Materials **I**maging and **D**ynamics Workshop

ESRF, Grenoble
October 28-29, 2009

http://www.xfel.eu/events/workshops/mid_workshop_2009/

The Materials Imaging and Dynamics (MID) instrument aims at the investigation of nanosized structure and nanoscale dynamics using coherent radiation. Applications to a wide range of materials from hard to soft condensed matter and biological structures are envisaged

Place and time: ESRF, October 28-29, 2009

Organizers: I. Gimbales & T. Tschentscher (XFEL), E. Jahn & A. Madsen (ESRF)

65 registered participants from Europe, USA and Japan

Day 1: plenary session; Day 2 parallel sessions (CXDI and XPCS) and discussions

Day 1: Plenary session

8.30 – 9.00	Registration	
Session I.	**X-Ray FELs and MID instrument**	
9.00 – 9.05	**H. Reichert**	*Welcome note*
9.05 – 9.20	**M. Altarelli**	*Status of the European XFEL*
9.20 – 9.45	**Th. Tschentscher**	*The MID instrument at the European XFEL*
9.45 – 10.15	**I. Vartaniants**	*Coherent Diffraction Imaging using X-ray FELs*
10.15 – 10.45	**C. Gutt**	*Photon Correlation Spectroscopy using X-ray FELs*
10.45 – 11.00	General discussion: MID instrument scope	
11.00 – 11.20	Coffee break	
Session II.	**Coherent Diffraction Imaging**	
11.20 – 11.50	**S. Ravy**	*Coherent diffraction for condensed matter physics*
11.50 – 12.20	**T. Salditt**	*imaging of supported bio-objects*
12.20 – 12.50	**E. Vlieg**	*Study of the initial stages of crystallization*
12.50 – 14.00	Lunch	
Session .	**X-ray Photon Correlation Spectroscopy**	
14.00 – 14.30	**P. Wochner**	*X-ray Cross Correlation Analysis*
14.30 – 15.00	**B. Stephenson**	*Large-q photon correlation spectroscopy*
15.00 – 15.30	**L. Cipelletti**	*Soft condensed matter studies*
15.30 – 15.50	Tea/Coffee break	
Session .	**Instrumentation**	
15.50 – 16.20	**H. Sinn**	*X-ray optic and beam transport effects to FEL radiation properties*
16.20 – 16.50	**A. Robert**	*The XPCS instrument at LCLS*
16.50 – 17.20	**S. Boutet**	*experiments at the LCLS*
17.20 – 18.00	**H. Graafsma**	*Area detector developments for and XPCS experiments*
Session IV.	**Instrumentation working groups**	
18.00 – 18.30	Definition of working groups and their tasks - Suggested Working Groups:	
	WG I	(O. Thomas & I. Vartaniants)
	WG II	XPCS (Ch. Schüßler-Langeheine & G. Grübel)

CXDI:

I. Vartaniants (DESY)

S. Ravy (Soleil)

A. Beerlink (Salditt, Göttingen)

XPCS:

C. Gutt (DESY)

B. Stephenson (ANL)

L. Cipelletti (Montpellier)

Emerging techniques & new ideas:

E. Vlieg (Nijmegen)

P. Wochner (MPI Stuttgart)

LCLS beamlines:

A. Robert and S. Boutet

Detectors and optics:

H. Graafsma (DESY)

H. Sinn (XFEL)

Day 2: Discussions in working groups & Conclusion

Session V.	**WG I : CDI - AUDITORIUM**	
9:00 – 13:00	**N. Vaxelaire**	Coherent Diffraction Imaging of strains as a tool to investigate the mechanics of polycrystals (15 min)
	H. Poulsen	Material research studies with coherent x-rays at XFEL (15 min)
	I. Robinson	Coherent diffractive imaging at XFEL (15 min)
	Coffee/Tea will be available during the sessions	
Session VI.	**WG II: XPCS – EMBL SEMINAR ROOM**	
9:00 – 13:00	**B. Sepiol**	Atomic diffusion investigation by XPCS (15 min)
	A. Madsen	Recent XPCS activities and their relation to XFEL experiments (15 min)
	H. Sinn	Phonons with XPCS (15 min)
	Coffee/Tea will be available during the sessions	
13:00 – 14:00	Lunch break	
14.00 – 15.00	WG I & II: Preparation of initial drafts of working group report	
15.00 – 15.20	Coffee/Tea break	
Session VII.	**Concluding Session - AUDITORIUM**	
15.20 – 15.50	WGI & WGII chairs	Presentation of working group findings
15.50 – 16.50	General discussion: MID instrument scope & realization	
16.50 – 17:00	**T. Tschentscher**	Summary of the Workshop

CXDI:

Chairs: I. Vartaniants (DESY) & O. Thomas (Marseille)

N. Vaxelaire (Marseille)
H. F. Poulsen (DTU, Risø)
I. K. Robinson (LCN & Diamond)

XPCS:

Chairs: G. Grübel (DESY) & C. Schüßler-Langeheine (Köln)

B. Sepiol (Vienna)
A. Madsen (ESRF)
H. Sinn (XFEL)

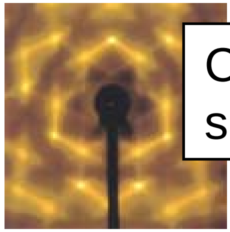
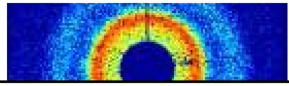
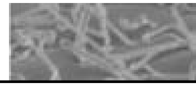
What can we do now and *What would we really like to do*

I CXDI and XPCS are both s/n ratio limited techniques with today's sources and detectors. **Potential gain with XFEL is enormous !**

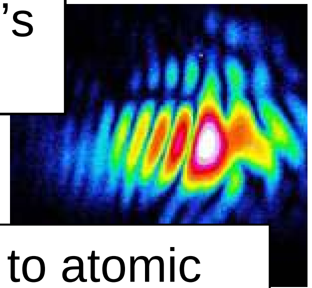
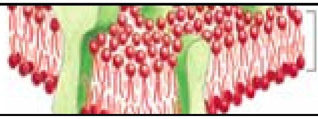
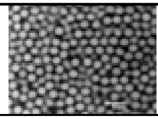
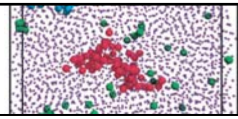
II How is the AC nature of the XFEL going to change the way we conduct and think about experiments?

III What would be the specifications of a dream detector and what is realistic to have for the XFEL startup?

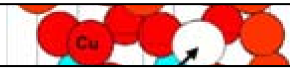
IV What would be the specifications for optical elements, beamline components and instrumentation?

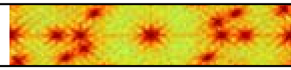
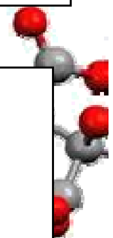




CXDI and XPCS are both s/n ratio limited techniques with today's sources and detectors. Potential gain with XFEL is enormous

- Structure (~1nm resolution, 3D, holography) and dynamics (ps-ns, down to atomic scales) by single shot images or series of speckle patterns.
- 3D lens-less imaging of nano-structured material (order, disorder, hard matter, soft-bio matter). Dynamics of atoms and molecules (diffusion, rotation, switching,…)
- Combination of the two: Time resolved CXDI and XCC

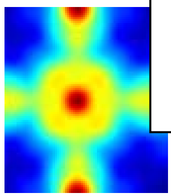
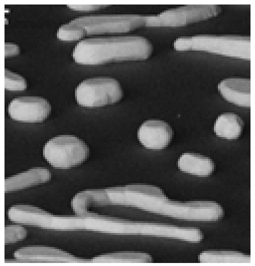
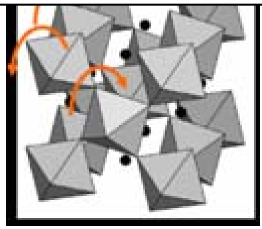
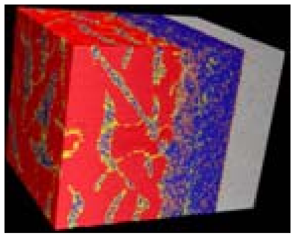
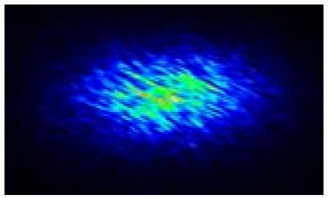
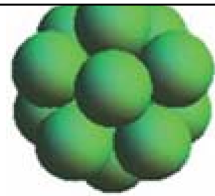
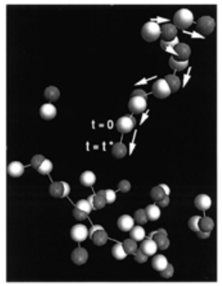



Scientific case CXDI: diffraction imaging of poly-crystals, crystallization, nucleation and growth, ablation, shock wave deformation, quantum dots…

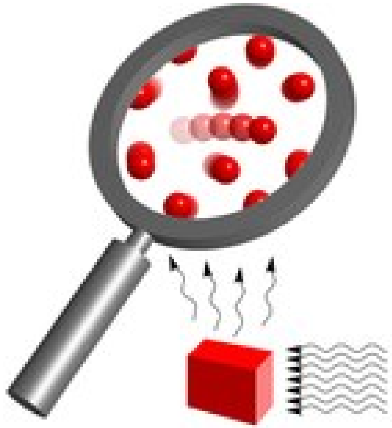
Scientific case XPCS: molecular dynamics in fluids, charge & spin dynamics in crystalline materials, atomic diffusion, phonons, pump-probe XPCS…

See also: XFEL TDR Ch. 6

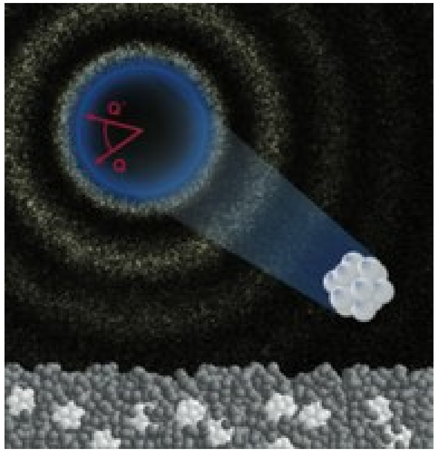
CXDI and XPCS are both s/n ratio limited techniques with today's sources and detectors. Potential gain with XFEL is enormous

Leitner et al.
Nature Materials (2009)



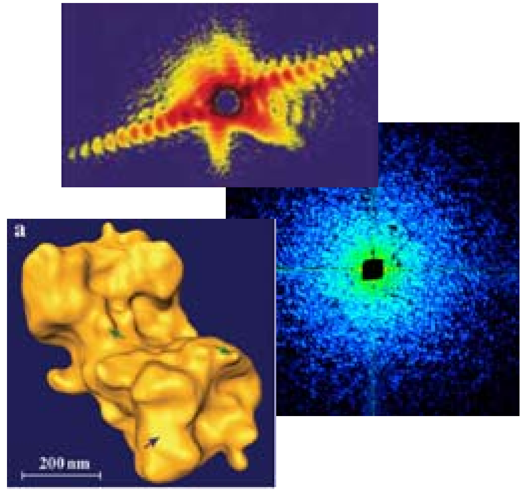
Fast atomic diffusion in materials

Wochner et al.
PNAS (2009)



Cross-correlations on molecular length scales (glasses, amorphous ice, polymer melts…)

Lima et al. PRL (2009)
Miao et al. PRL (2006)
Williams et al, PRL (2003)

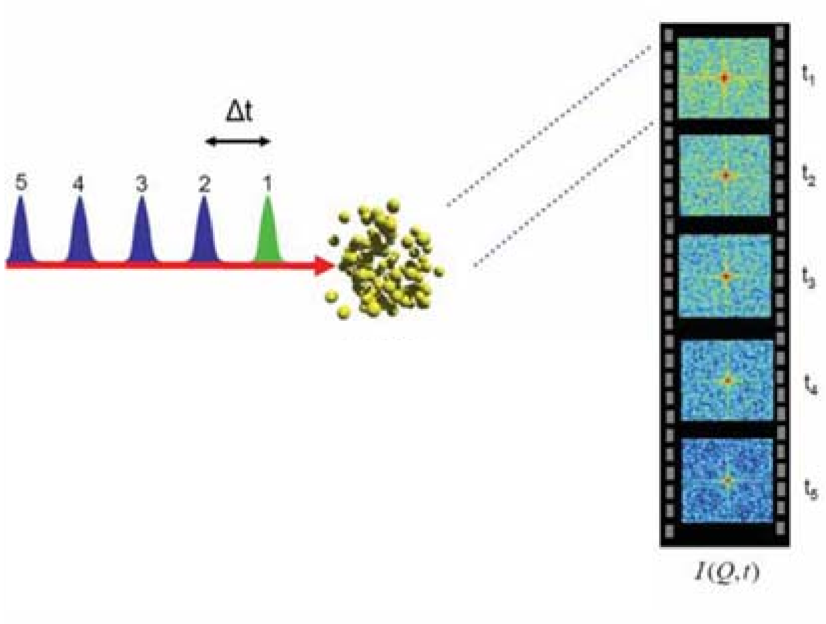


3D diffraction microscopy with ultimate resolution

Follow the fluctuations and time-evolution of all Fourier components of the electron density and eventually perform a time-resolved 3D reconstruction

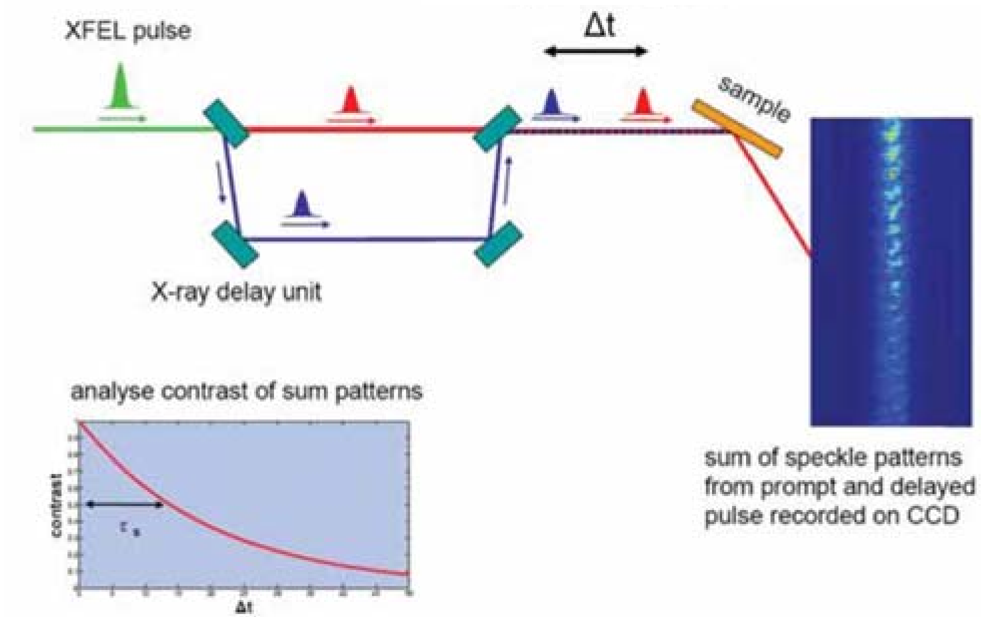
How is the AC nature of the XFEL going to change the way we conduct and think about experiments?

CXDI: some samples need not to survive more than one shot
XPCS: single shot experiments in general not possible



Sequential mode
(time, angle, new sample?)

Split-delay mode (XPCS)



Beam damage, optics, absorbers, coherence diagnostics of each shot, vertical polarization
X-PP, OL-PP, 3D, E-range

What would be the specifications of a dream detector and what is realistic to have for the XFEL startup?

General: Single ph sensitivity, Integrating pixel detector, on chip storage,
5 MHz source → 5 MHz detector

CXDI WG:

200 μm pixel size
As fast as possible (5 MHz)
Storage: as many as possible
1k x 1k (better 4k x 4k)
Dyn. range 10^4 (better 10^5)
6-36 keV operation, maybe lower?

XPCS WG:

4 μrad ang. res. (40μm @ 10m)
As fast as possible (5 MHz)
Storage: as may as possible
10^8 (or a many as possible, high-Q annulus)
Dyn. range: 100 ph/pixels may be enough
6-36 keV operation

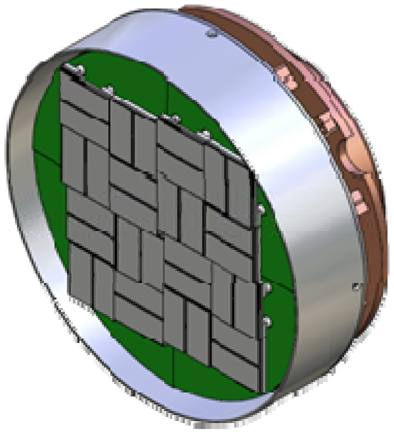
AGIPD

Heinz Graafsma: AGIPD
200 μm pixels
5 MHz framing speed
200-400 images storage depth
2e4 dyn/range
Prototype 2010

Several detectors (SAXS, WAXS, single shot, seq. mode)? Mask for XPCS?
s/n- considerations
Focusing?

For comparison: Detectors at LCLS (120 Hz!)

S. Boutet
(CXI instrument)



- 2D Pixel Array Detector
  - High resistivity Silicon (500 µm) for direct x-ray conversion.
  - Reverse biased for full depletion.
  - Bump-bonding connection to CMOS ASIC.
- <1 photon readout noise
- 110x110 µm^2 pixels
- 1520x1520 pixels
- 10^3 dynamic range
- 120 Hz readout
- **Tiled detector, permits variable 'hole' size**

Collaboration with the Gruner Group at Cornell University

A. Robert
(XCS instrument)

- 2D Pixel Array Detector
- <<1 photon readout noise
- 55x55 µm^2 pixels
- 1024x1024 pixels
- 10^2 dynamic range
- 120 Hz readout
- **More modules, tiled detector**

Collaboration with P. Siddons at BNL

What would be the specifications for optical elements, beamline components, instrumentation and layout?

Difficult experiment:

To observe speckles from disorder (liquids) at the peak in S(Q) (Q≈1-3 $Å^{-1}$) from a single shot with a reasonable ΔT of the sample

Depending on Z, up to ~10 ph/speckle/pulse can be expected with moderate temp rise (≲10K) with the current XFEL design parameters if the beamline features:

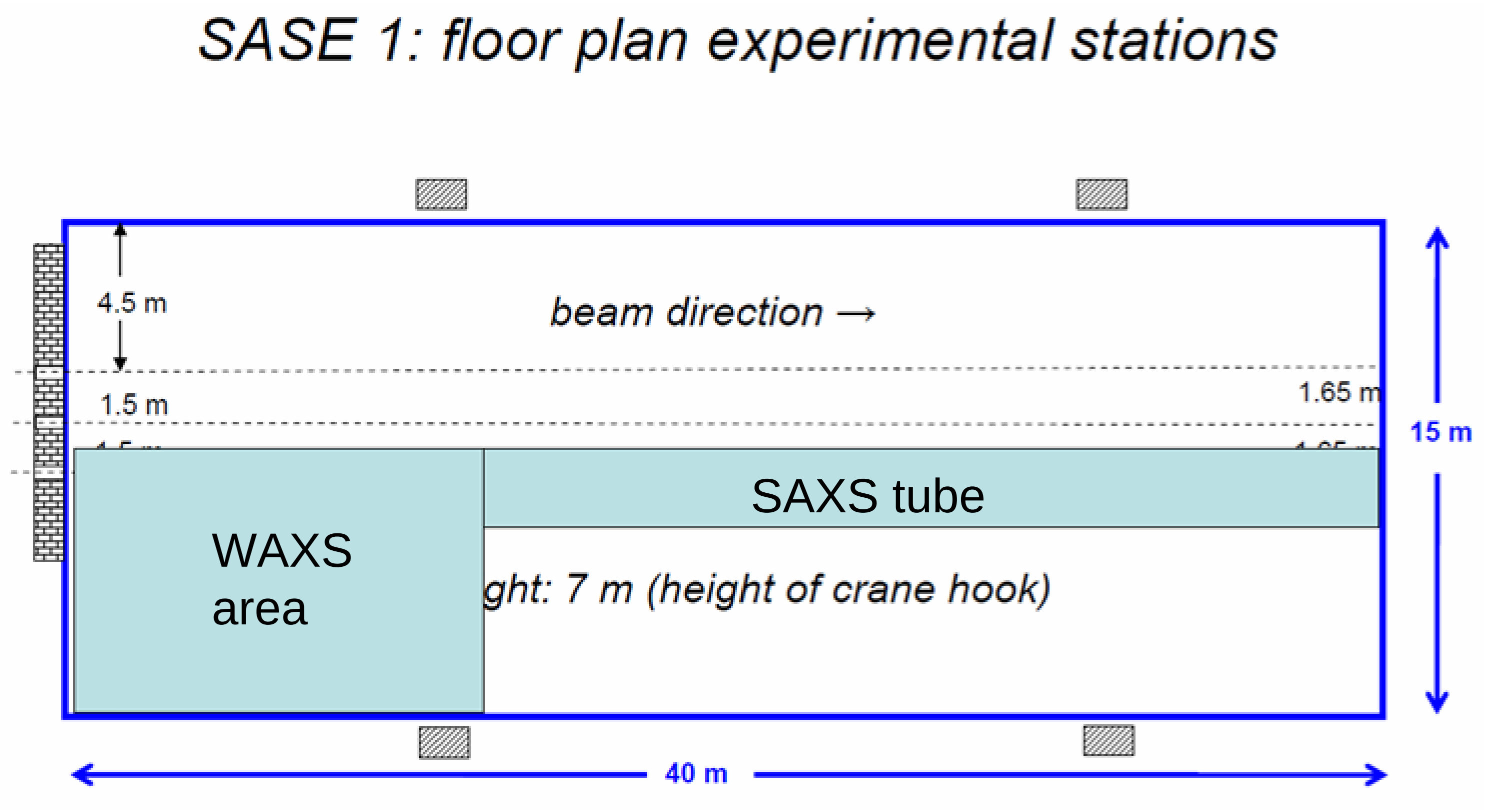
- High monochromaticity
- Focusing
- Camera with small pixels
- High-E option (up to 36 keV)

XPCS WG talk by H. Sinn: The case of water

What would be the specifications for optical elements, beamline components, instrumentation and layout?

- E range 6-36 keV (SASE-1, 1st and 3rd order), lower energies?
- Polarization control (vertical, waveplate)
- Monochromaticity 10^{-2} – 10^{-5}, delay line
- Focusing optics: spot size 100nm-100μm
  - KB optics for small spots (<1μm)
  - CRLs (Be and Si for moderate focusing and collimation)
- Slits, filters and absorbers
- Diagnostics (pulse length, intensity, beam position & coherence)
- Pulse pattern: Interest in sub 200 ns times (delay line)
  modification of the pattern in the e^--gun?
- Pulse length: Interest in sub 100 fs pulses (rad. damage)
- Diffractometer with necessary degrees of freedom, WAXS, SAXS (large dist.), multiple Q, multiple detectors,..
- High precision positioning, confocal microscope, SEM, cryostat, laser heating, external fields, pump lasers, high pressure, liquid jet,…

What would be the specifications for optical elements, beamline components, instrumentation and layout?



Detailed report addressing all these issues is under preparation for the MID instrument

Acknowledgements

Thanks to all participants for a very stimulating workshop

Thanks to everyone I borrowed text and images from for this presentation
and to I. Vartaniants, O. Thomas, G. Grübel, C. Schüßler-Langeheine,
and T. Tschentscher for driving the discussions

Thank you for listening