Single-crystal Diffraction
Outline

- Scientific Scope
- Time resolved Laue Diffraction
- Synchrotron Beamline characteristics
  (ESRF, APS, KEK-AR)
- expected LCLS performance
- 'future' LCLS capabilities
- previous Experiments
  (SPPS, Synchrotron)
- LCLS Experiments
- Conclusion
Scientific capabilities

- Protein crystals
  - ligand movement
  - complete 3-D reorganisation

- Small molecule crystals
  - structural changes
  - photo induced phase transition

- Inorganic crystals
  - shock waves
Why Laue?

- uses full X-ray flux – fast data collection
- gives maximum per shot coverage of reciprocal space
- single shot can give sufficient I/sigma
  - fast data collection
- allows self normalisation
  (intensity ratios/ energy)
- independent of machine fluctuations
  (single shot characterisation needed)
- less damage by optical pump pulses
Synchrotron Laue Diffraction

- Time resolved laue beamlines
  - ESRF
    - $10^{10}$ photons/pulse
    - 100 ps
    - 3% bandwidth
    - 1(3) kHz
  - APS
    - $10^{10}$ photons/pulse
    - 100 ps
    - 3% bandwidth
    - 1 kHz
  - KEK
    - $10^9$ photons/pulse (13-20 keV)
    - 50 ps
    - 1 kHz
    - up to 15% bandwidth
LCLS – Expected Performance

- $10^{12}$ photons/pulse
- 0.8-8.4 keV
- 250 fs
- 0.3 % bandwidth
- 120 Hz

- coherent radiation
- few micron focus possible
- single pulse data acquisition
- 'energy resolved' Laue possible

- reflection conditions
  - 0.3% 8265-8290 eV (0.05°/0.1° at $\theta=15°/30°$)
  - 0.5% 8265-8315 eV (0.09°/0.2° at $\theta=15°/30°$)
X-ray spectrum comparison

ESRF - ID09b

Intensity

Energy (keV)

ESRF - ID09b

LCLS-FEL

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Office of Science/U.S. DOE

XPP workshop June 2008
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ASSOCIATION
TTF-CA Laue diffraction

ESRF ID09b
unpublished data
d=50 mm
beamsize 161x56 um
crystal 70x60x10 um
room temperature
measurement
50 ms at 1 kHz
<5·10^{10} photons on sample
~250 reflections measured
LCLS – extended operation

- energy of the e-beam
  shot by shot variation (+/-1% tuning possible)

- spontaneous radiation (1.5·10^8 photon/pulse)
  chirped single pulse
  tapered undulator modules
  broader bandwidth (>1%)
  smooth envelope
Wide bandwidth undulator performance

M. Tischer DESY-Hamburg – based on XFEL parameters
Time resolved studies

- APS (14-ID-B/BioCARS)
  - Protein Single Crystal (PYP, MbCO, Heme)
  - Small Molecule Single Crystal (Metallorganics)

- ESRF (ID09b)
  - Protein Single Crystal (MbCO)
  - Dynamics in solution (CH2I2 Isomers)
  - Photo induced Phase transitions (TTF systems)

- KEK - (PF-AR/NW14)
  - Protein Single Crystal (Hemoglobin)
  - shock induced deformations (CdS)
  - Small Molecule Single Crystal (Metallorganics)
  - Photo induced Phase transitions (TTF systems)
PtPOP Laue pattern

Philip Coppens et al.
unpublished data
difference image
KEK-AR NW14
5 pulses
<5 · 10^9 photons
Time resolved studies at SPPS

~2x10^6 photons/pulse  9.4 keV
220 x 500 µm²  CCD with fiber-coupled phosphor
1% bandwidth  at ~54 mm
300 s, 10 Hz, ΔΦ ~24°

Laser off  Laser on (Δt=-1ns)

Christian Blome, Thomas Tschentscher (DESY)
Simone Techert (MPI for biophysical Chemistry, Göttingen)
Time Resolved 'Laue' Crystallography at LCLS

Simone Techert (MPI for biophysical Chemistry, Göttingen)
Conclusion

- Laue like diffraction uses full flux
  broadband can further increase data per shot

- applicable to a wide range of single crystals
  small molecules, proteins, inorganic

- well established and growing field
  ESRF, KEK, APS

- per bunch characterisation needed
  e-beam diagnostics
  single shot spectrometer?
Acknowledgement

Shin-ichi Adachi
Philip Coppens
David Fritz
Jerry Hastings
Jochen Schneider
Peter Stefan
Simone Techert
Thomas Tschentscher
Michael Wulff

ID09b
NW14
BioCARS