consuming, Limited spatial resolution

The Neutron Powder Diffractometer at LANSCE

* Discussion of residual strain adapted from viewgraphs by M. Bourke (LANSCE)
Why use Metal Matrix Composites?

- Higher Pay Loads
- High temperatures
- High pressures
- Reduced Engine Weights
- Reduced Fuel Consumption
- Better Engine Performance

**MMC Applications**

- Rotors
- Fan Blades
- Structural Rods
- Impellers
- Landing Gears

**Engineering Examples**

- **F117 (JSF)**
- **Landing Gear**
- **National AeroSpace Plane Engine**
W-Fe: Fabrication, Microstructure & Composition

- 200 μm diameter continuous Tungsten fibers,
- Hot pressed at 1338 K for 1 hour into Kanthal (73 Fe, 21 Cr, 6 Al wt%) – leads to residual strains after cooling
- Specimens: 200 * 25 * 2.5 mm³

![Image of Tungsten fibers with different volume percentages: 10 vol.%, 30 vol.%, 20 vol.%, 70 vol.%](image)

Powder diffraction data includes Bragg peaks from both Kanthal and Tungsten.
Neutron Diffraction Measures Mean Residual Phase Strains when Results for a MMC are compared to an Undeformed Standard

Symbols show data points
Curves are fits of the form $<\varepsilon> = <\varepsilon_{11}[^{\cos^2\alpha}] + <\varepsilon_{22}[^{\sin^2\alpha}]$

Pressure Vessels and Piping, Vol. 373, “Fatigue, Fracture & Residual Stresses”, Book No H01154
Load Sharing in MMCs can also be Measured by Neutron Diffraction

- Initial co-deformation results from confinement of W fibers by the Kanthal matrix
- Change of slope (125 MPa) is the typical load sharing behavior of MMCs:
  - Kanthal yields and ceases to bear further load
  - Tungsten fibers reinforce and strengthen the composite
• Important Programmatic Answers.
  1. Material is Single Phase Monoclinic (α”).
  2. Lack of New Peaks Rules out Stress Induced Phase Transition.
  3. Changes in Peak Intensity Indicate That Twinning is the Deformation Mechanism.
Macromolecular Crystallography using Synchrotron Radiation provides Detailed Molecular Structures

- The principle steps are:
  - Isolation, purification
  - Cloning and expression (several mg are required)
  - Crystallization
  - Preliminary x-ray survey – cell dimensions, space group, quality of crystal, sensitivity to radiation damage
  - Data collection (perhaps including MAD) – 1 Å resolution usually requires measurement of several x 100,000 unique Bragg reflections
  - Phase determinations
  - Electron density maps
  - Structure refinement

For neutrons we must add:
  - Producing even bigger crystals (several mm$^3$)
  - Deuteration (may reduce crystal size needed)
  - Largest MW is less than x-rays
    - Current neutron record same as synchrotron record in 1990

Large lysozyme crystal grown on the space shuttle
The Reciprocal Lattice for Multiple Wavelengths

- With a continuous band of wavelengths, each reciprocal lattice point becomes a line pointing towards the origin.
What does the Scattering Pattern look like for Multiple Wavelengths?

- Many of the radial rods intersect the Ewald sphere and given rise to Bragg reflections.
- The Laue pattern reflects the crystal symmetry.

Note that diffraction orders overlap for a broad wavelength band.
What is the Role for Neutron Scattering in Protein Crystallography?

• Even the highest resolution synchrotron x-ray studies have trouble locating protons in protein crystals
  – Especially true if there is a close-by metal atom (e.g. in enzymes)
  – X-rays measure electron density – if a proton and its electrons are displaced x-rays will give a false impression of proton location

• Neutron diffraction can locate protons even in moderate resolution studies (~2 Å)
  – Neutrons locate nuclei not (generally) electrons
  – Either H or D scatter comparably with other nuclei

• There are many cases were H plays a vital role in proteins
  – Primary motive power for many enzymatic reactions
  – Hydrogen bonding and hydration contribute to structural stability
The Laue Method is a Powerful Tool for Neutron Protein Crystallography

- “Quasi-Laue” technique implemented at continuous neutron sources
  - “quasi” because it uses restricted wavelength band (1.5 to 2 Å typically) to avoid overlapping Bragg peaks
  - Use image-plate detectors that measure over a wide range of scattering angles but with relatively low efficiency
  - Typically requires crystals of several mm$^3$ and MW less than ~50 kDa

- Full Laue method implemented at LANSCE*
  - Uses wavelengths from ~0.6Å to ~6.5Å, separated by TOF
  - Peak-to-background ratio is excellent because bgr is spread over many TOF channels
  - Has recently solved structure with MW ~ 160 kDa

The Protein Crystallography Station (PCS) at Los Alamos

- The PCS sees a broad wavelength neutron beam, pulsed at 20 Hz
- The time-of-flight of a neutron from source to detector determines
  \[ \lambda (\text{Å}) \sim 4 \frac{t(\text{ms})}{L(\text{m})} \]

The heart of the PCS is an advanced neutron detector that subtends 16° x 120° at the sample position (0.3 m² active area with a spatial resolution of ~1.5mm)
Neutron TOF Laue Patterns for Cubic Insulin*

Detector image integrated over $\lambda$ – equivalent to the pattern obtained at a reactor

The same data, integrated over $x$, showing how the reflections are separated in TOF i.e. in $\lambda$.

The data are color coded with the shortest wavelength (hot) neutrons in red and the longest wavelength (cold) neutrons in blue

Preparing a Neutron Protein Crystallography Experiment

• Need to know x-ray structure and have a good scientific case for needing to know H positions

• X-ray crystals are ~0.1 mm³; neutrons need 1 mm³ or larger for hydrogenated samples

• Scattering power increases by ~10x if crystal is deuterated

• Typically, insert gene that encodes protein in *E Coli* and grow up using D₂O and deuterated nutrient – probably need about 5 L of final medium for neutron experiment (this can be done at LANSCE)

• Extract protein and grow deuterated crystal – crystal mosaic needs to be 0.2° to 0.3°

• MW limit is currently about 150 kDa for good quality crystals
The Process of Obtaining Neutron Laue Patterns

- Detector response correction – use incoherent scatterer
- Check crystal centering – telescope
- Collect data (~12 hours per crystal orientation)
- Check diffraction quality – intensity & standard deviation
- Locate diffraction spots in x, y and $\lambda$
- Check no spurious peaks
- Index reflections & determine crystal orientation
- Predict reflection positions & overlay on observations
- Integrate reflections
- Perform wavelength normalization ($I \sim \lambda^2$)
- Average intensities of equivalent reflections
- Refine crystal structure (use x-ray structure)
A Recent Example: Preliminary Measurements on D-xylose Isomerase*

- X-ray structure known with very high resolution (<1 Å) (MW=160kDa)
- Unable to decide between postulated catalytic mechanisms
  - Enzyme action transfers an H from one C atom of substrate to an adjacent C
  - Three different mechanisms proposed – each involves differences in H-atom orientations at active sites

Neutron data show that the ring N atom on Trp137 is deuterated: cannot see this in electron density deduced from x-ray data

Pair Distribution Functions

- Modern materials are often disordered.
- Standard crystallographic methods lose the aperiodic (disorder) information.
- We would like to be able to sit on an atom and look at our neighborhood.
- The PDF method allows us to do that (see next slide):
  - First we do a neutron or x-ray diffraction experiment
  - Then we correct the data for experimental effects
  - Then we Fourier transform the data to real-space
Obtaining the Pair Distribution Function*

\[ G(r) = \frac{2}{\pi} \int_{0}^{\infty} Q[S(Q) - 1] \sin QrdQ \]

* See http://www.pa.msu.edu/cmp/billinge-group/
Structure and PDF of a High Temperature Superconductor

The structure of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ looks like this: (copper [orange] sits in the middle of octahedra of oxygen ions [shown shaded with pale blue].)

The resulting PDFs look like this. The peak at 1.9Å is the Cu-O bond.

So what can we learn about charge-stripes from the PDF?
Effect of Doping on the Octahedra

- Doping holes (positive charges) by adding Sr shortens Cu-O bonds.
- Localized holes in stripes implies a coexistence of short and long Cu-O in-plane bonds => increase in Cu-O bond distribution width with doping.
- We see this in the PDF: $\sigma^2$ is the width of the CuO bond distribution which increases with doping then decreases beyond optimal doping.