FEL's and X-ray Photon Correlation Spectroscopy

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Layout

- Storage Ring based Synchrotron sources versus Free Electron Lasers : Realities from experimentalists
- X-ray Photon Correlation Spectroscopy with an FEL

Storage Ring based Synchrotron sources versus Free Electron Lasers

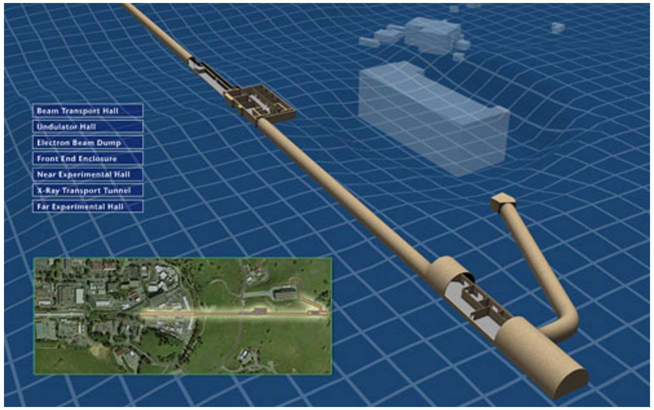
Realities from the experimentalist side

Synchrotron Sources

Highly stable (intensity, position, pointing, energy) and partially coherent storage rings sources with high brilliance in the hard X-ray Regime

Parameter	Comment
Time Structure	Continuous
Intensity	Stable
Position/ pointing	Stable
Energy spectrum	Stable
Timing	Stable
Coherence	Partial

Free Electron Lasers



FEL's are chaotic sources : they jitter

Parameter	Storage Ring	FEL
Time Structure	Continuous	**Pulsed**
Intensity	Stable	**Fluctuations**
Position/ pointing	Stable	**Fluctuations**
Energy spectrum	Stable	**Fluctuations**
Timing	Stable	**Fluctuations**
Coherence	Partial	**Full**

Typical LCLS parameters

Parameter	Hard X-ray	Unit
Photon Energy	≤ 10 (1st harm)	keV
Photons per Pulse	2-0.1	10^{12}
Repetition Rate	Up to 120	Hz
Single shot Pulse Bandwidth	0.2	%
Pulse Duration (FWHM)	80-2	fs

FEL X-ray beam is coherent over its size

For Si(111) beam : 0.1-1x10^9 ph pulse^{-1}

Very similar per shot to what is obtained per second on a storage ring

Experimental Tutorial : SR vs. FEL

SLAC

- Storage Ring based 3rd generation synchrotron sources technology and its development for the past 20 years (such as at the APS, ESRF and Spring-8) have been opening a new robust way of using X-rays to investigate material science questions thanks to their unique properties :

① Very large average flux (with undulators)
② Very collimated beam
③ Highly stable beam position
④ VERY stable intensity (with or without pop-up injection)
⑤ Short pulse durations
⑥ Temporal fluctuations
⑦ Energy tunability
⑧ Well define Energy spectrum and access to high Energies (>20keV)
⑨ Very efficient detectors (single photon counting, E-resolved, etc…)
⑩ A certain degree of coherence

Experimental Tutorial : SR vs. FEL

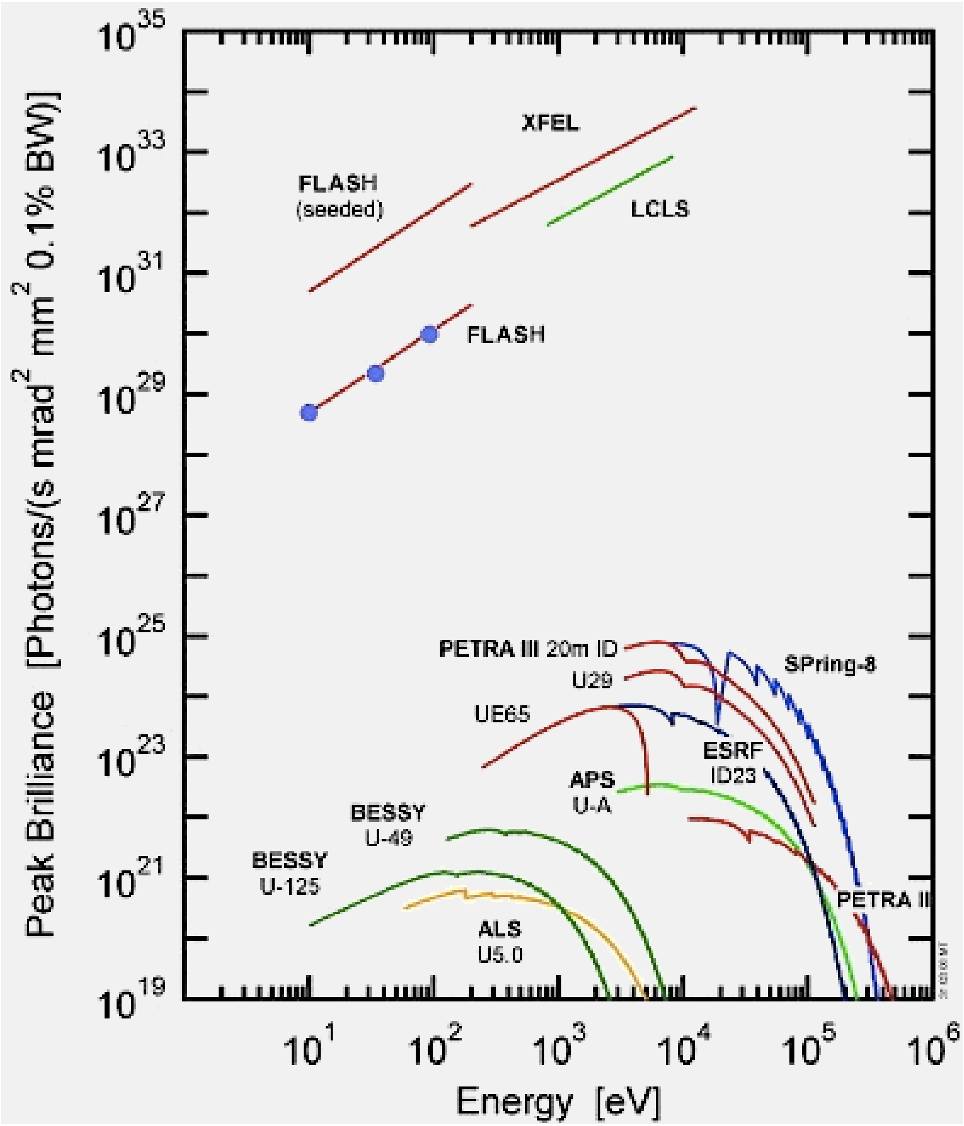
SLAC

"Free Electron Lasers offer the promise to provide unprecedented brilliant , ultra short and coherent X-ray beams down to Angstrom wavelengths."

It's still hard X-ray : so it should be very similar experimentally from what we know from 3rd generation storage rings, right ?

Let's re-visit every point one by one :

(1) FLUX



- FEL sources provide unprecedented peak brilliance as compared to Storage Ring (SR) sources.
- This originates from the pulsed nature of these sources.
- One typically gets per shot what one gets per second on a SR

(2) Collimated beams

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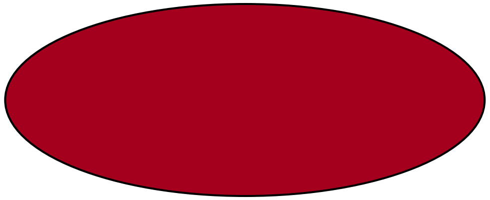
Storage Ring



Typ. beam size @40-50m

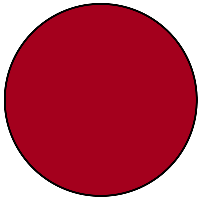
2-3 x0.5-1mm (h,v)

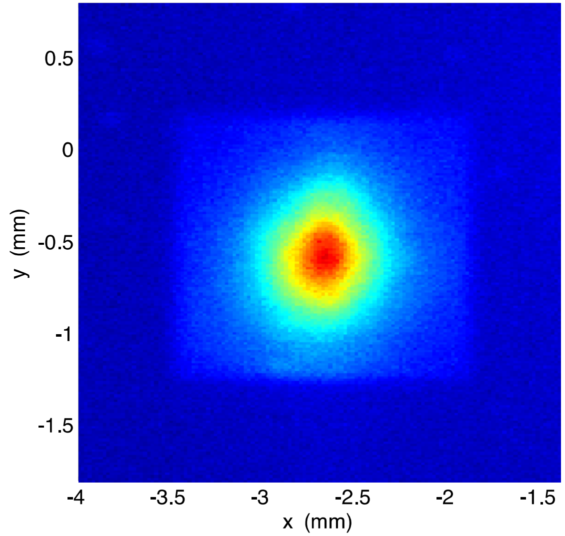
Typ. divergence high-β

30 x 15μrad (h,v)

(example : Troika ID10A at the ESRF)

FEL





Typ. beam size @200-400m

0.5-1 x0.5-1mm (h,v)

Typ. Divergence

1-2 x 1-2μrad (h,v)

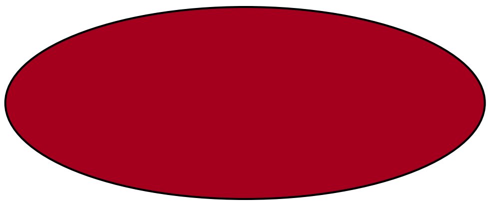
MOIANB01 Proceedings of BIW10, Santa Fe, New Mexico, US H. Loos et al.

OPERATIONAL PERFORMANCE OF LCLS BEAM INSTRUMENTATION*

It can have a huge impact on X-ray optics (e.g. focusing)

(3) position stability

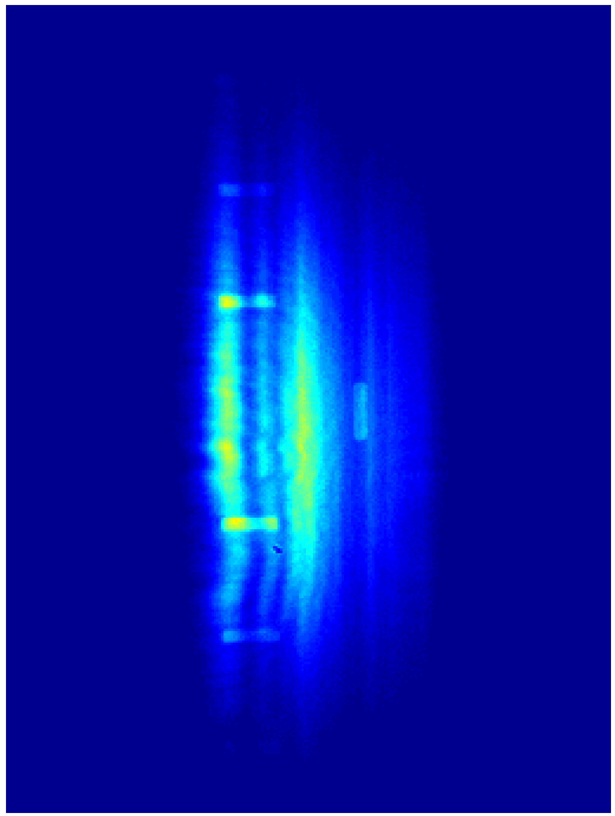
Storage Ring



Rock Stable !

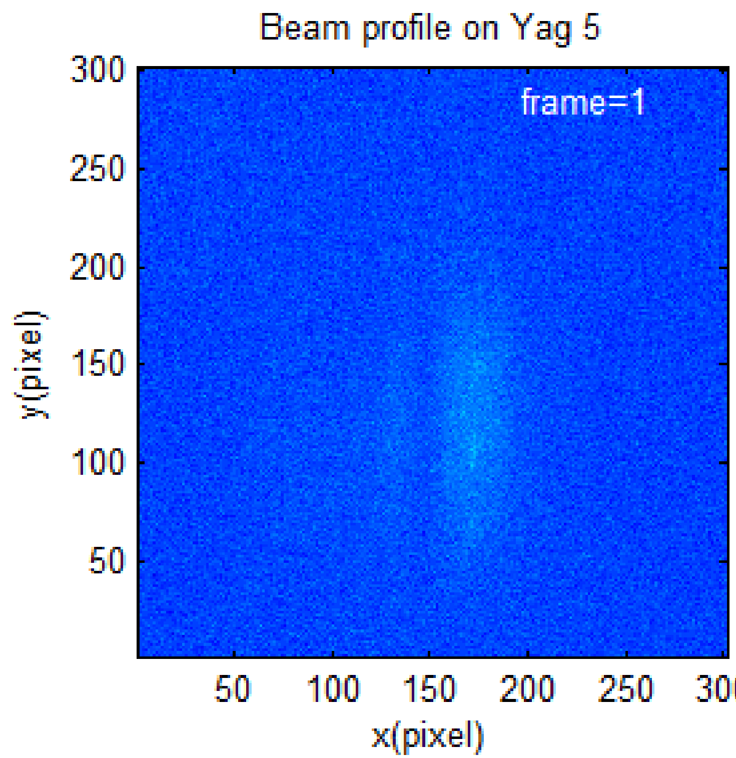
FEL

XPP



120Hz

XCS



Fluctuates in position by about 10% of its size

(4) Intensity stability

Storage Ring

Rock Stable !

With

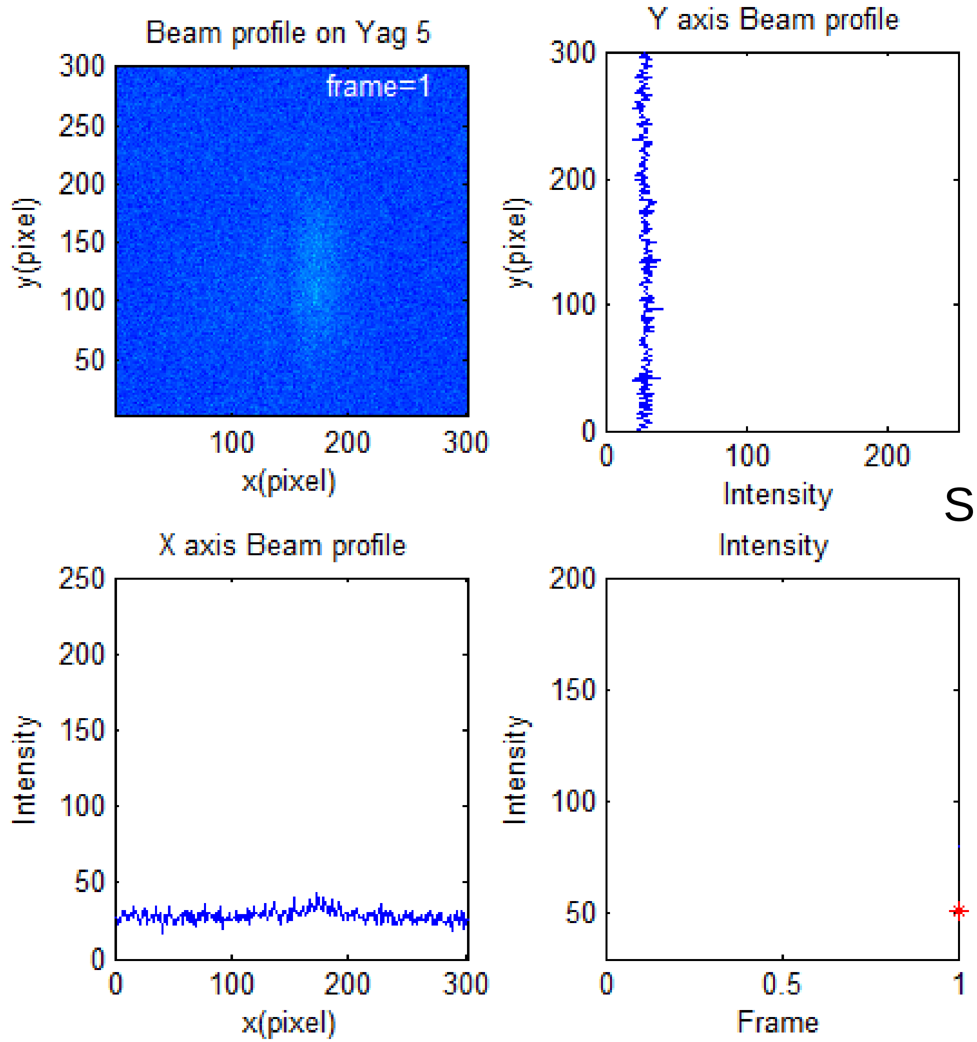
Or

Without

Top-up

FEL

Intrinsic intensity fluctuation coming from the SASE process itself, in addition of machine instability and special behavior in monochromatic beam



Si(111)

(4) Intensity stability

Storage Ring

Rock Stable !

With

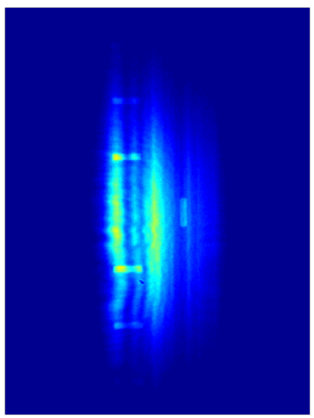
Or

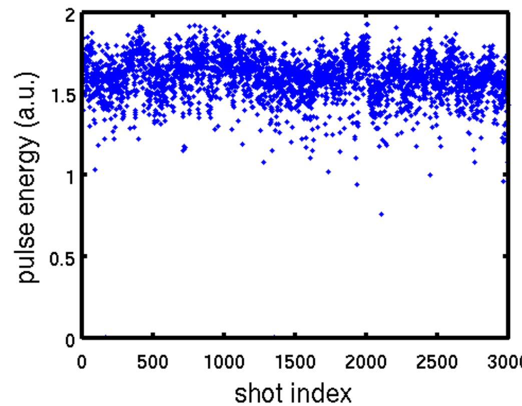
Without

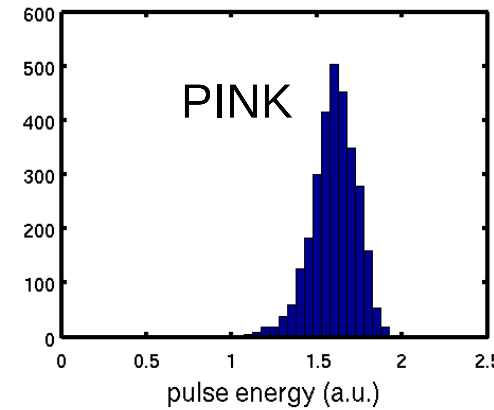
Top-up

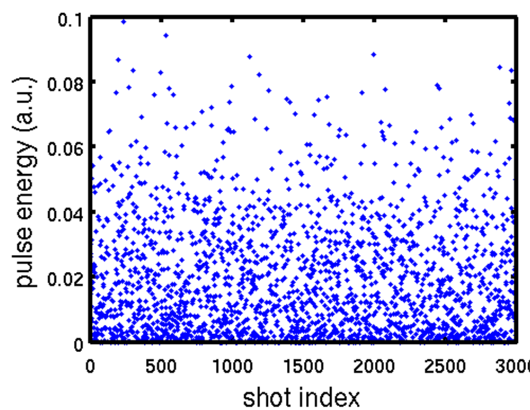
FEL

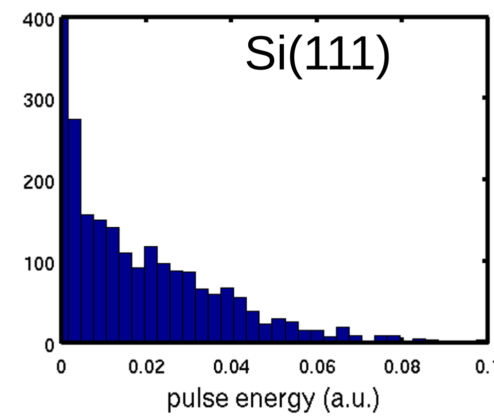
Drastic difference between pink and monochromatic beams











Courtesy of XPP

(5) Short Pulse Duration

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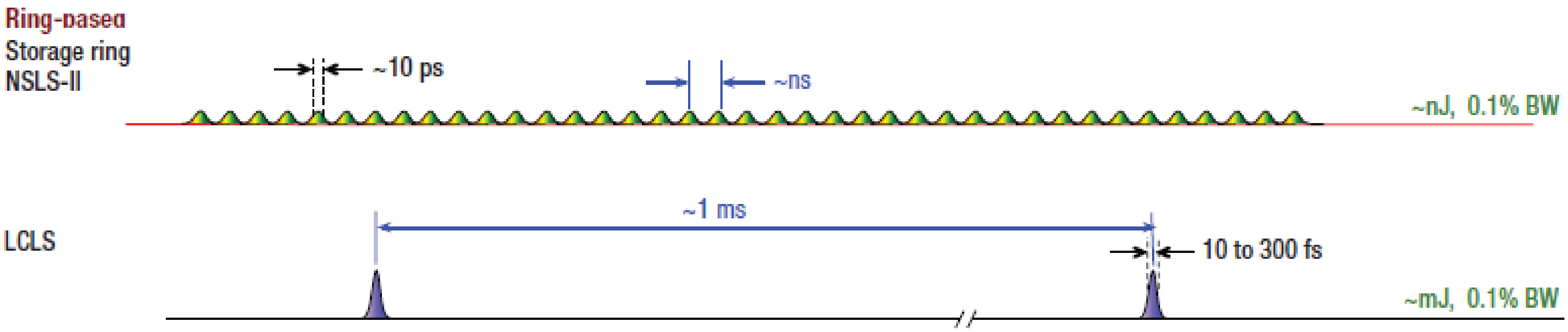
Storage Ring

Typ. 50-100ps

FEL

Below 100fs down to a couple of femtosecond.

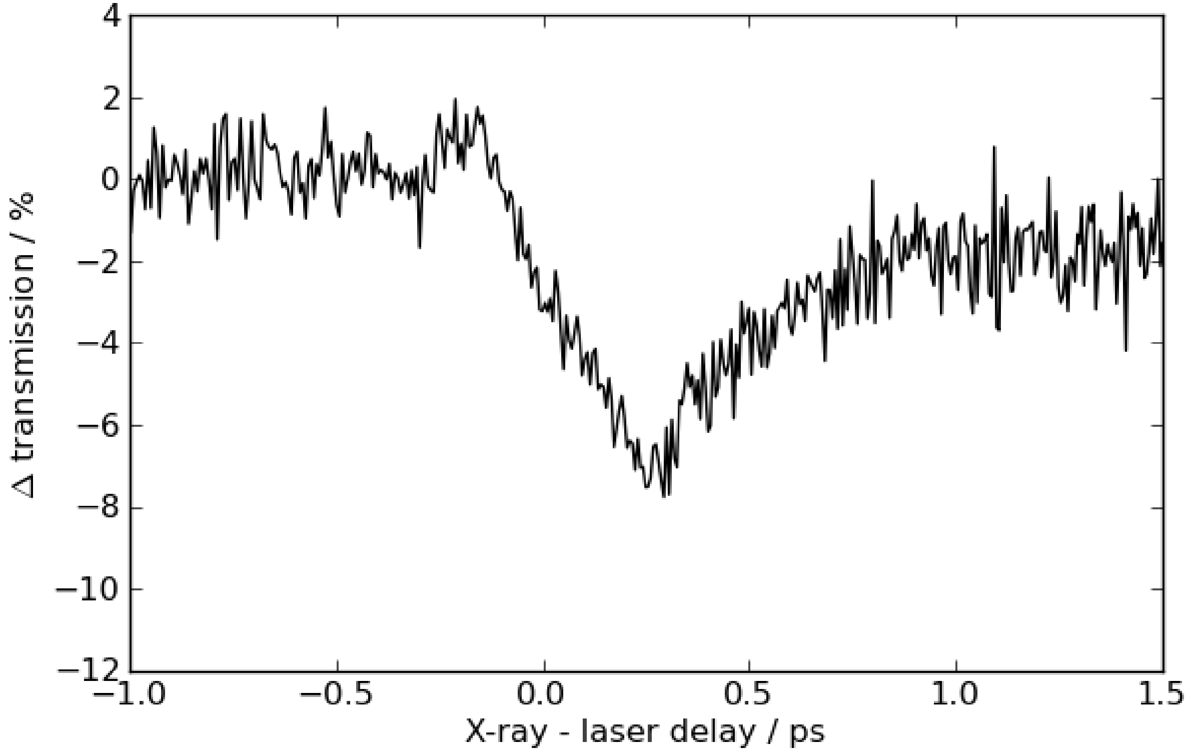
FEL sources are providing ultra-short pulse duration



(5) Temporal fluctuations

Storage Ring

FEL



(7) Energy Tunability

Storage Ring	FEL
One adjust the gap at the request of a specific user experiment.	One primarily adjust the Energy of the Linac (and all its electron optical path starting from the electron gun).
Energy range is a little bit limited by the undulator gap performances, but not much	If tunable gap undulator are available, one can then further tune the energy with the gap.
	It offers a very large flexibility in terms of the energy requested (at LCLS with a fixed gap undulator it offers energies from 500eV up to 10keV on the first harmonic)

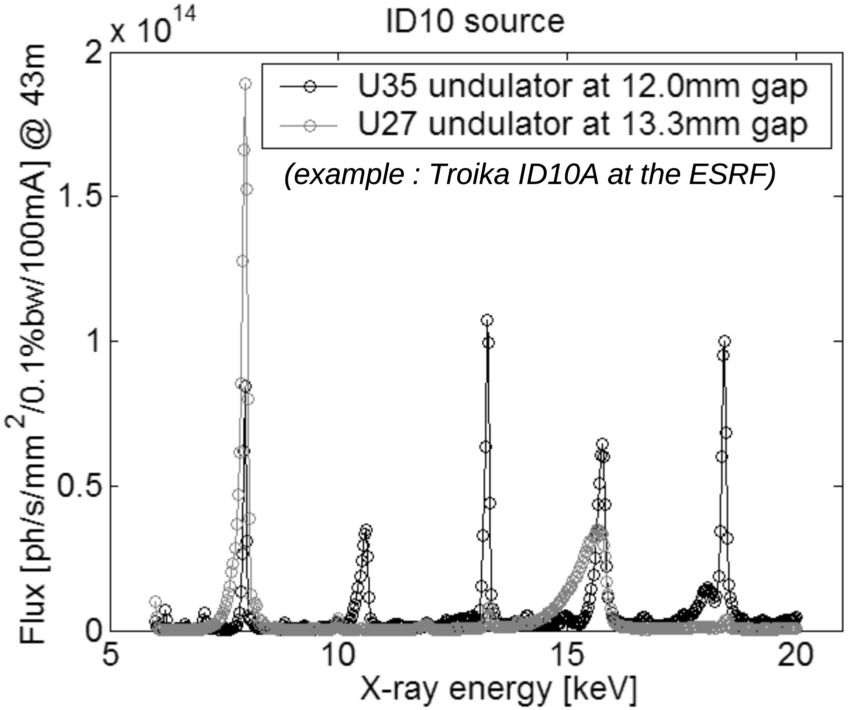
(8) E-spectrum

Storage Ring

Access to high Energies with 3rd harmonic

Stable and well define energy spectrum

1st harmonic width : 1-4%

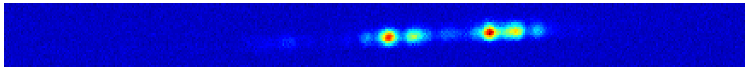


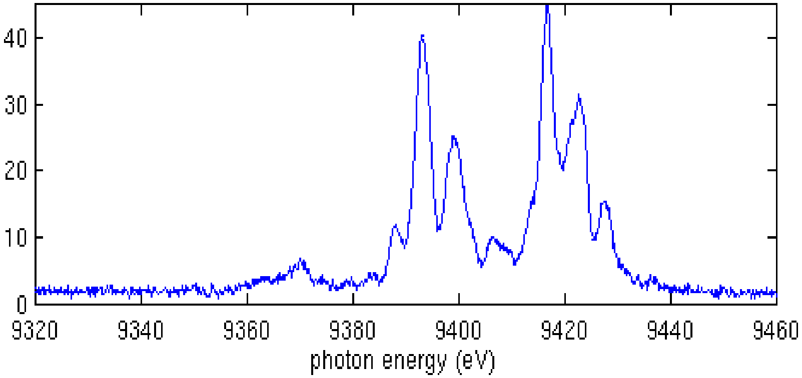
FEL

Access to high Energies with 3rd harmonic

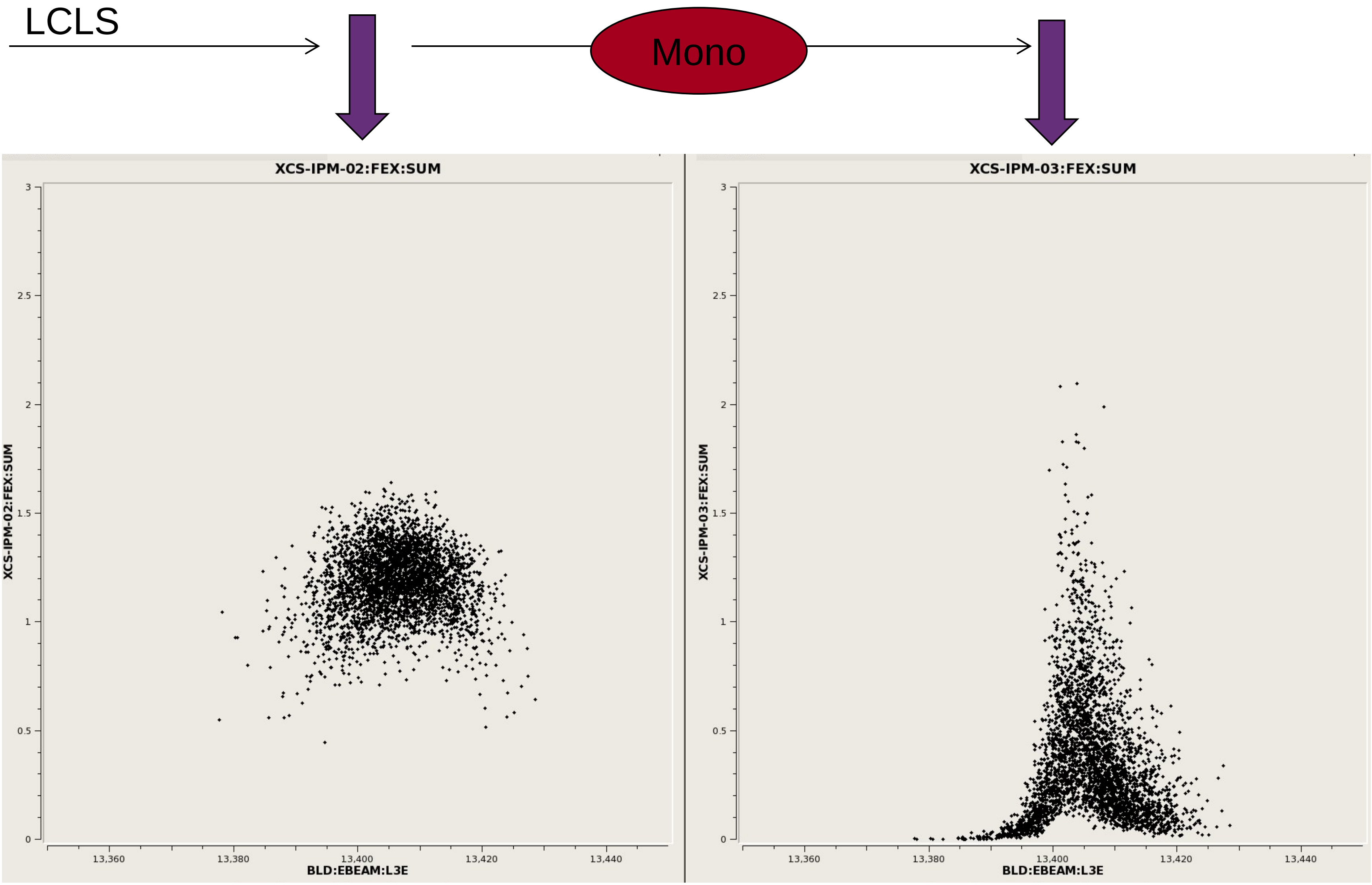
Fluctuating spectrum as a result of the energy jitter and complicated detailed E-structure

1st harmonic width : 0.2% (<dE/E>=0.7%)





(8) Spectrum Fluctuations

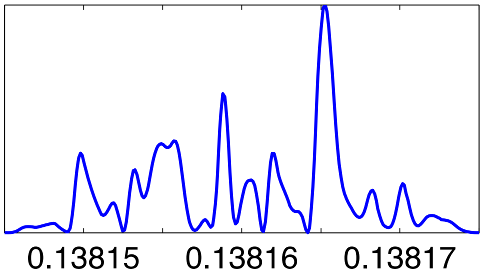


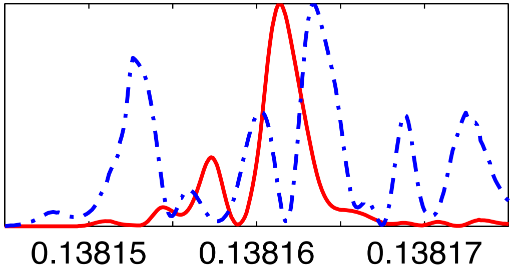
(8) E-spectrum

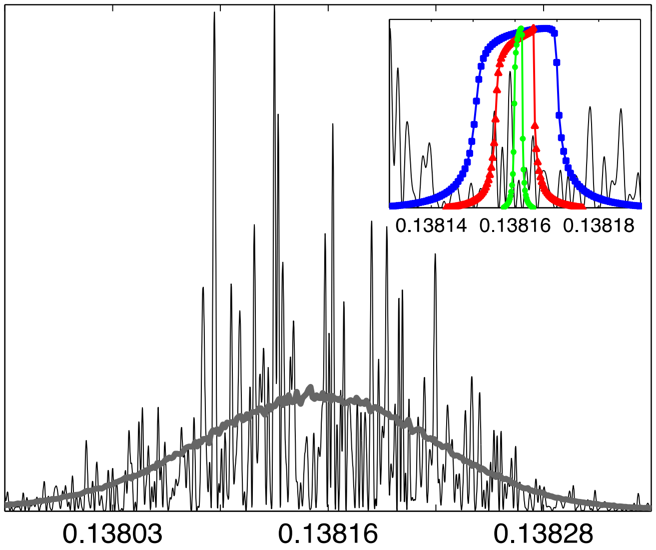
“High wavevector temporal speckle correlations at the Linac Coherent Light Source”, S. Lee,W. Roseker, C. Gutt, Z. Huang,Y. Ding, G. Gruebel and A. Robert

FEL

Optics Express **20** (9),9790 (2012)

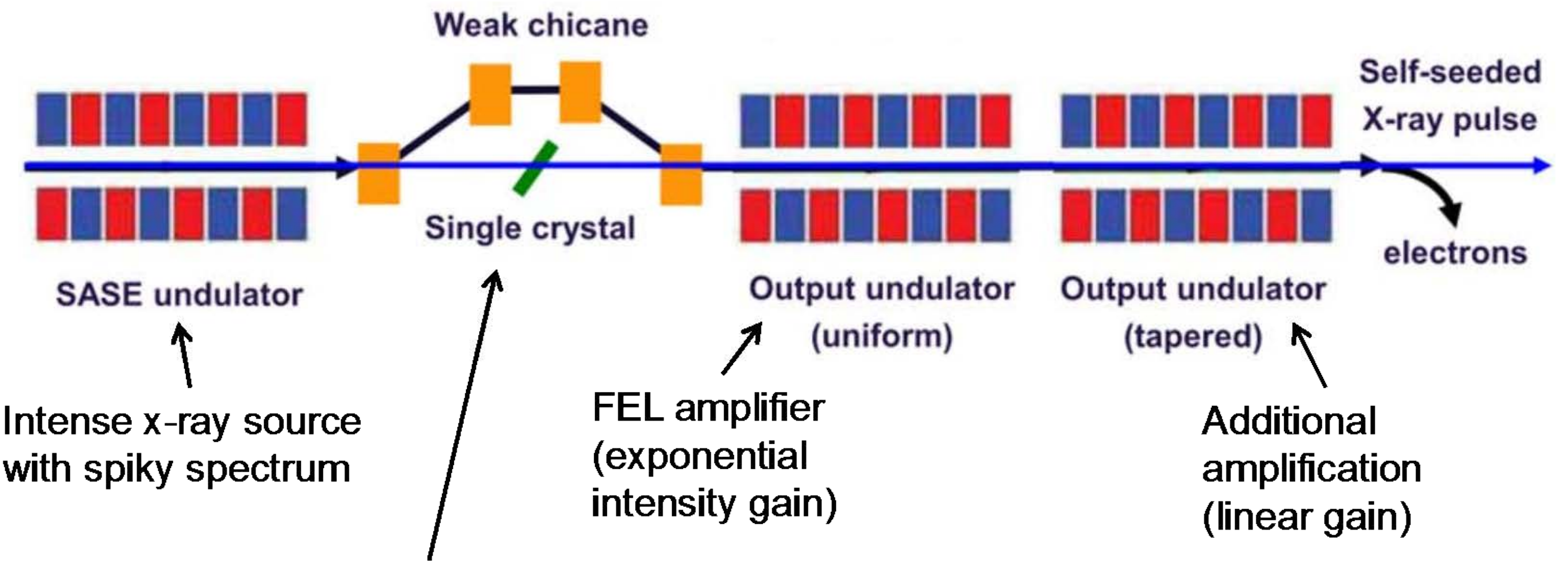




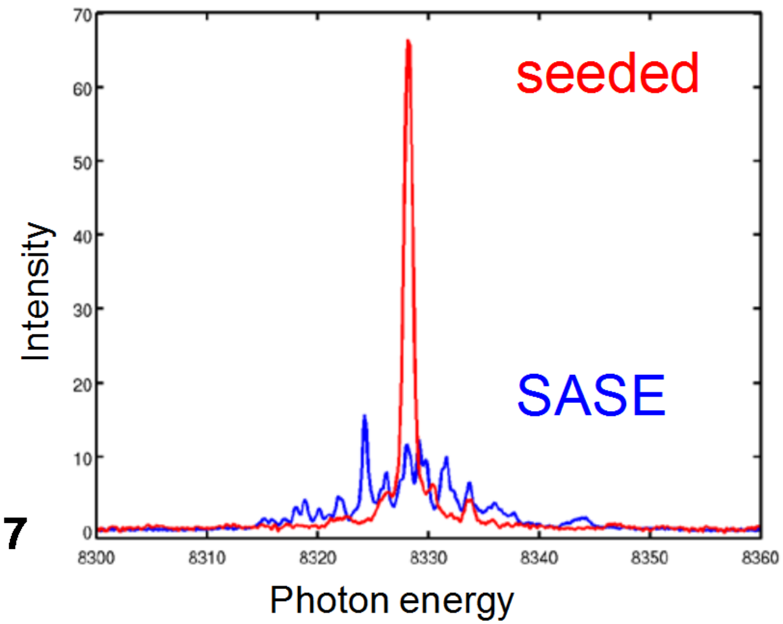


(8) E-spectrum : Self-Seeding : the FUTURE of FEL's !

SLAC



Bragg C*(400)



ΔE/E ≈ 5.10-5

As of last week :
1mJ on a good
shot

(9) Detector Efficiency

SLAC

Storage Ring

Availability of robust, efficient and diverse detectors :

- Single photon counting
- Integration
- Energy Resolved
- Large pixelated detectors
- APD's
- ...

FEL

All photons come at once ! We can only use integrating detectors :

- Use of Si diodes
- Each facility had to develop a dedicated pixelated detector program focused on specific application of using FEL measurements

(10) Degree of Coherence

Storage Ring

Limited degree of coherence because of the source size.

One is constrained to slit down the beam to typ. 20x20 micron beams in order to extract the coherent portion of the beam.

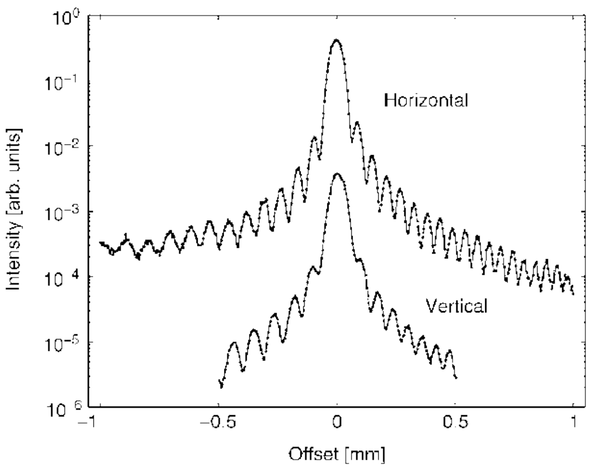


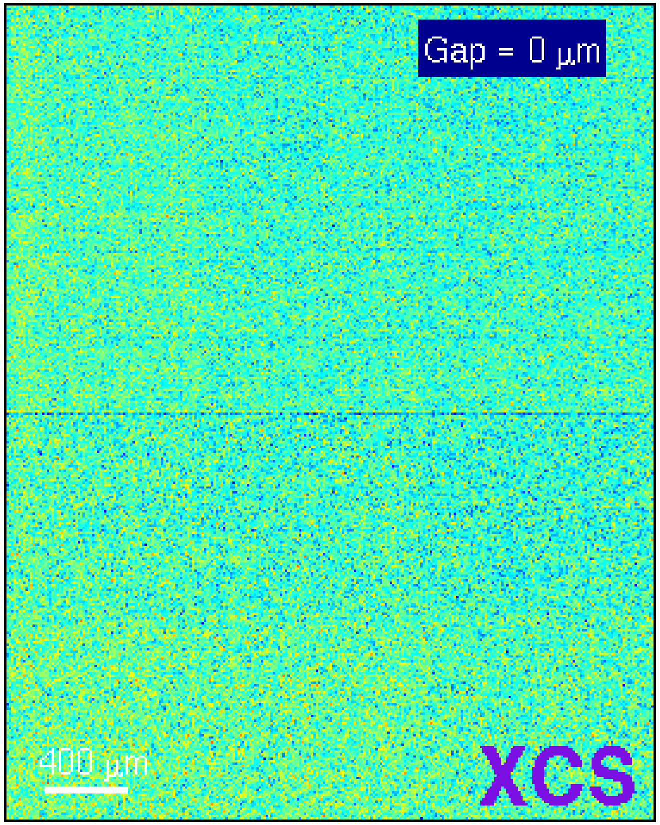
Figure 18-2

Airy fringes from a 5 × 5 mm^2 slit, recorded with I = 1.54 Å radiation at 1.5 m from the slit. The visibility V of the fringes can be quantified by $V = (I_{max}\ I_{min})/(I_{max} + I_{min})$, where I_{max} is a fringe maximum and I_{min} is an adjacent minimum

Grübel, Madsen, Robert ,XPCS , Springer (2008)

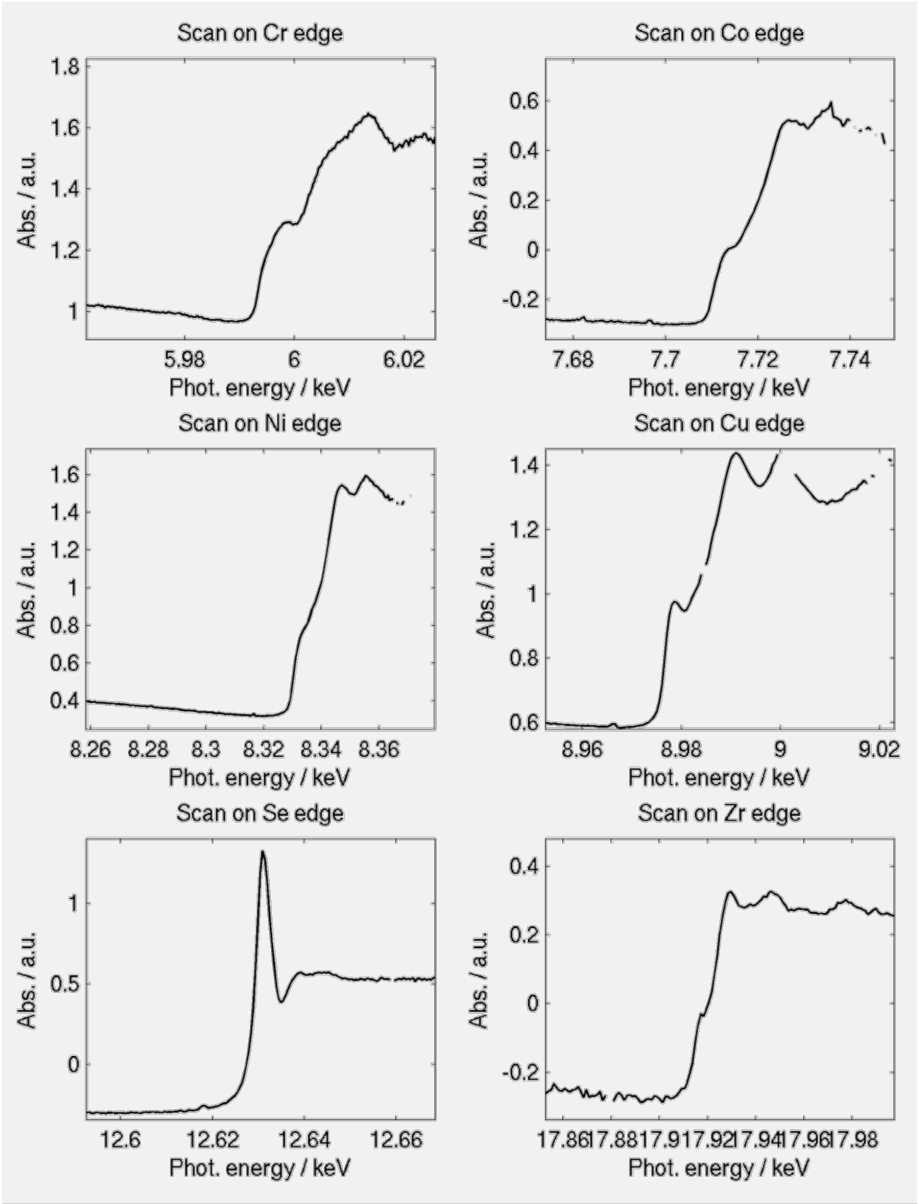
FEL

The beam is fully transversely coherent . Here is the proof !



A. Robert at al., J. Phys : Conf. Ser. **425,** 212009 (2012)

Can we really renormalize all these fluctuations ?



<u>Example</u>

EXAFS spectra measured at XPP, during the commissioning of the Si(111) channel cut monochromator

Courtesy of XPP

Now let's be honest , how does it perform ?

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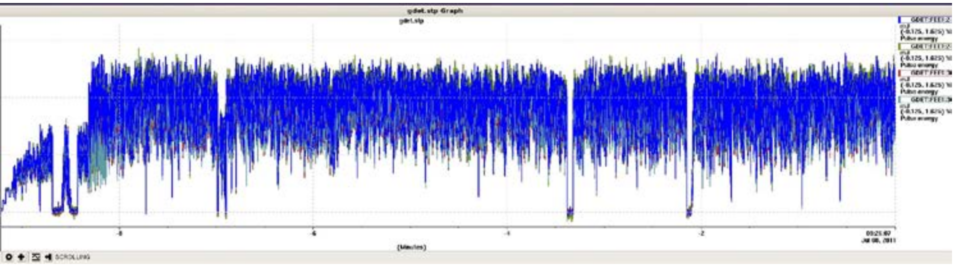
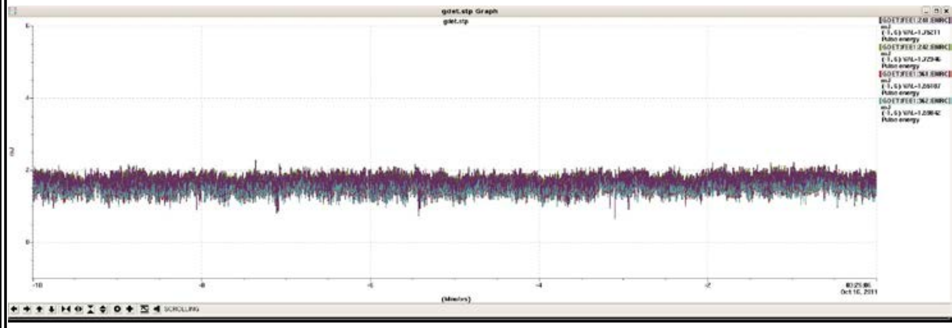
Something very different from SR sources , we have :

" BAD" days and **"GOOD" days**

- a little less than 1mJ
- Very large intensity fluctuations

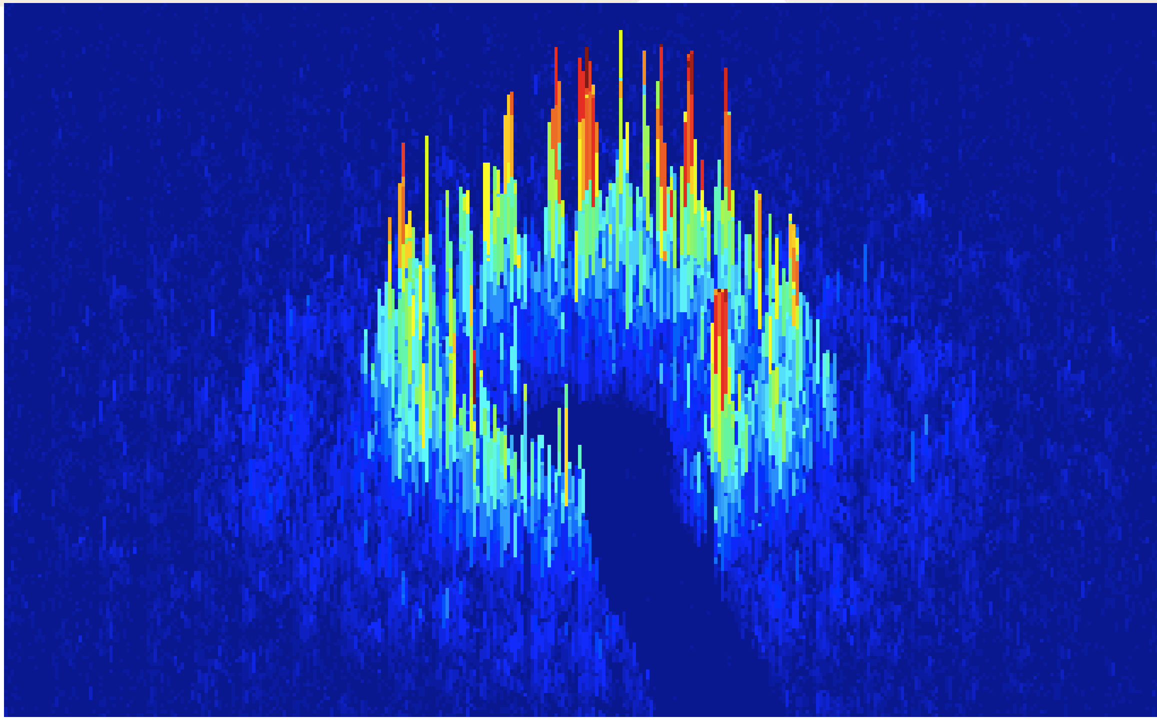


- more than 1.5mJ up to 3-3.5mJ
- 10-15% intensity fluctuation and no loss at all



How does it look ?

How does it look experimentally when it fluctuates at full speed ?

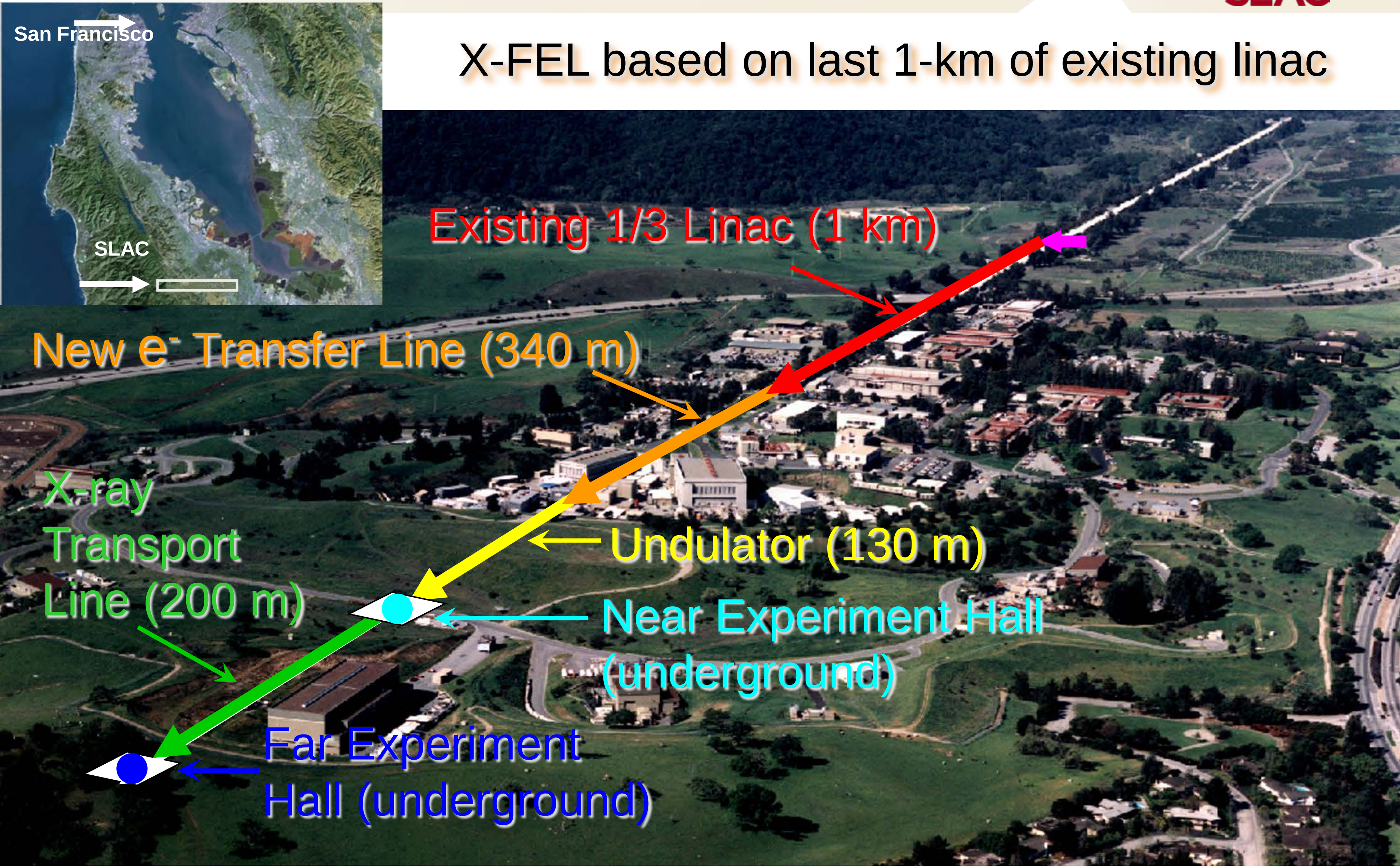


Experimental Reality Summary

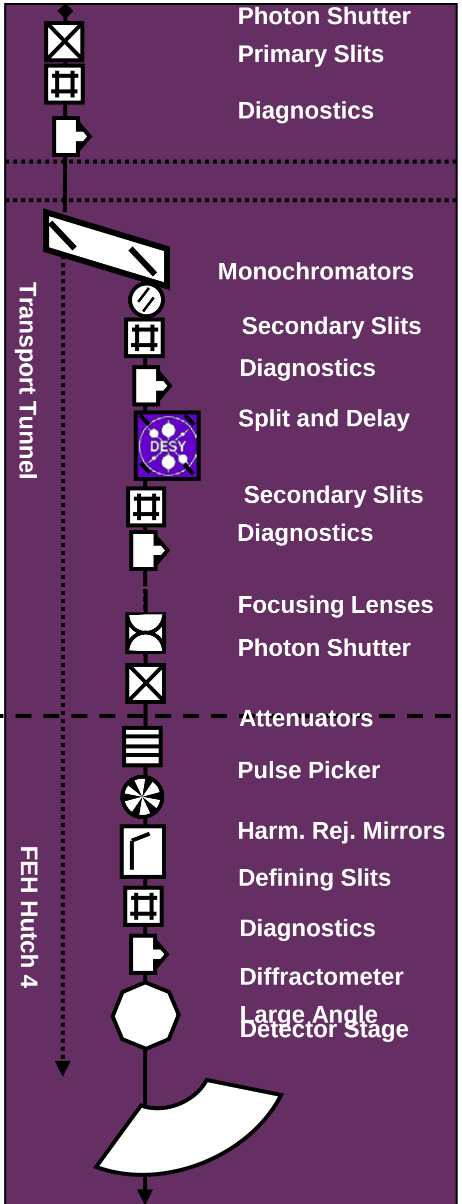
- FEL sources are fundamentally different from Storage Ring sources.
- We have to re-invent how to do experiments with hard X-rays in order to fully explore the potential of these revolutionary machines.
- The key is to develop the necessary diagnostics suite to be able to fully characterize each pulse and to correct or account for it.
- We keep developing novel schemes to use these machines and perform pioneering experiments.
- FEL’s are always mutating and offering new capabilities ever since.

Linac Coherent Light Source

X-FEL based on last 1-km of existing linac



HXR Dept : XCS Instrument

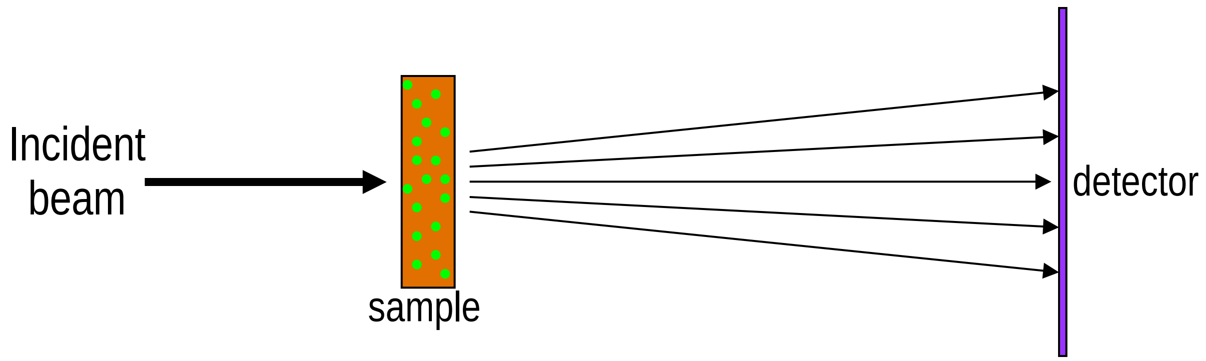


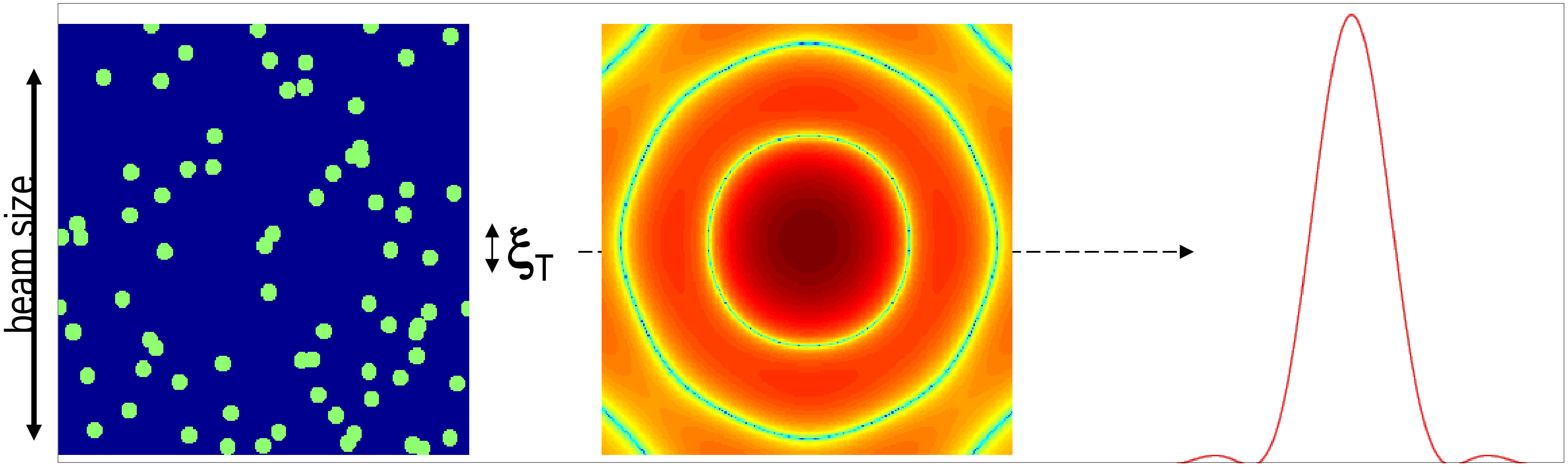
- Energy Range : 4-25keV
- Monochromators :
Si (111), (220), (511)
- Focusing capabilities with CRL's
- Fixed Energy Split and Delay
- Four-Circle Diffractometer
- Sample-detector distance: 4-8m

Now back to one of the applications of FEL's:

X-ray Photon Correlation Spectroscopy

Introduction to (Incoherent) Scattering

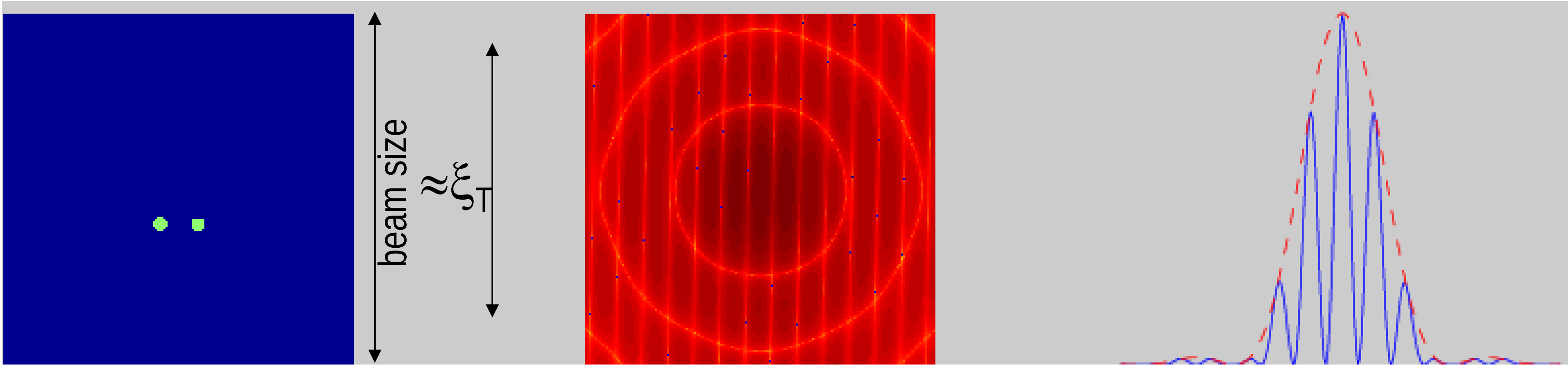




incoherent beam : beam size larger than transverse coherence length ξ_T

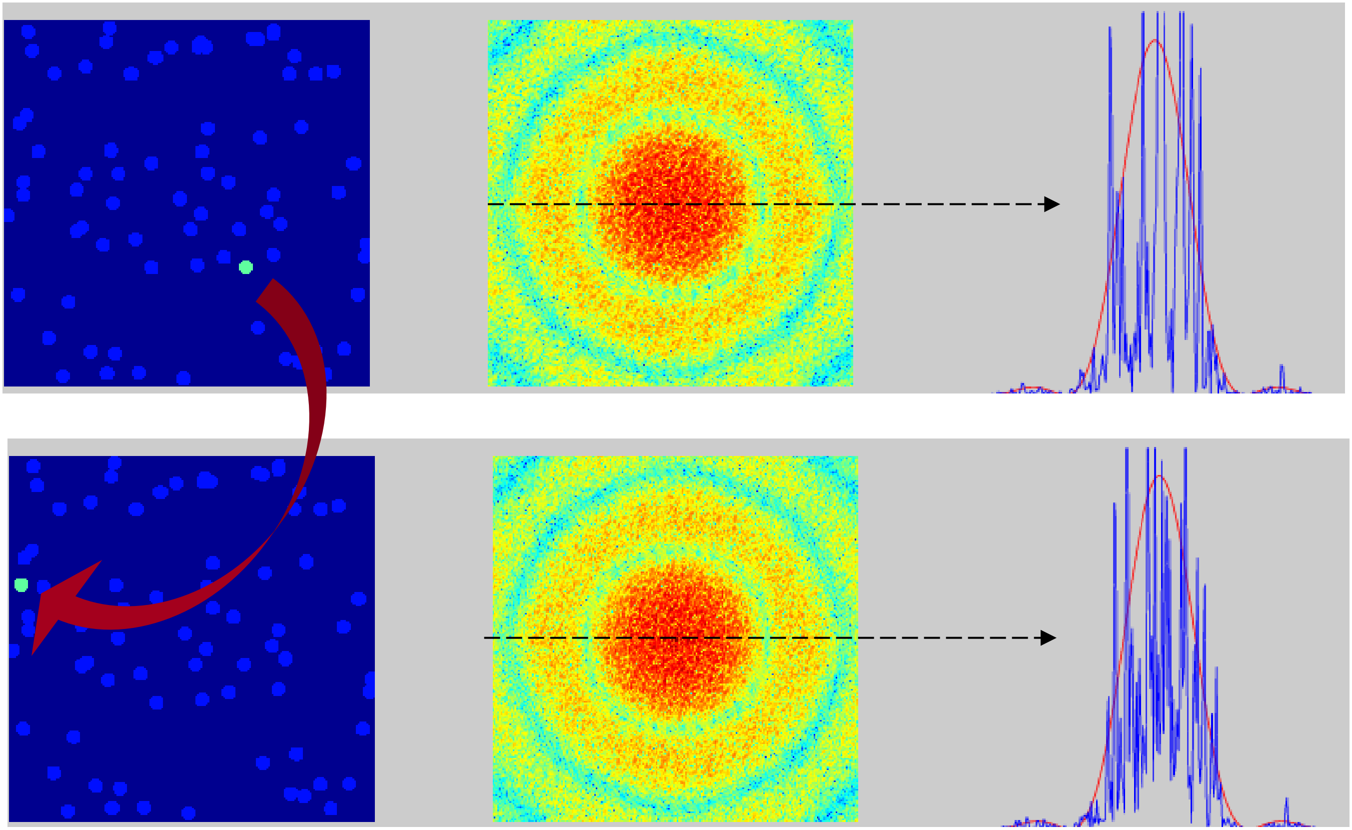
Basics on Coherent Scattering

Young’s double slit interference experiment : i.e. interference pattern



Coherent Scattering = speckles

Speckles : complicated interference pattern related to exact arrangement of the scatterers

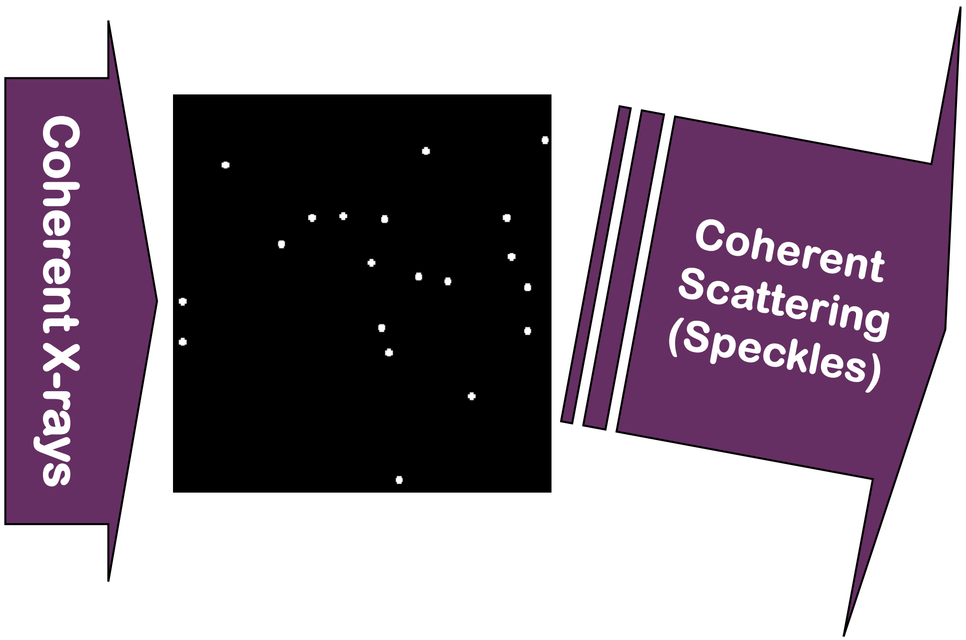


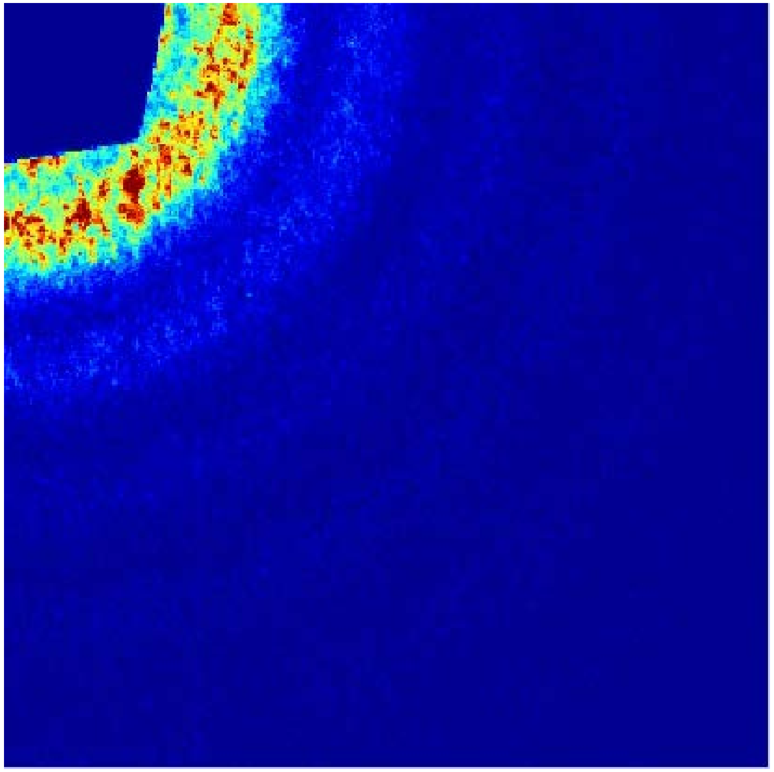
X-ray Photon Correlation Spectroscopy

SLAC

Speckles : scattering patterns produced by the coherent illumination of the sample
XPCS : observation of the time-fluctuation of speckle patterns
Characterization of the underlying dynamics of the system
XPCS is <u>independent of the scattering geometry</u> (SAXS, Diff., GI-SAXS, Refl.,…)
XPCS probes dynamical phenomena

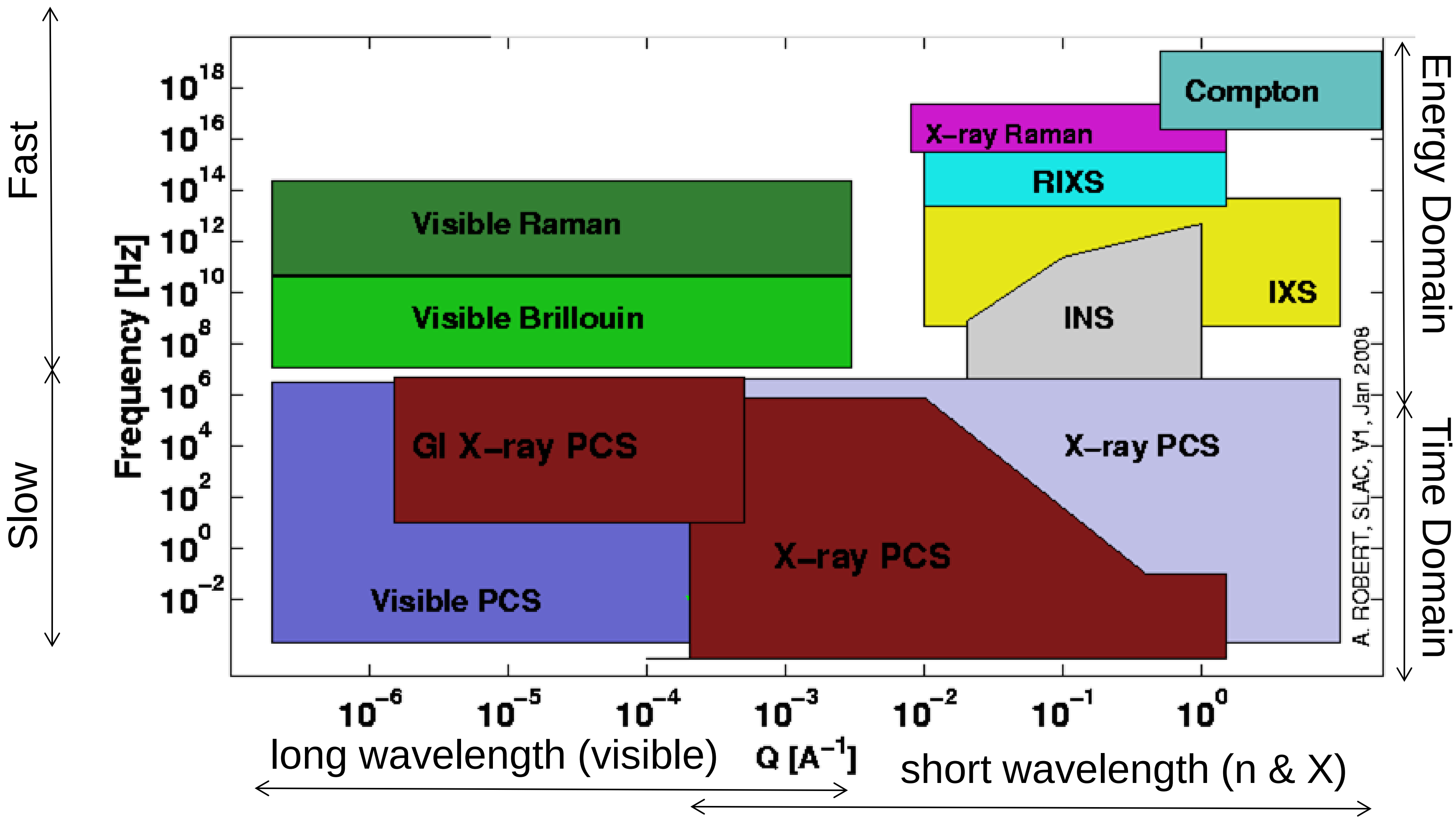
A. ROBERT, J. Appl. Cryst **40**, s34-s37 (2007)





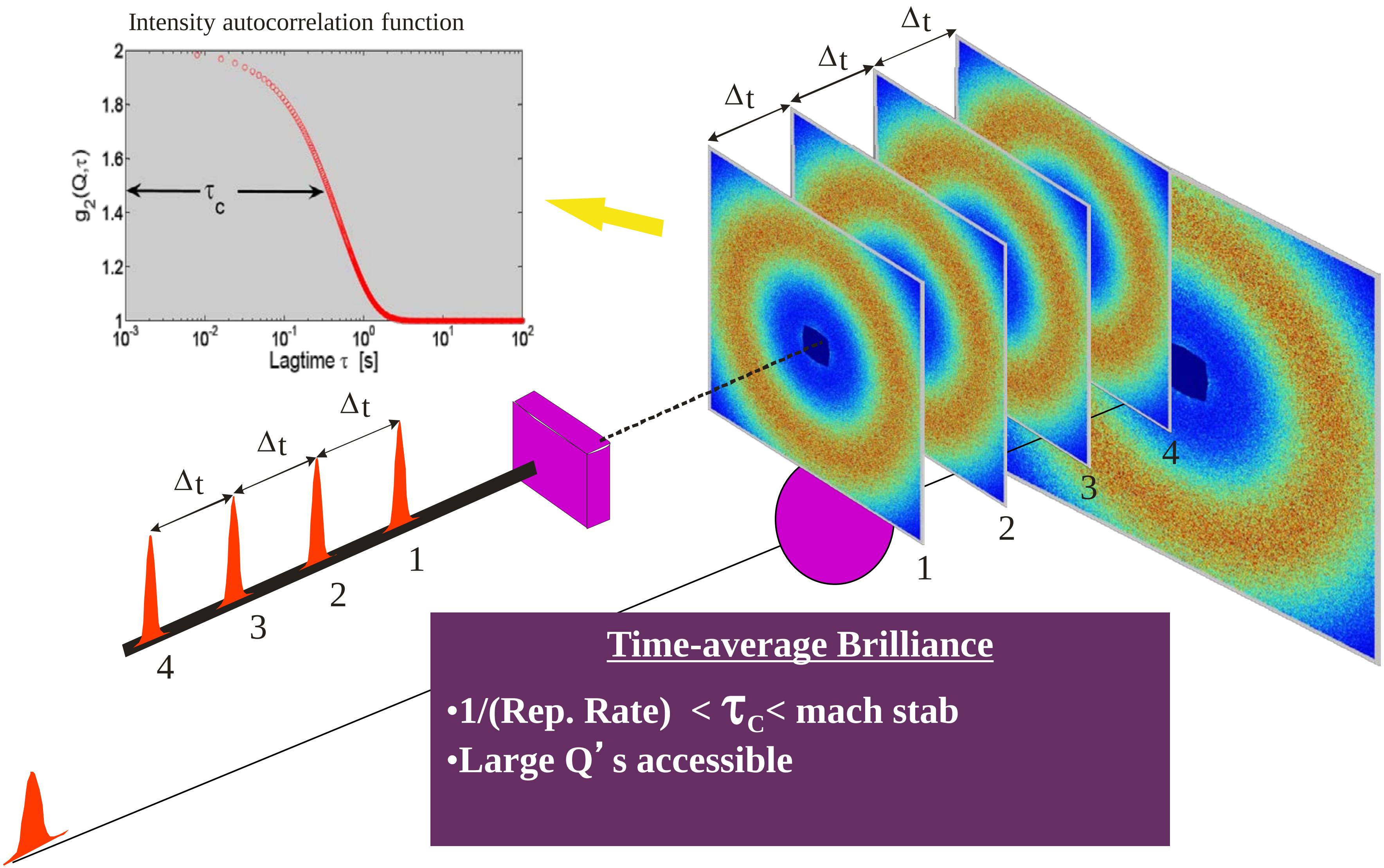
Current XPCS capabilities from 3rd gen. synchrotrons

Fundamental quantity describing the structure and dynamic of condensed matter systems is the dynamic structure factor S(Q,ω) or S(Q,t)



XPCS / Coherent Scattering at XFEL's

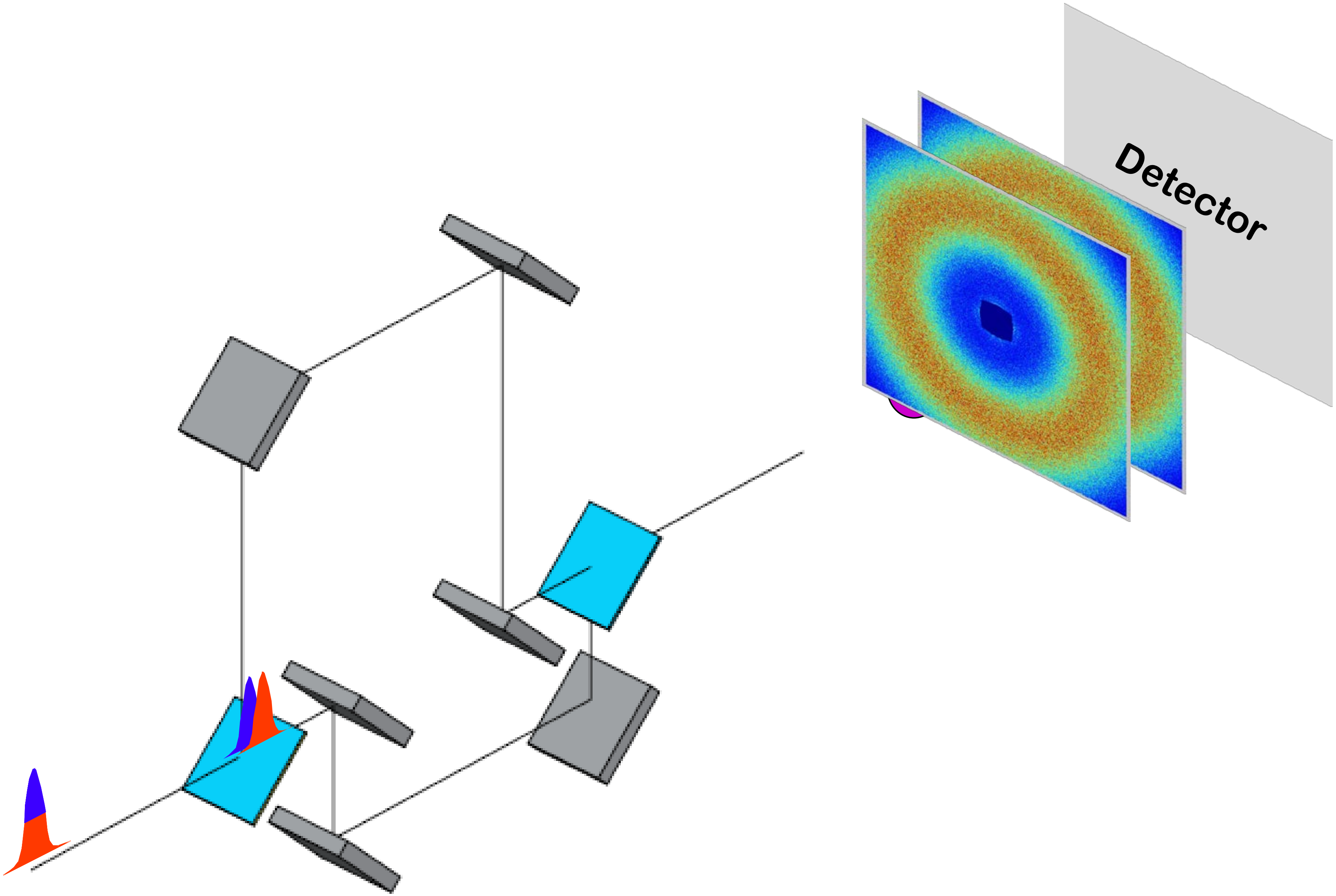
G.B. Stephenson, A. Robert, G. Grübel, Nature Materials **8** (2009), p 705



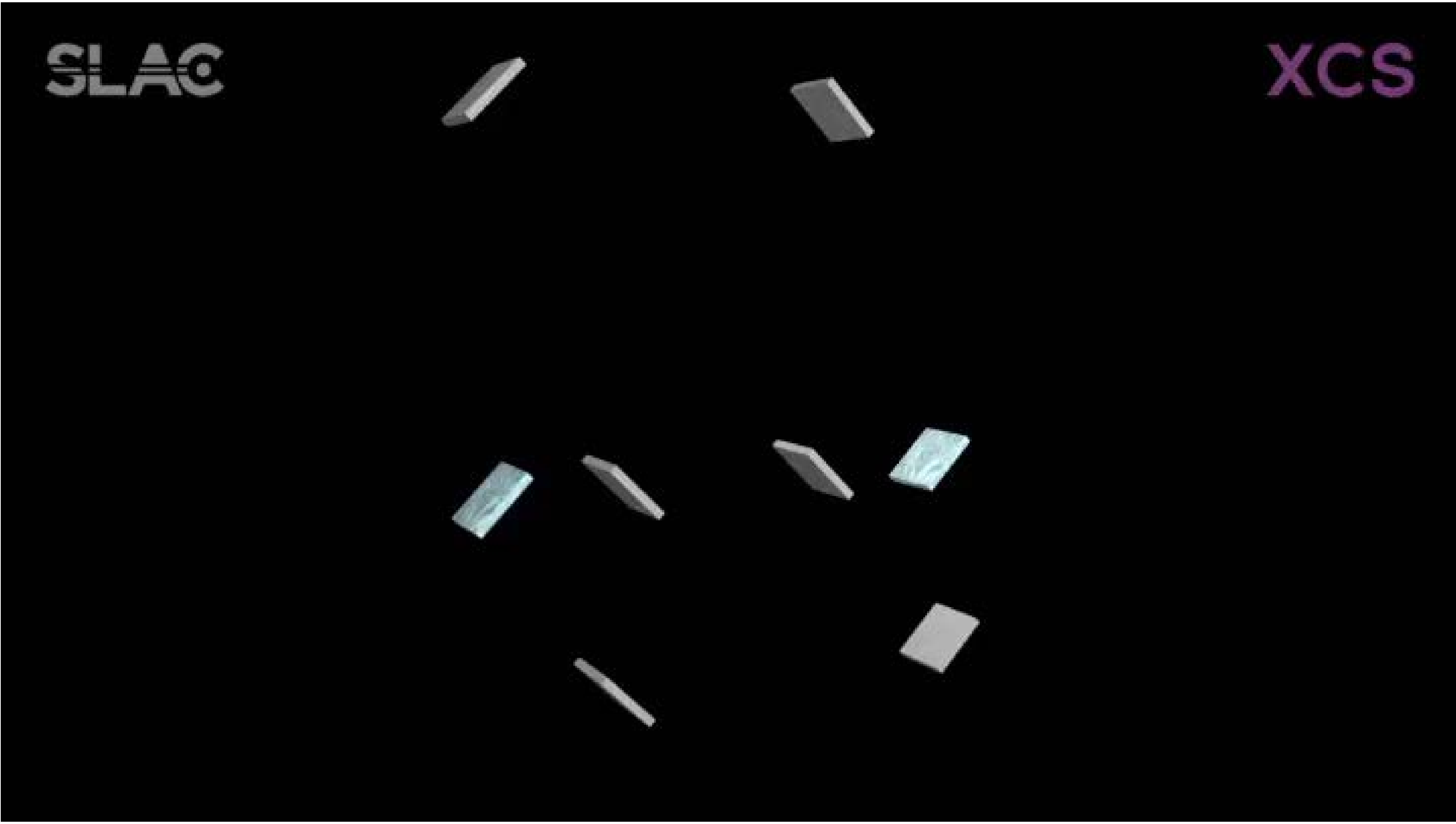
Time-average Brilliance

- 1/(Rep. Rate) < τ_C < mach stab
- Large Q's accessible

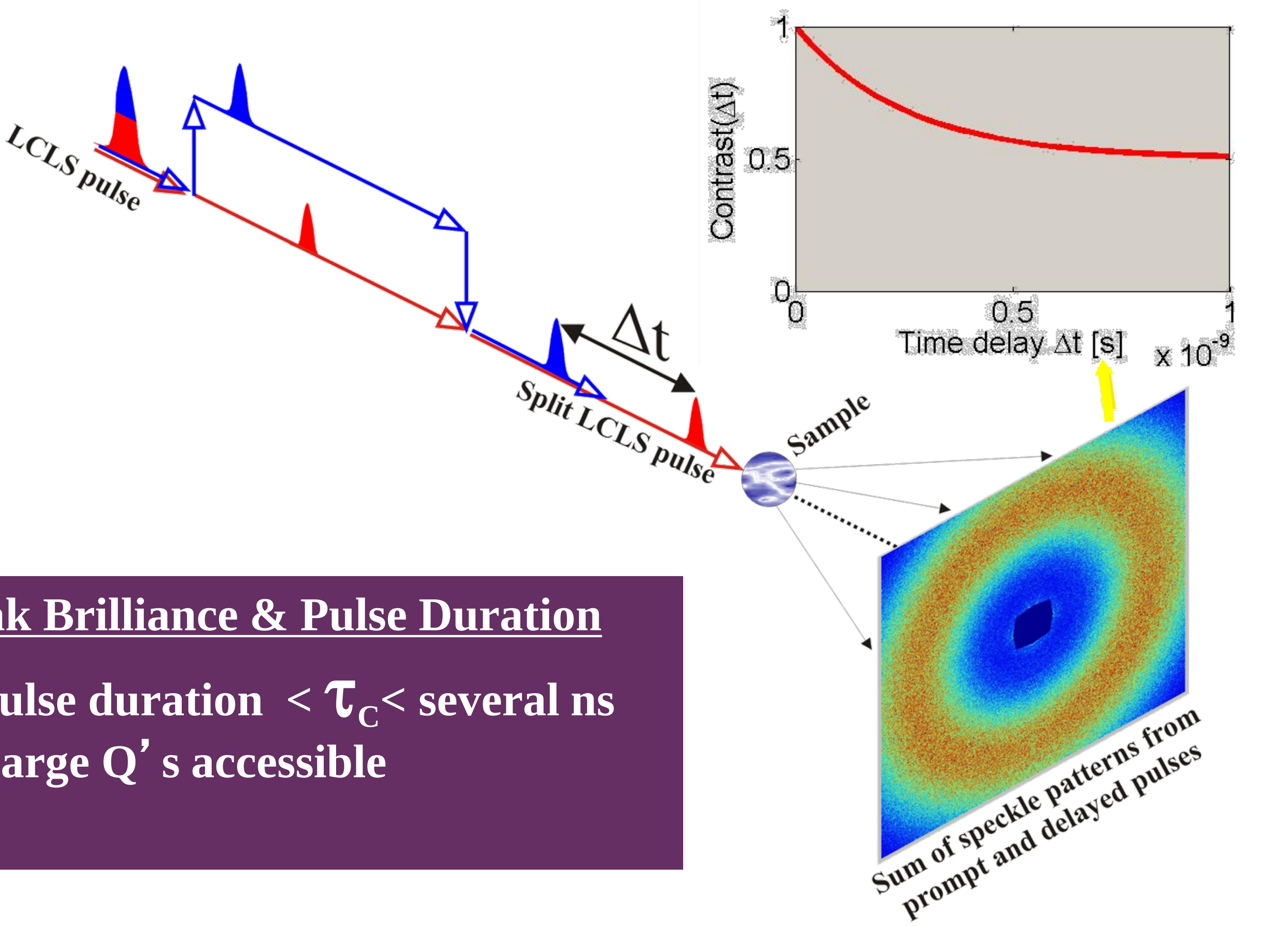
Ultrafast XPCS with a Split and Delay Unit



Ultrafast XPCS with a Split and Delay Unit



Ultrafast XCS : Split & Delay



Peak Brilliance & Pulse Duration

- Pulse duration < τ_C < several ns
- Large Q's accessible

Split and Delay technology is crucial to success in Ultrafast dynamics with XFEL's

Split and delay

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The Split and Delay is provided by DESY (Coherence group of G.

1768 OPTICS LETTERS / Vol. 34, No. 12 / June 15, 2009

Performance of a picosecond x-ray delay line unit at 8.39 keV

Wojciech Roseker,[1,*] Hermann Franz,[1] Horst Schulte-Schrepping,[1] Anita Ehnes,[1] Olaf Leupold,[1] Federico Zontone,[2] Aymeric Robert,[3] and Gerhard Grübel[1]

research papers

Journal of
Synchrotron
Radiation

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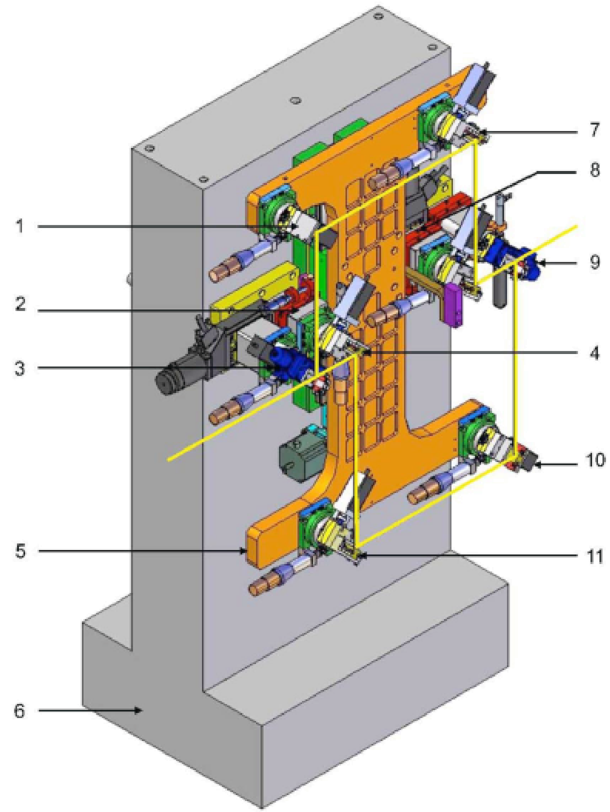
Development of a hard X-ray delay line for X-ray photon correlation spectroscopy and jitter-free pump–probe experiments at X-ray free-electron laser sources

Wojciech Roseker,[a*] Hermann Franz,[a] Horst Schulte-Schrepping,[a] Anita Ehnes,[a] Olaf Leupold,[a] Federico Zontone,[b] Sooheyong Lee,[a,c] Aymeric Robert[c] and Gerhard Grübel[a]

5 January 2009 / Vol. 17, No. 1 / OPTICS EXPRESS 55

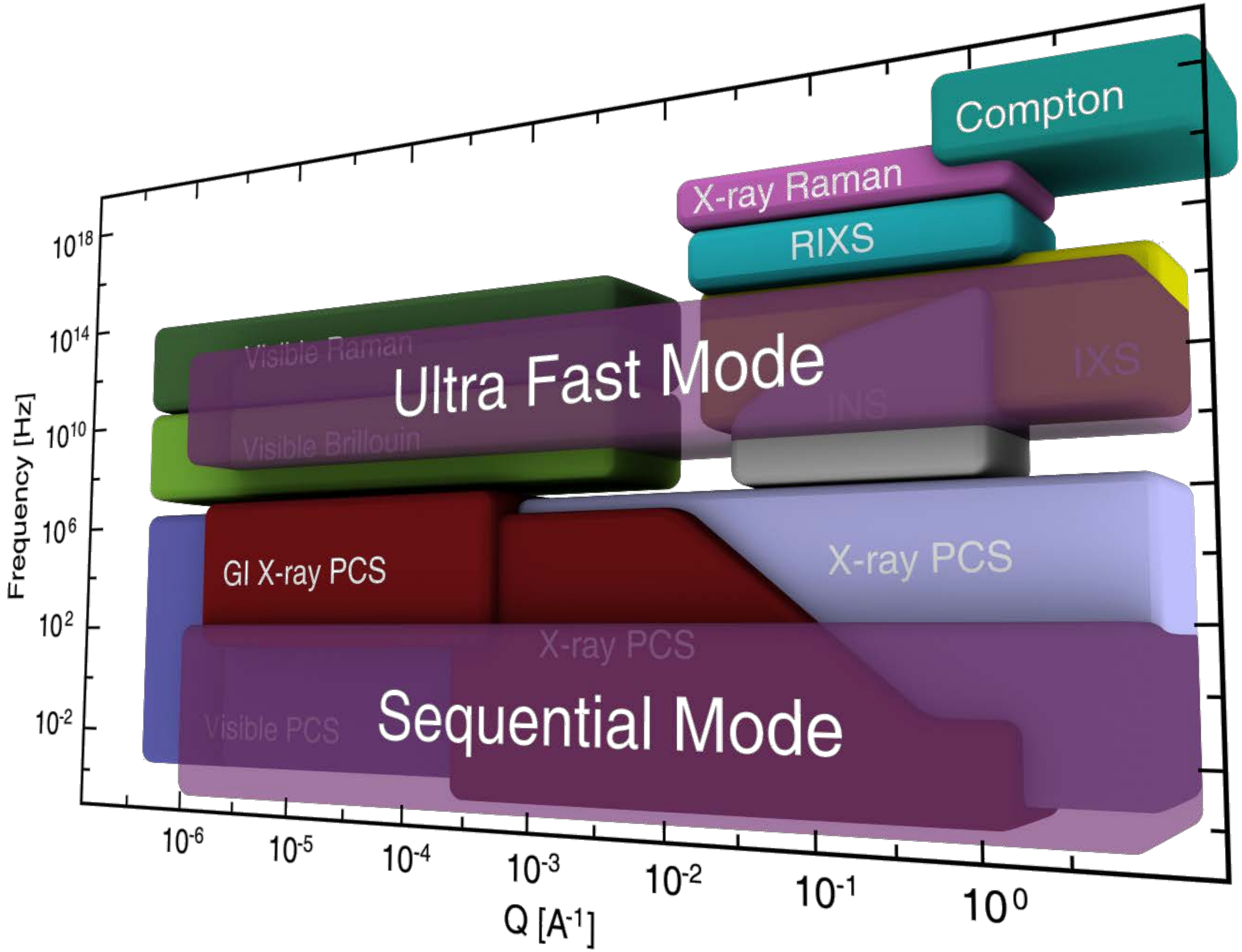
Measuring temporal speckle correlations at ultrafast x-ray sources

C. Gutt[1*], L.-M. Stadler[1], A. Duri[1], T. Autenrieth[1], O. Leupold[1], Y. Chushkin[2], G. Grübel[1]



Uses Si(511) crystals with 90 degrees scattering angles at 8.39keV

XPCS capabilities at LCLS



Early Coherence result

PRL 108, 024801 (2012) PHYSICAL REVIEW LETTERS week ending 13 JANUARY 2012

Single Shot Spatial and Temporal Coherence Properties of the SLAC Linac Coherent Light Source in the Hard X-Ray Regime

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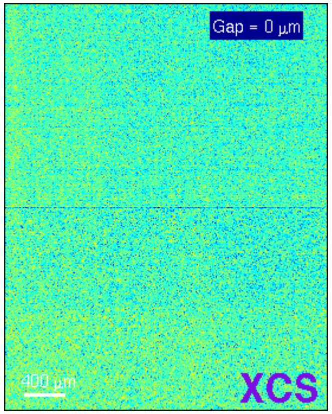
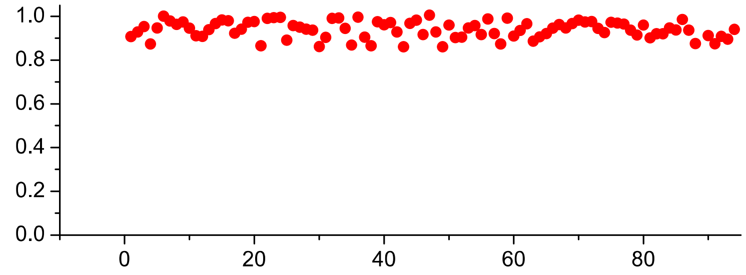
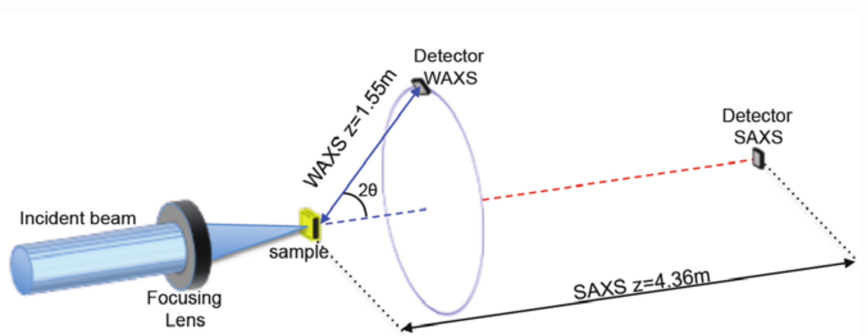
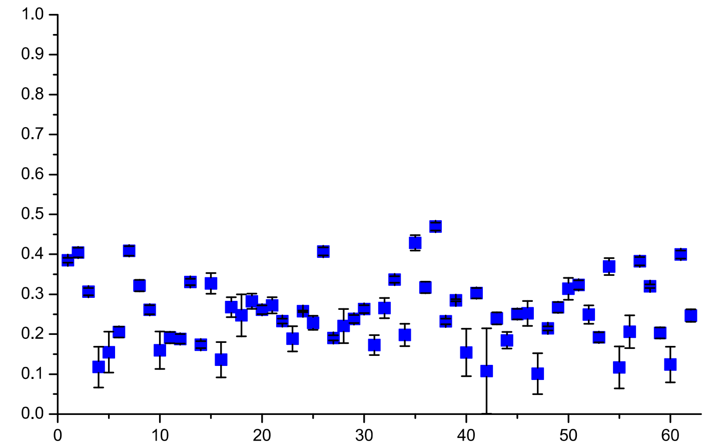
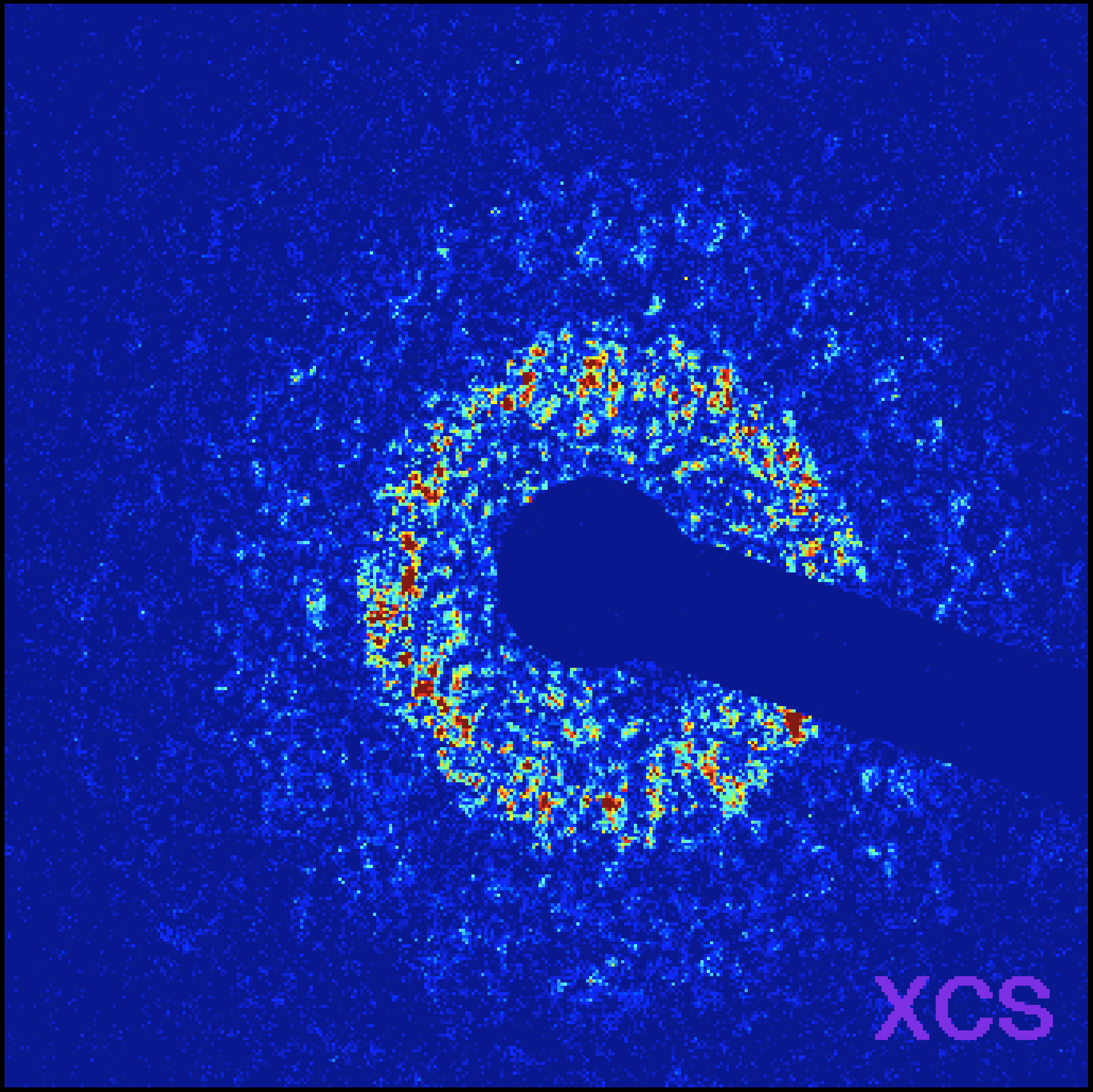








First Speckles at XCS



Coherence Characterization II

PRL 109, 185502 (2012) PHYSICAL REVIEW LETTERS week ending 2 NOVEMBER 2012

High Contrast X-ray Speckle from Atomic-Scale Order in Liquids and Glasses

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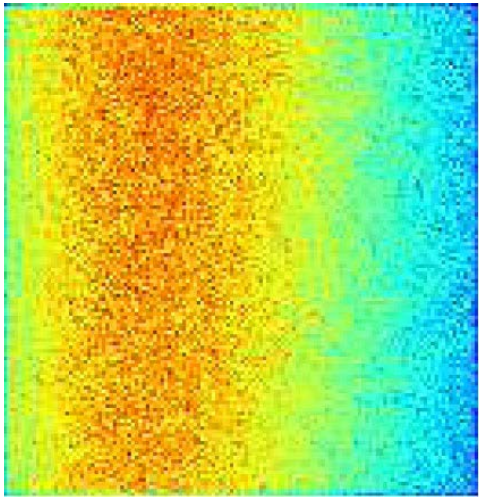

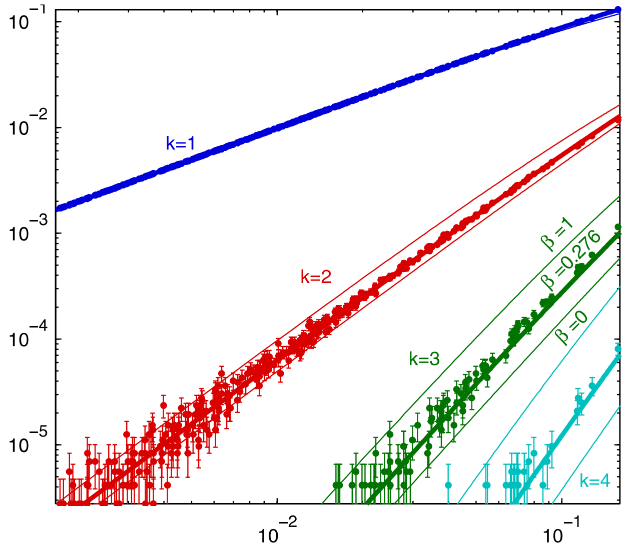

Where are we at ?

- XPCS (similar to SR) has been recently demonstrated on various systems
  - In the small angle regime with soft matter systems
  - At wide angle with atomic resolution

- Ultra-fast XPCS is still not demonstrated but coming soon

Supplement

Experimental Tutorial : SR vs. FEL

SLAC

REVIEW ARTICLE | FOCUS
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nature photonics

X-ray free-electron lasers

Brian W. J. McNeil[1*] and Neil R. Thompson[2]

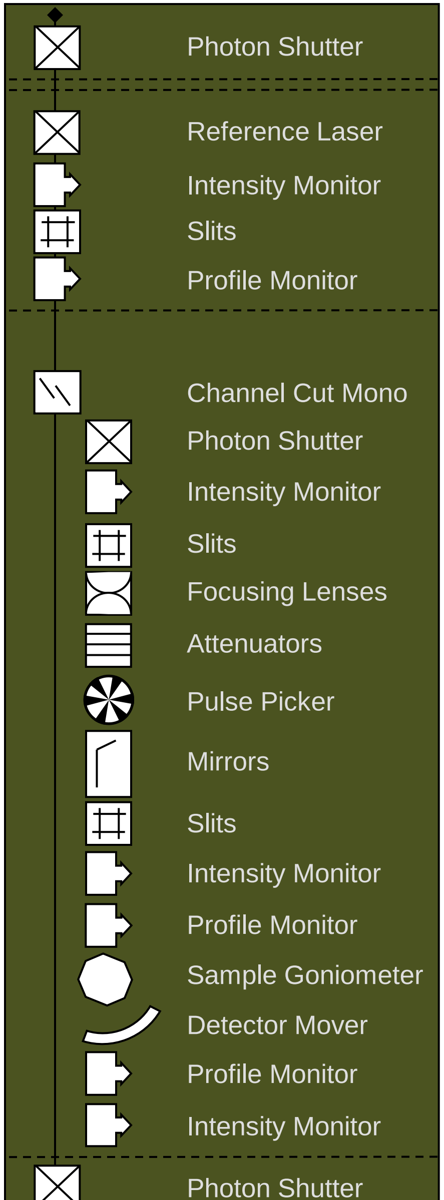
With intensities 10^8–10^{10} times greater than other laboratory sources, X-ray free-electron lasers are currently opening up new frontiers across many areas of science. In this Review we describe how these unconventional lasers work, discuss the range of new sources being developed worldwide, and consider how such X-ray sources may develop over the coming years.

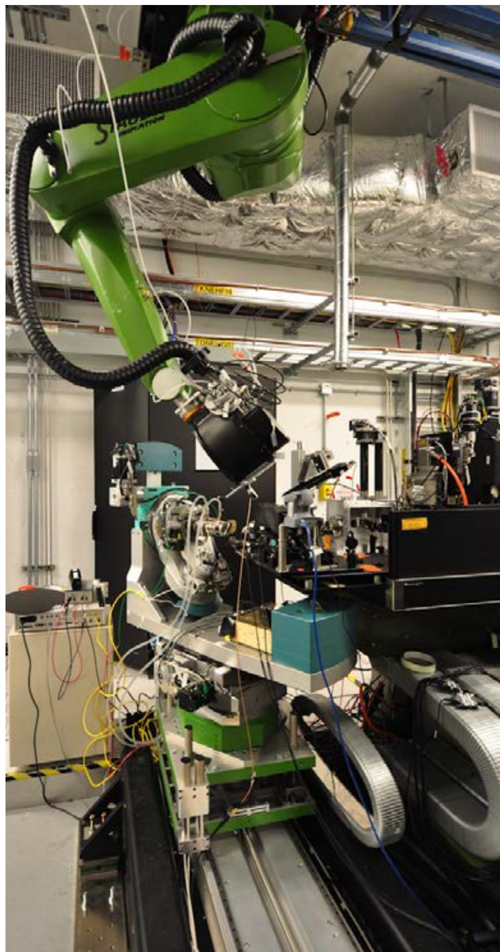
Table 1 | Current X-ray facilities that are either operational (O), under construction (C) or undergoing advanced technical design work (D). 'Accelerator technology' refers to either normal conducting (NC) or superconducting (SC) accelerating cavities. The wavelength given is the minimum proposed. Emittance values (ε_n) are estimates for C- and D-type facilities.

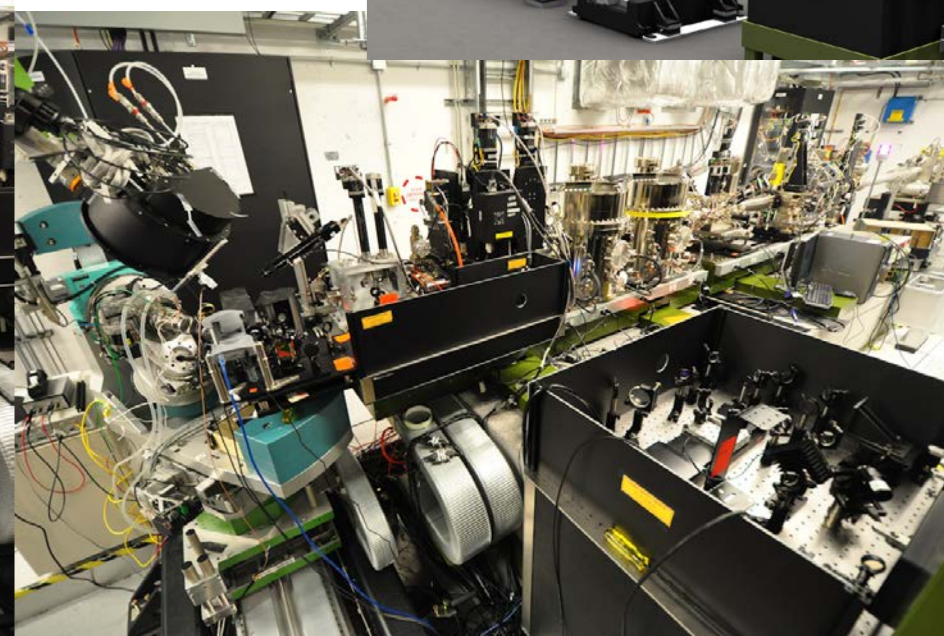
Name	Location	Status	Type	Energy (GeV)	ε_n (μm)	λ_{min} (nm)	Maximum pulses per second	Radiation polarization control
LCLS[51]	USA	O	NC	14	1	0.12	120	No
FLASH[101]	Germany	O	SC	1.2	<2	4.45	8×10^3	No
XFEL[52]	Germany	C	SC	17.5	1.4	0.10	27×10^3	Yes
XFEL/SPring-8[53]	Japan	C	NC	8	0.8	0.10	60	No
FERMI@Elettra[57]	Italy	C	NC	1.7	1	4	50	Yes
SwissFEL[56]	Switzerland	D	NC	6	0.4	0.1	100	Yes
PAL XFEL[102]	Korea	D	NC	10	1	0.1	60	No
LCLS-II[103]	USA	D	NC	14	1	0.6	120	Yes
SPARX[104]	Italy	D	NC	2.4	1	0.6	100	Yes
FLASH-II[54]	Germany	D	SC	1.2	1–1.5	4	10	No

HXR Dept : XPP Instrument , 1st Hard X-ray LCLS Inst.

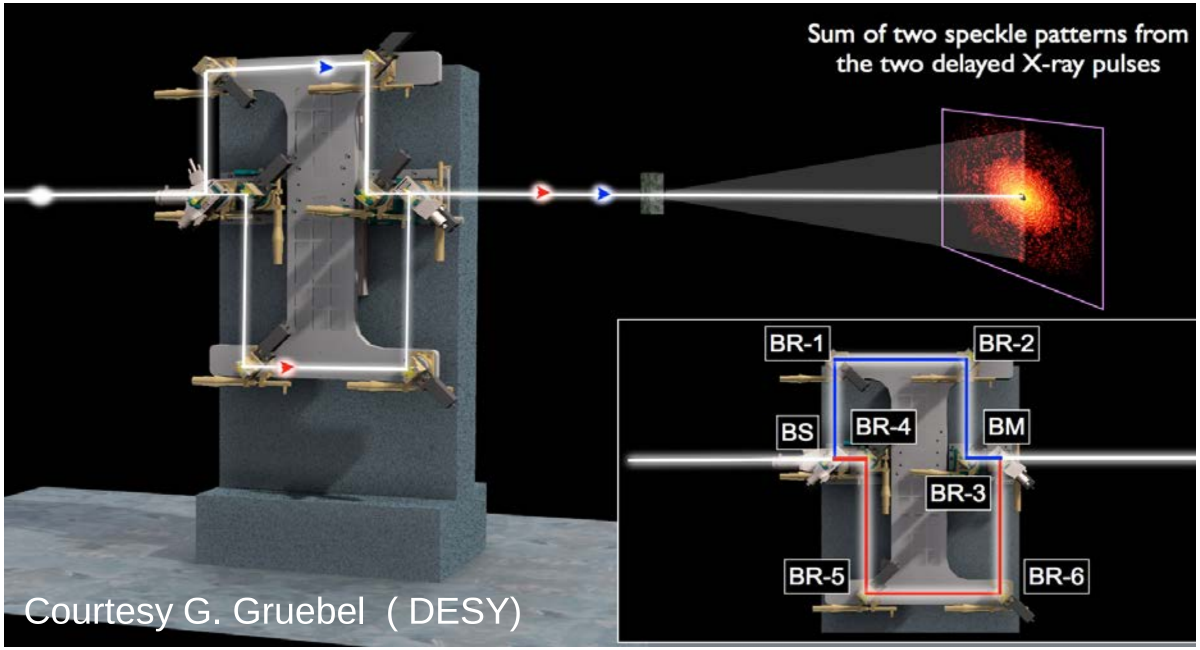
- Energy Range : 4-25keV
- Monochromators :Si (111), (220)
- Focusing capabilities with CRL's
- Flexible Robot arm
- Four-Circle Diffractometer
- Pump Laser system







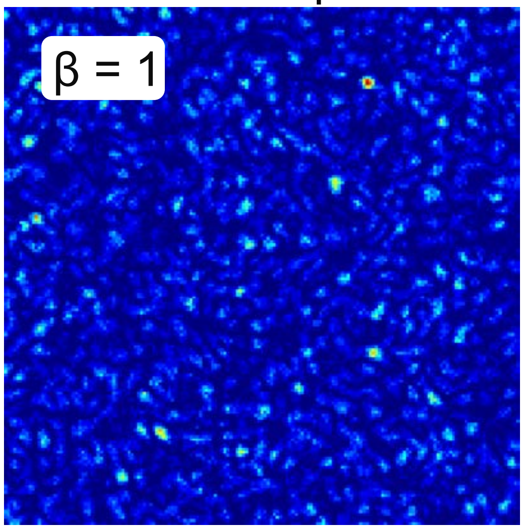
XCS Inst. : Split and Delay Experiment Concept



- Technology in development (DESY/LCLS)
- Measuring the sum of two single shot speckle patterns separated by ultra fast time scales to probe equilibrium dynamics in the picosecond timescales

Atomic Speckles

Coherent Speckle

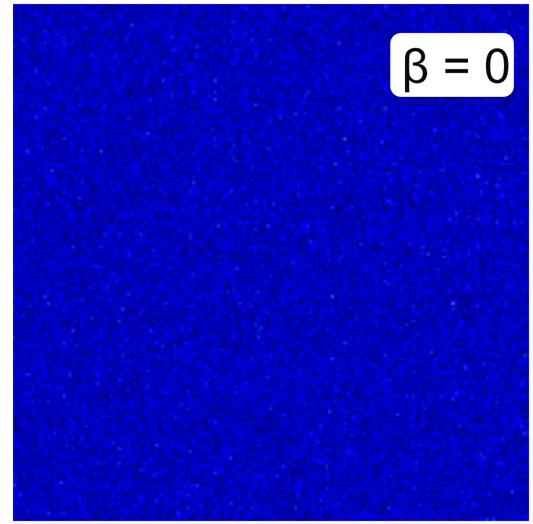


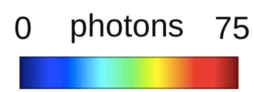
Contrast,

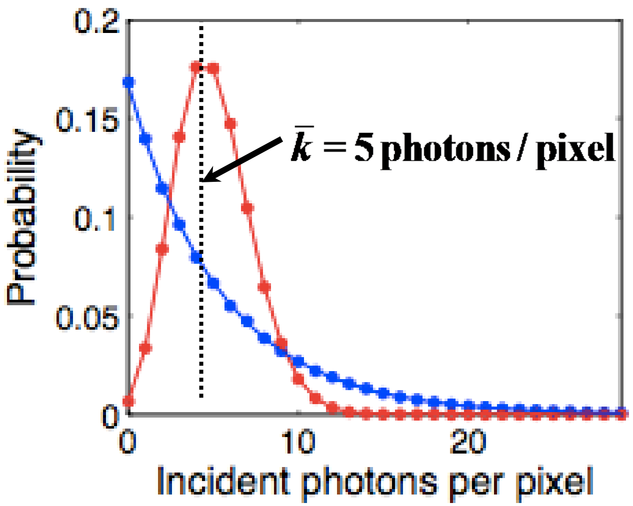
$$\beta \equiv \frac{1}{M}$$

Mean count rate:
5 photons / pixel

Poisson "Shot Noise"







Observed probabilities

- Poisson image (red)
- Coherent speckle image (blue)

Probability distribution functions

Poisson: $P_{pois}(k,\bar{k}) = \bar{k}^k e^{-\bar{k}} / k!$

Negative Binomial (M=1):

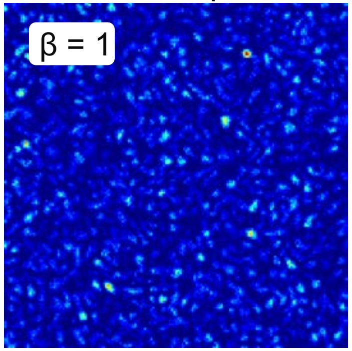
$$P_{NB}(k,\bar{k},M) = \frac{\Gamma(k+M)}{\Gamma(M)\Gamma(k+1)}\left(1+\frac{M}{\bar{k}}\right)^{-k}\left(1+\frac{\bar{k}}{M}\right)^{-M}$$

Atomic Speckles

Courtesy P. Fuoss

SLAC

Coherent Speckle



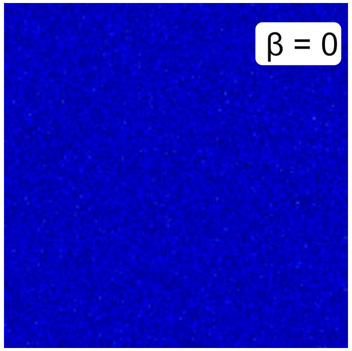
Contrast,

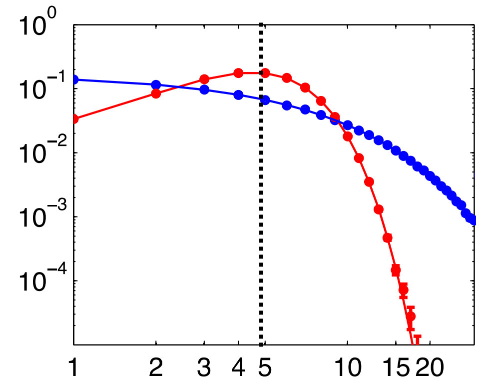
$$\beta \equiv \frac{1}{M}$$

Mean count rate:
5 photons / pixel

0 photons 75

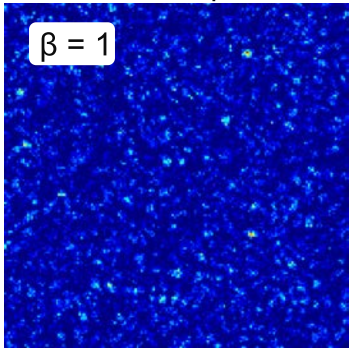
Poisson "Shot Noise"





k=5

Coherent Speckle



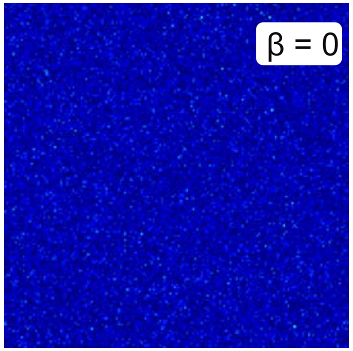
Contrast,

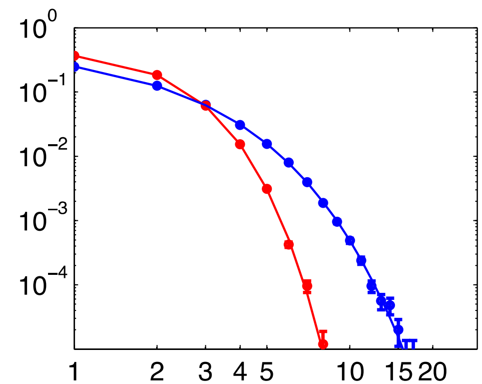
$$\beta \equiv \frac{1}{M}$$

Mean count rate:
1 photons / pixel

0 photons 18

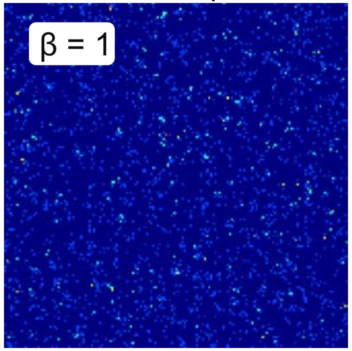
Poisson "Shot Noise"





k=1

Coherent Speckle



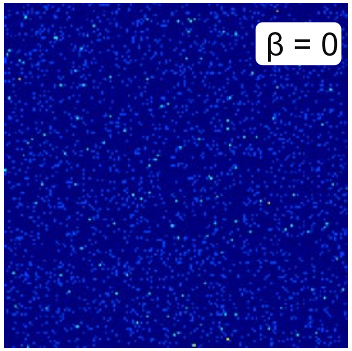
Contrast,

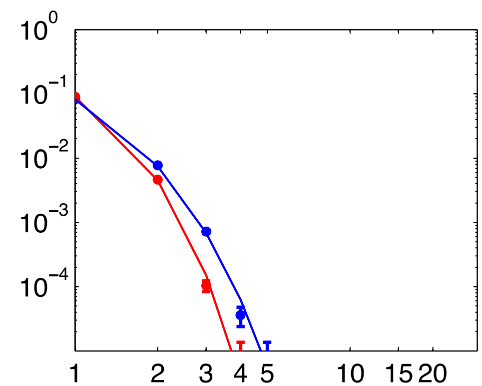
$$\beta \equiv \frac{1}{M}$$

Mean count rate:
0.1 photons / pixel

0 photons 6

Poisson "Shot Noise"

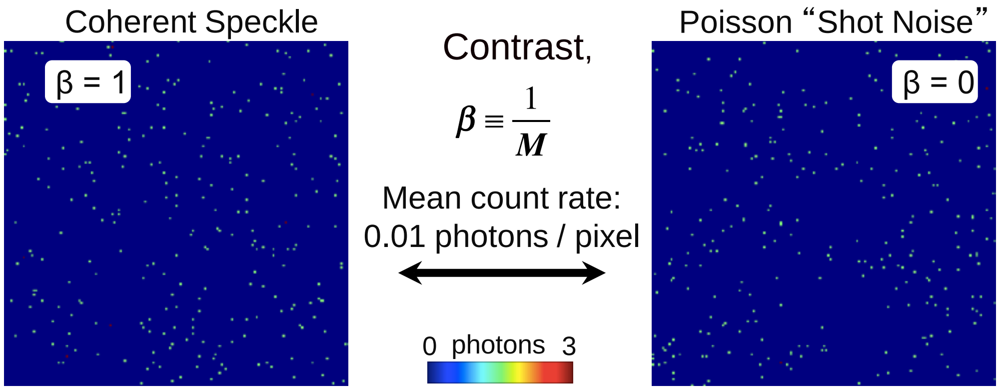


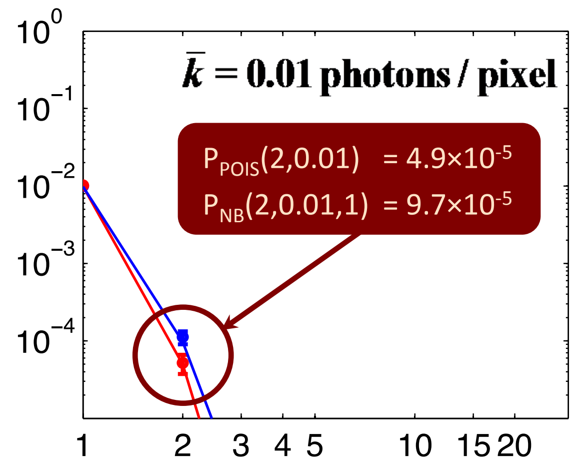


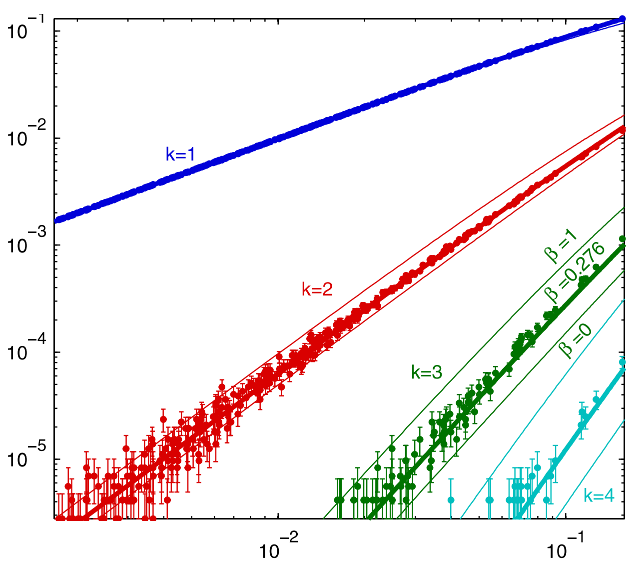
k=0.1

Atomic Speckles

Courtesy P. Fuoss







<u>Result :</u> one can characterize the contrast of very weak speckle patterns with atomic resolution