Coherent X-ray Imaging

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Outline

1. Fundamentals
   contrast
   resolution
   coherence
   X-ray sources, optics, detectors
   imaging regimes, coherent scattering

2. Direct methods
   projection
   full-field

3. Indirect methods
   coherent diffractive imaging
   scanning CDI (ptychography)
   holography
Imaging

image [ˈɪmɪdʒ]

Noun:
The optical counterpart of an object produced by an optical device (as a lens or mirror) or an electronic device.

Verb:
Make a visual representation of (something) by scanning it with a detector or electromagnetic beam.

- *Merriam-Webster Dictionary*

Contrast mechanisms in x-ray imaging

Access a wealth of information

- **Absorption** measure electron density
- **Phase** measure real part of refractive index
- **Fluorescence** measure elemental distribution
- **Spectroscopy** measure chemical state, atomic neighborhood
- **Diffraction** probe atomic lattice structure and strain
- **Polarization** probe magnetic and orbital states

- Natural sample contrast is possible; staining not required
- Image structure of thick samples, sectioning not required
- More penetrating, less damage, less charging than with electrons
Refractive index and contrast in the x-ray region

\[ n = 1 - \delta - i\beta = 1 - \frac{r}{2\pi} \lambda^2 \sum_{i} n_i f_i(0) \]
\[ A = A_0 \exp(-inkt) \]
\[ k = \frac{2\pi}{\lambda} \]

- Absorption contrast:
  sensitive to \( \text{Im}(n) \)
  \( \sim 4\pi\beta(x,y)t/\lambda \)

- Phase contrast:
  sensitive to \( \text{Re}(n) \)
  \( \sim 2\pi\delta(x,y)t/\lambda \)

Absorption edges provide elemental and chemical specificity
Polarized x-rays give sensitivity to electron spin

![Graph showing x-ray energy and intensity](image)

**Image formation as a scattering process**

Incident waves with initial momentum $k_{inc}$ are elastically scattered into new direction $k_{scatt}$ with momentum transfer $\Delta k$.

Ewald sphere is defined by conservation of momentum. Only spatial frequencies on the Ewald sphere are accessible to the imaging process, limiting attainable resolution.
**Diffraction limits to resolution**

**Point-spread function**

\[ P(x,y) = \frac{\sin x \sin y}{x/y} \]

with \( x = \frac{kax}{z} \), \( y = \frac{kay}{z} \)

\[ \text{Transverse} \quad R = 0.5 \frac{\lambda}{NA} \]

\[ \Delta k = k_{\text{inc}} - k_{\text{scatt}} \quad (0 \leq \Delta k \leq 2k_{\text{inc}}) \]

For extreme-angle ray (xz plane, \( k_y = 0 \)) with

\[ k_x = \frac{2\pi}{2R} = \frac{2\pi}{\lambda NA} \]

\[ k_z = \frac{k_{\text{inc}}}{2k_{\text{inc}}} \quad (k_x \ll k_{\text{inc}}) \]

**Bragg’s law**

\[ \Delta k = k_{\text{inc}} - k_{\text{scatt}} \]

\[ k_x^2 + k_y^2 + (k_x + k_{\text{inc}})^2 = k_{\text{inc}}^2 \]

\[ \text{Longitudinal} \quad \text{DOF} = \frac{\lambda}{(NA)^2} \]

\[ \Delta \text{f} = \frac{0.813/\text{NA}}{f_{\text{cut}}} \]

**What do we mean by “resolution”?**

- Point sources are spatially coherent
- Mutually incoherent
- Intensities add
- Rayleigh criterion (25.5% clip)

Conclusion: With spatially coherent illumination, objects are “just resolvable” when

\[ \text{Res}_{\text{res}} = \frac{0.61 \lambda}{\text{NA}} = 1.22 \Delta \tau \]
Coherence

**longitudinal coherence**

\[ \Delta \lambda \]

\[ \lambda \]

\[ \frac{\lambda^2}{\Delta \lambda} \]

\[ \tau_c \sim \frac{\lambda^2}{c \Delta \lambda} \]

\[ w_c \sim \frac{\lambda z}{d} \]

\[ d \cdot \theta = \lambda / 2\pi \]

\[ \Delta x \Delta p \approx h / 2 \]

**transverse coherence**

Coherent vs. incoherent

**Scanning and full-field microscopy are incoherent methods**

- Transfer function is linear in the field intensities
- Characterized by sloping function down to 2NA

**Diffraction and holographic microscopy are coherent methods**

- Transfer function is linear in the field amplitudes
- Characterized by flat top, sharp cutoff at limiting NA
Why use synchrotron radiation?

Synchrotron sources offer:

- Brightness (small source, collimated)
- Tunability (IR to hard x-rays)
- Polarization (linear, circular)
- Time structure (short pulses)

➢ Source brightness is the key figure of merit for coherent imaging

\[ B = \text{photons/source area, divergence, bandwidth} \]

\[ F_c \sim \lambda^2 B \]

Coherent flux from synchrotron sources

- SR sources (except FELs) are incoherent, but highly forward directed due to relativistic effects

\[ \theta \sim \frac{1}{\gamma} \]

- Spatial and temporal filtering (pinholes, monochromators) are needed to select the coherent flux

\[ F_c \sim \lambda^2 B \]

- Only the coherent flux can be focused into a diffraction-limited spot or be used to form interference fringes
**X-ray source brightness**

Flux per spatially coherent mode: \[ F_c = B \frac{\lambda^2}{4} \]

**Discovery of x-rays**

**We are here**


**Diffraction limited focusing requires coherent light**

Achieving high NA is challenging because x-rays interact weakly

\[ n = 1 - \delta - i\beta \quad \delta,\beta \sim 10^{-3} \text{ to } 10^{-6} \quad \Rightarrow \quad |n| \approx 1 \]

- **Refractive** (compound refractive lenses)
  - Low efficiency, highly chromatic, aberrations
  - ~50 nm

- **Reflective** (Kirkpatrick-Baez mirrors)
  - High efficiency, achromatic, limited to ~10 nm
  - ~40 nm

- **Diffractive** (Fresnel zone plates, MLLs)
  - Moderate efficiency, limited to ~10 nm except MLL
  - ~15 nm

- **Waveguides**
  - Low efficiency, 2D is challenging
  - ~10 nm
Fresnel zone plate

\[ f^2 + r_n^2 = \left( f + \frac{n\lambda}{2} \right)^2 \]

\[ r_n^2 = \frac{n\lambda + \frac{n^2\lambda^2}{4}}{2n\lambda} \]

\[ r_n = \sqrt{n\lambda} \]


Large-format, single-photon sensitive x-ray CCD cameras opened the door to coherent x-ray imaging

Fairchild Peregrine 486 CCD Camera
- 4K x 4K pixel array (61.4 mm square area)
- 15 µm pixels, 100% fill factor
- Back-illuminated for up to 80% QE
- Readout noise < 5 e- at 50 Kpixels/s
- Dynamic range > 86 dB in MPP
- 6 s readout with four on-chip amplifiers
- Pixel binning for more rapid readout
- Peltier-cooled to -50 C for low dark current
Pixel array detectors: revolutionizing coherent imaging

A Three Layer Hybrid Device
- Diode layer → converts x-rays to photocurrent.
- ASIC layer → custom signal processing electronics.
- A layer of metallic interconnects (bump bonds) between corresponding pixels on the diode and ASIC layers.

PADs can be read out in ~1 ms.
(CCDs take seconds!)

PAD pixels are 55-150 µm.
(CCDs are 12-24 µm)

Pilatus 6M detector (PSI/Dectris)

Imaging regimes with coherent x-rays

X-ray beam

near-field Fresnel

phase contrast

in-line holography

coherent diffraction

far-field Fraunhofer

absorption radiograph

Kagoshima (1999)

Jacobsen (1990)

Miao (1999)

absorption

2a

z ∼ a²/λ

z >> a²/λ
**X-ray scattering from a disordered sample**

- **(a) Incoherent scattering**, giving rise to a continuous diffraction ring.
- **(b) Coherent scattering**, resulting in a speckled diffraction ring.


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**2. Direct methods**

- Imaging regimes with coherent light
- Projection imaging
- Full-field imaging

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**References:**

**Direct methods**

- Scanning
- Full-field
- Projection

**Phase contrast: tool of choice for low absorption samples**

(a) Dust mite and (b) tomographically reconstructed fly leg joint, recorded with ~8 keV x-rays and propagation phase contrast.


Small fish, recorded with three-grating method and standard x-ray tube (40 kV/25 mA). (a) Transmission. (b) Differential phase.


Moth wing, recorded with 4 keV x-rays.  
(a) Bright-field.  (b) Differential interference contrast.

B. Kaulich, T. Wilhein, JOSA A19, 797 (2002)
Full-field x-ray microscope


Resolution of a Fresnel zone plate lens

\[ R = \frac{0.6i\lambda}{NA} \]

\[ NA = \frac{\lambda}{2\Delta r} \]
Quantitative phase tomography

- Defocus series (a, b, c) and phase (d) of a silicon AFM tip
- Quantitative 3D reconstructions of real part of refractive index from ±70° tomographic projections through tip

Calculated $\delta = 5.1 \times 10^{-6}$

Measured $\delta = 5.0 \pm 0.5 \times 10^{-6}$


3. Indirect methods

- Coherent diffractive imaging
  - Isolated sample (single-view)
  - Extended sample (ptychography)

- Bragg coherent diffractive imaging

- Holography

- Time-resolved imaging

References:
Indirect methods: CDI and holography: "Lensless" imaging

- Object wave (diffraction) is detected directly
- Diffraction intensity corresponds to autocorrelation of object
- Coherent reference wave interferes with object wave to form hologram
- Hologram intensity corresponds to convolution of object and reference

\[
\text{Resolution:} \quad \begin{align*}
\text{transverse} & \sim \frac{\lambda}{\text{NA}} \\
\text{longitudinal} & \sim \frac{\lambda}{(\text{NA})^2}
\end{align*}
\]

\[
\text{Contrast:} \quad \propto |f_1|^2 + |f_2|^2
\]

Coherent diffractive imaging

**Lensless method**
Resolution \( \sim \frac{\lambda}{\text{angular size}} \) limited only by wavelength and signal

- Two-step process: record coherent diffraction pattern, recover object structure numerically (iterative phase retrieval)
- Sensitive to phase as well as absorption of the specimen
- Get 3D by tomographic methods; no depth of field limit
- But: must assume some information to recover phase, e.g. known object extent or illumination profile

**Iterative phase retrieval**

- **Real Space**
  - N x N Object in 2N x 2N Matrix
  - Force Intensity Outside Of Object to Known Value

- **k-Space**
  - Set Magnitude to Speckle Image


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**Error reduction algorithm**

\[
g \xrightarrow{\mathcal{F}} G = |G| e^{i\phi} \\
\text{SATISFY OBJECT CONSTRAINTS} \\
\xrightarrow{\mathcal{F}^{-1}} G' = |F| e^{i\phi} \\
\text{SATISFY FOURIER CONSTRAINTS}
\]

R.W. Gerchberg, W.O. Saxton, Optik 35 237 (1972)  
ER and Hybrid Input-Output algorithms

**ER**

\[ s_{n+1} = P_s P_F s_n \]

**HIO**

\[
\begin{cases} 
  P_s g_n(r) & \text{if } r \in \text{support} \\
  g_n(r) - \beta P_s g_n(r) & \text{otherwise}
\end{cases}
\]

where \( G(r) = \mathcal{F}[g(r)] \),

\[
P_s G(q) = \begin{cases} 
  \sqrt{\mathbb{R}(r)} \frac{G(q)}{G(q)} & \text{if } I(r) \text{ is known and } |\mathcal{F}(r)| \neq 0 \\
  0 & \text{otherwise}
\end{cases}
\]

and \( g_n \) and \( g_{n+1} \) are the \( n \)th and \( (n+1) \)th iterates, \( P_s \) and \( P_F \) are Fourier modulus and support projections, \( \beta \) is a "feedback" parameter.


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Reconstruction

Real space

Magnitude

Far field

Magnitude

Real space

Phase

Far field

Phase

Error (a.u.)

0.100

0.010

0.001

1

10

100

1000

Iteration number

Reconstruction error
**Iterative phasing: simple example**

High harmonic generation of XUV radiation from femtosecond laser, illuminating two pinholes

Data  Support constraint (loose)  Reconstruction


**First demonstration with x-rays**

diffraction pattern  reconstruction

Difference Map algorithm

The Difference Map is defined by:

\[ g_{n+1} = g_n + \beta (g_{n-1} - g_n) \]

with \( n \)th Fourier and support estimates, \( g_s = \beta^{-1} \) and \( g_F = \beta^2 \).

A common choice for DM is \( \beta = 1 \), giving:

\[ g_{n+1} = P_F \left[ (\gamma_F + i) P_F (g_n) - \gamma_S g_n \right] \]
\[ g_{n-1} = P_S \left[ (\gamma_F + i) P_F (g_n) - \gamma_S g_n \right] \]

With \( \beta = 1 \), we get back Fienup’s HIO algorithm.

A metric used to monitor convergence is:

\[ \varepsilon_n = \| g_{n+1} - g_n \| = \| g_{n-1} - g_n \| \]

V. Elser, JOSA A 20, 40 (2003)

Freeze dried yeast cell imaged by CDI

Diffraction reconstruction (data taken at 750 eV; absorption as brightness, phase as hue).

Stony Brook/NSLS STXM image with 45 nm Rayleigh resolution zone plate at 520 eV (absorption as brightness).

D. Shapiro, PNAS 102, 15343 (2005)
**CDI setup at APS beamline 2-ID-B (1-4 keV)**

![CDI setup diagram]

**Buried structures can be probed with element specificity**

In contrast to weak segregation theory, Bi is locally concentrated in Bi-doped Si crystals

(a) Image below Bi M5 edge (2550 eV)  
(b) Image above the Bi M5 edge (2595 eV)  
(c) Difference  
(d) SEM image

C. Song, PRL 100, 025504 (2008)
Curved object illumination aids unique phase recovery

- Lens illuminates object with curved wavefront, defines field of view
- Object illumination is reconstructed by back-propagation, used to retrieve phase of object wave by iterative methods


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Fresnel diffraction

\[
\begin{align*}
\text{"object wave"} \quad a(\xi, \eta) &= e^{ikz} \int \int a(x, y) \frac{ik}{2z} \left( (x - \xi)^2 + (y - \eta)^2 \right) \, dx \, dy \\
&= e^{ikz} e^{\frac{i k}{2z} (\xi^2 + \eta^2)} \left\{ \frac{ik}{e^{\frac{i k}{2z} (x^2 + y^2)}} \, \text{FT} \left[ a(x, y) \right] \right\}
\end{align*}
\]
... and converges faster

Original

curved beam illumination  plane wave illumination

Unique solution
Fresnel coherent diffraction imaging of a gold test pattern

Images reconstructed by FCDI

G. Williams, PRL 97, 022506 (2006)
"Keyhole" FCDI

Use reconstructed illumination profile to determine support in extended sample


Ability to study extended samples is essential for many real-world problems!


"Fuse bay" structure

B. Abbey, APL 93, 214101 (2008)
I. McNulty
NX2014
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Bragg gratings that diffract to a certain angle represent a specific transverse and longitudinal periodicity (Ewald sphere).

Data collection over a series of rotations about an axis fills in 3D Fourier space for phasing.

3D coherent diffraction imaging

(a) SEM of pyramidal indentation in a 100-nm Si$_3$N$_4$ membrane lined with 50-nm Au spheres.
(b) 3D image reconstructed from 123 diffraction projections spanning -57° to +66°, using reality and positivity constraints.
(c) Large DOF projection. (d) Enlarged region of (c).

3D CDI of biological specimens is feasible, too

Ptychography: scanning approach enables solution to extended object and unknown probe

\[ \hat{P}_n(r) = \sum_j \frac{\hat{O}_n^*(r, r_j) \psi_n(r, r_j)}{\sum_j |\hat{O}_n(r, r_j)|^2} \quad \text{is the Probe} \]

\[ \hat{O}_n(r) = \sum_j \frac{P_n^*(r, r_j) \psi_n(r, r_j)}{\sum_j |P_n(r, r_j)|^2} \quad \text{is the Complex Object} \]

\[ \psi_n(r, r_j) = \hat{O}_n(r) \hat{P}_n(r, r_j) \]

\[ \psi_{n+1}(r, r_j) = \psi_n(r, r_j) + p \left[ 2 \hat{P}_n(r, r_j) \hat{O}_n(r) - \psi_n(r, r_j) \right] - \hat{P}_n(r, r_j) \hat{O}_n(r) \]
Thibault et al. algorithm

Recipe:

1. Start with guess for $\hat{O}$ and $\hat{P}$, use these guesses to define $\psi_0$.
2. Update $\psi_{n+1}$ for all $j$ probe positions, holding $\hat{O}$ and $\hat{P}$ constant.
3. Update $\hat{O}$ using sum on previous page, using current $\hat{P}$ and $\psi_n$.
4. Update $\hat{P}$ using sum on previous page, using current $\hat{O}$ and $\psi_n$.
5. Back to step 1, repeat.

Good convergence in 10s of iterations

![Image of good convergence in 10s of iterations]
**Magnetic multilayers: model magnetic storage media**

- Fabricated by sputtering; can be nano-patterned lithographically
- Perpendicular anisotropy spontaneously forms "worm" domains with antiparallel out-of-plane magnetization
- Artificial ferrimagnets with strong coupling at domain interfaces

Magnetic force micrograph of 200 nm thick GdFe multilayer (courtesy E. Fullerton, UCSD)

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**Resonant x-ray scattering**

\[
I \approx \sum \exp(i \cdot \mathbf{r}_n)f_n \\
\]

\[
f_n \approx f^{(0)}_{\text{nonres}} + f^{\text{magn}}_{\text{nonres}} + f' + if''
\]

J.P. Hannon, PRL 61, 1245 (1988)
Magnetic domain structure can be visualized in-situ by resonant x-ray ptychography

Resonant scattering vs. photon energy
Reconstructed domain structure and probe function

Sample scan: \((14 \times 3 \, \mu m)^2 \times (40 \times 1 \, \text{s})\) exposures

Magnetic domain evolution with increasing field

Hysteresis loop of sample magnetization as a function of magnetic field applied normal to the film surface. (b-f) Reconstructions from a series of diffraction patterns taken at indicated points in hysteresis curve. Bright domains are anti-parallel to the applied magnetic field.
Decreasing field

Domain evolution as the magnetic field was decreased from saturation towards zero. (a) Sample hysteresis loop as a function of applied field; (b-f) reconstructions from series of scanned diffraction patterns taken at various points in (a).

A. Tripathi, PNAS 108, 13393 (2011)

Bragg diffraction from crystals

\[ Q = k_f - k_i \]
Coherent diffraction from crystals

Each Bragg spot contains the shape information
Bragg coherent diffractive imaging

- Bragg CDI is uniquely sensitive to crystalline order and lattice strain
- The Ewald sphere can be tiled by rocking the crystal to get 3D information

Three-dimensional Bragg method

- Select coherent part of hard x-ray beam with double crystal monochromator and precision slits
- Locate sample in beam and Bragg peaks (ideally, 3 to get complete strain tensor)
- Rock sample around Bragg peaks to record diffraction vs. angle
- Assemble 3D XYθ data set, align to central peak
- Reconstruct via iterative phase retrieval, using constraint applied in pixel coordinates

Setup at APS 34-ID-C beamline
Diffractometer and cryo setup at 34-ID-C

Mapping crystal strain in 3D by CDI

0.5 µm Pb crystal grown on SiO$_2$ substrate

Reconstructed diffraction data
Asymmetries in the Bragg spots arise from lattice strain

I. Robinson and R. Harder, Nature Mater. 8, 291 (2009)

3D strain is expressed as a tensor

\[
\epsilon_{ij} = \begin{bmatrix}
\epsilon_{xx} & \gamma_{xy} & \gamma_{xz} \\
\gamma_{yx} & \epsilon_{yy} & \gamma_{yz} \\
\gamma_{zx} & \gamma_{zy} & \epsilon_{zz}
\end{bmatrix}
\]

\[
\epsilon_x = \frac{\partial u_x}{\partial x}, \quad \epsilon_y = \frac{\partial u_y}{\partial y}, \quad \epsilon_z = \frac{\partial u_z}{\partial z}
\]

\[
\gamma_{yz} = \gamma_{zy} = \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}, \quad \gamma_{zx} = \gamma_{xz} = \frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}
\]
Vector displacement field around a lattice defect (Au crystal)

Produced by combining reconstructions from (11-1), (020), and (-111) reflections

3D strain map in ZnO nanorods

Nanoscale structures can be highly strained because of confinement effects, resulting in dramatically different electronic, magnetic and optical properties

\[
\epsilon_\alpha = \begin{pmatrix}
\frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \\
\frac{\partial u_i}{\partial x_k} \\
\frac{\partial u_j}{\partial x_k}
\end{pmatrix},
\quad
\epsilon_{ij} = \frac{\partial u_i}{\partial x_j}
\]

M. Newton, Nature Mater. 9, 120 (2010)
Unusual internal core-shell strain in zeolite crystals

Calcination of ZSM-5 zeolite crystals results in a surprising triangular strain distribution.

Nano-engineering of local strain by organic templating could be used to develop new catalysts.

Internal strain distribution undergoes phase transition at ~200 °C, as seen by Bragg CDI.


X-ray Bragg ptychography

- Extension of scanning small-angle CDI methods to the Bragg regime.
- Algorithm enables reconstruction of both unknown probe and object wave
- More robust reconstruction than single-view; Bragg gives crystal strain as well as structure
- First experiments on ferroelectric materials are yielding structure at ~6 nm resolution and strain at the $10^{-5}$ $\Delta c/c$ scale
Initial experiments

Scan along vertical arm of ZnO tetrapod
- 11.5 keV x-rays, ~1.3 µm focus, < 0.5 µm steps
- Collect 3D diffraction pattern (rock) at each scan position
- Reconstructed real-space voxels: 14x19x14 nm

Local polarization in ferroelectric thin films

Critical phenomena such as domain fluctuations and order parameter pinning can lead to unexpected behavior at the nanoscale

(left) Ferroelectric polarization domains in thin-film PbTiO₃, mapped by piezoresponse force microscopy.
(right) Domains imaged by x-ray Bragg ptychography to 5.7 nm.

S. Hruszkewycz, PRL 110, 177601 (2013)
Holography

Gabor

Fourier transform

Record hologram

Reconstruct

Reference wave encodes magnitude and phase of object wave

Reconstruct object wave by "re-illuminating" hologram with reference wave (or its C.C.)

Gabor holography

Reconstructed hologram (right) of a NIL8 hamster neural fibroblast recorded with 656 eV x-rays.
Estimated dose was 7.5 x 10^5 Gy

S. Lindaas, JOSA A13, 1788 (1996)
**FT hologram formation**

\[
a(\xi, \eta) = \frac{e^{ikz}}{iLz} \iint a(x-s,y) e^{-ikz(x-s)^2 + (s-x)^2} \, dx \, dy
\]

object wave

\[
b(\xi, \eta) = \frac{e^{ikz}}{iLz} b_0 e^{-ikz(x-s)^2 + (s-x)^2}
\]

reference wave

\[I = |a|^2 + |b|^2 + a^*b + ab^*
\]

hologram intensity

**Reconstruction**

- Numerically take FT of hologram intensity to reconstruct
- Spatially separated primary, conjugate object waves result
- Weak curvature \(f(x,y)\) on object wave can be ignored

Image terms:

\[a^*b + ab^* = q(s,\xi) F(\xi,\eta) + q(s,\xi)^* F(\xi,\eta)^*
\]

where:

\[F(\xi,\eta) = \frac{e^{ikz}}{iLz} f(\xi,\eta) \iint a(x,y)f(x,y) e^{-ikz(x-s)^2 + (s-x)^2} \, dx \, dy
\]

\[q(s,\xi) = e^{-ikz(s-x)^2}
\]

and

\[f(\xi,\eta) = e^{-ik\xi^2}
\]

\[\text{FT}^{-1} \{ a^*b + ab^* \} = f(x-s,y) a(x-s,y) + f(-(x-s),-y)^* a(-(x-s),-y)^*
\]
UE56-SGM beamline and ALICE

Fourier transform holography with a pinhole mask

Single-shot compatible

Sample: [0.7 nm Pt/1.2 nm Co]_{10} multilayer on Si_{3}N_{4} membrane
(a) MFM image
(b) Gold proximity mask

S. Flewett, PRL 108, 223902 (2012)
CDI can be done on a tabletop!

R. Sandberg, PNAS 105, 24 (2008)

First ultrafast CDI of a virus with an x-ray laser

Linac Coherent Light Source at Stanford University, CA

1.8 keV x-rays, 70 fs exposure!

M. Seibert, Nature 470, 78 (2011)
Imaging lattice dynamics: Laser pump - CDI probe

Diffraction pattern as a function of laser delay.
fast period = 400ps
slow period = 5.56ns


Imaging lattice dynamics: Laser pump - CXD probe

\[ \text{DifferenceMap} = FT\left[ (A_1^{\text{Exp}} - A_2^{\text{Exp}}) \exp(i\phi_1^{\text{recon}}) \right] \]

- \( A_1^{\text{Exp}} \): Measured Amplitudes of the reference structure (no laser)
- \( \phi_1^{\text{recon}} \): Phases retrieved for the reference data.
- \( A_2^{\text{Exp}} \): Measured Amplitudes of modified structure (laser fixed time offset)
Phonon modes in a laser-shocked gold nanocrystal

(top) Orthogonal slices taken either side of the center of a gold nanocrystal.
(middle) Projected displacement obtained from experiment.
(bottom) Simulated (1, 1) mode for a cylinder.

Comparison is for a delay time of +110 ps for a separation of 180 nm between z-y and 120 nm between x-z slices.

J. Clark, Science 341, 56 (2013)

Imaging resolution by x-ray holography

3rd Gen SR’s
Coherent vs. total flux of SR sources

Flux per spatially coherent mode: \( F_c = B \lambda^{2/4} \)

Large emittance, low brilliance, small coherent fraction and flux

Small emittance, high brilliance, large coherent fraction and flux

APS source today and proposed “MBA lattice”

**Today**

- Bunch structure, flux:
  - Pump-probe diffraction/crystallography
  - Pump-probe scattering
  - Imaging
  - CDI

**Future: 100-fold increase in brightness**

- Brightness:
  - XPCS
  - Imaging
  - CDI
  - IXS
APS brightness with MBA lattice

Figure 1: Comparison of brightness from the present APS to selected hybrid-permanent magnet and superconducting undulators in the MBA lattice design described here.

M. Borland (ANL)

Coherent fraction of proposed DLSR's

I. McNulty  NX2014  18 June 2014

M. Borland (ANL)
Partial coherent light can be treated as a distribution of coherent modes

\[ J(r_1, r_2) = \sum_{n=1}^{N} \mu_n \psi_n(r_1) \psi_n^*(r_2) \]

Coherent modes for the lower-coherence set of experimental data. The square delineates the edge of the physical aperture. (a) (0,0) mode, (b) (1,0) mode, (c) (0,1) mode.


Diffractive imaging with partially coherent light

- Conventional phase retrieval algorithms that assume full coherence break down with partially coherent light

\[ I(k) = \sum_{n=1}^{N} \mu_n I_n(k) \]

- If you know (or guess) the modal distribution (i.e. its weighting \( \mu_n \)), you can fold this into the algorithm to optimize for each mode

SEM of Au test pattern  Conventional reconstruction with partial spatial coherence  Reconstruction incorporating 3 spatially coherent modes

L. Whitehead, PRL 103, 243902 (2009)
Going broadband: use polychromatic light

Use of entire first undulator harmonic (~2.5% BW) gives 60x gain in measurement speed.

B. Abbey, Nature Photonics 5, 420 (2011)
Summary

- Contrast, resolution, sources, optics and detectors; x-ray imaging regimes
- Direct methods: projection and full-field
- Indirect methods: coherent diffractive imaging, ptychography, holography, and time-resolved
- Brighter sources, partially coherent methods

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... and thank you!