X-ray Coherence methods for LCLS

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Discussion Questions

• Coherent x-ray diffraction imaging
• How much information in a single shot?
• 3D solution from a single shot?
• XPCS or Imaging approach?
• Real or Reciprocal space view?
• Planning for initial LCLS experiments
Diamond
in-vacuum
X-ray
Undulator
Coherent X-ray Diffraction Imaging

APS $\xi_{\text{HOR}} = 20\mu\text{m}$, focus to $1\mu\text{m}$
LCLS $\xi_{\text{HOR}} > 500\mu\text{m}$, focus to $0.1\mu\text{m}$

Nothing moves!

High DR pixel detector

Coherence defining aperture

Sample grain

X-ray beam

Rotational axis

CCD X-ray detector
Chemically Synthesized Silver Nanocubes

Yugang Sun and Younan Xia,
Rocking scan of Ag cubes with 0.01° steps
Gold nanocrystal reconstruction
showing support used for 20 HIO followed by 10 ER
Coherent Diffraction from Crystals

Fourier Transform

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Diffraction by Strain of Point Defect

\[ A \sim \sum e^{i\mathbf{Q} \cdot (\mathbf{R}_j + \mathbf{u}_j)} \approx \sum e^{i\mathbf{Q} \cdot \mathbf{R}_j} (1 + i\mathbf{Q} \cdot \mathbf{u}_j) \]

Imaginary density

\[ + \]

\[ - \]

[Diagram of normalized intensity with arrows and concentric circles]
VLS growth of nanowires
Reconstruction of InP nanowire
CVD on Si, Suneel Kodambaka, UCLA

InP nanowires grown on Si (111)
Phase structure in nanowires
GaAs Nanowire “Barcode”
Vincent Favre-Nicolin, Joel Eymery (CEA), Rienk Algra (Philips), Ross Harder
Dark Field TEM of GaAs Nanowires
Models of Barcode Diffraction
(111) wires at (11-1) reflection

- Twinned stacking sequence
- Deformation faults

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Antiphase domains in faulted wires?
Contact strain of Zeolite ZSM-5
with Hyunjung Kim and K. B. Yoon at Sogang University
ZnO Sample Preparation

Dimensions: 4-5µm

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Density sections ZnO-39 (010)
Marcus Newton and Steven Leake (in preparation, 2008)
Phase maps from 2 Bragg peaks
Blue-Red is +2 radians. Slice at -1500nm from centre ZnO-5 -39

\[ \varphi = \vec{Q} \cdot \vec{u(r)} \]

Q=(100)

Q=(010)
Typical displacement field

$Q \cdot u \text{ small}$

$Q \cdot u \text{ large}$

$Q = (010)$
How to extract the contrast data
Five Bragg peaks

002 no fringe visibility

010 & 100 good fringe visibility

101 & 011 diminished fringe visibility but fringes still evident

010:011 & 101:100 show complementary fringes but not between each other

Error in coordinate transform ruled out

010 and 100 reflections fringe spacing difference ~ 20%
Fringe Visibility 96±2% @010
How much information in a single shot?

• Phase problem can be solved beforehand:
  – Low dose rocking curve before ‘shot’
  – Ptychography scan before ‘shot’

• Phased diffraction allows full imaging during transient

• Phases are little changed during perturbation
  – localised change in real space affects all of reciprocal space
  – traditional “difference map” principle
3D solution from a single shot?

• Keyhole imaging with curved beam
  – multiple views of sample?

• Reconstruction is of exit wave field
  – can’t propagate to general 3D object

• Phase problem easier to solve for real objects
  – logo physics and cowboys

• Free-space propagation of phased wave field
  – valuable for ptychography probe
XPCS or Imaging approach?

• Fluctuation-dissipation theorem:
  – transient response “=” fluctuation due to noise
  – complex susceptibility, eg shear modulus
  – 1-point or 2-point correlations?

• Beam ‘heating’ anyway, use as impulse:
  – Split-and-delay technique
  – “Dusty Mirror” experiment
“Dusty Mirror” experiment
Loss of fringe visibility in (ps) time
Real or Reciprocal space view?

• Free to choose once phase problem is solved
  – Low dose rocking curve before ‘shot’
  – Ptychography scan before ‘shot’
• “Dirty mirror” was recip space information
  – OK because many similar samples in beam
• Real space avoids drifts, pulse-to-pulse variations
  – good for localised changes, rare events
• Reciprocal space better for self-similar objects
  – average over multiple copies
Generic aspects of speckle

• First-order change is of intensity
• Second-order change in speckle positions
  – contrast is mostly sensitive to this
• ‘Persistent’ speckle observation
  – Martin Grant & Mark Sutton
• Contrast useful to quantify degree of coherence of the beam
Planning for initial LCLS experiments

• CXI and PCS not ready in initial phase
• XPP will be first diffraction station
  – Area detector can measure CXD pattern
  – Laser pump can ‘activate’ sample
• Fabricated Gold nanocrystal arrays
  – control size, shape, orientation (est 200nm)
• Pre-align each under low dose for phasing
• Explode with full pulse: changes or not?
  – Observe melt? front after laser pump
e-beam Lithography “Lift-off” method

Si (100) wafer
10(+-1) mm x 10(+-1) mm square/rectangle

Thermally grown Si O2,
~ 100nm thick
(Back side oxide remaining)

Au film 20nm thick (piece-to-piece accuracy within 10%?)
(with and without adhesion layer of Cr or Ti 2nm thick)
(EB or thermally evaporated)

ZEP (EB) resist for lift-off
Top View of basic layout plan with pickup marks

50 μm interval dot array with $31 \times 31 = 961$ dots

Size to be discussed
Top View of chip layout
S. Shimamoto (Waseda), T. Matsuura (UCL), Sept 2008

hexagon dots          square dots          triangle dots
1 um^2 area dots
0.25 um^2 area dots
4 um^2 area dots

Shimamoto-Matsuura-Robinson, September 2008

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Dewetting to coalesce into crystals
Garth Williams thesis (2005)
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