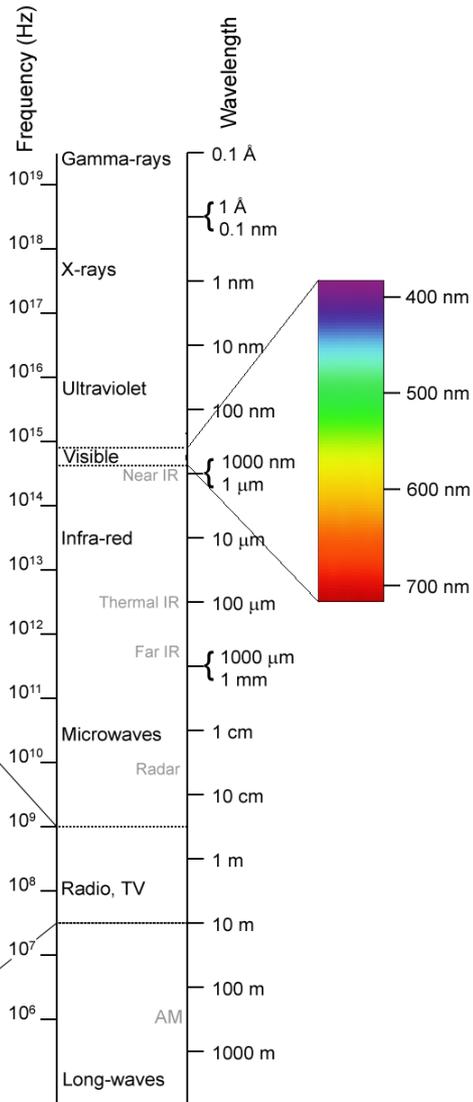# Progress and Prospects of X-ray Free Electron Lasers

Evgeny Saldin

The dream of an X-ray laser has motivated the laser community for many decades, but quantum lasers can only be operated to EUV range.

The history of coherent source for X-ray range began in 1977 with the conception of the Free Electron Laser by John Madey.

Today, XFELs are capable of operation over entire X-ray spectrum and of producing femtosecond fully coherent pulses with peak power up to 100 GW-level

Frequency (Hz) Wavelength

Electromagnetic Spectrum

Gamma-rays	0.1 Å
10^{19}	
	1 Å
10^{18}	0.1 nm
X-rays	1 nm
10^{17}	
	10 nm
10^{16}	
Ultraviolet	100 nm
10^{15}	
Visible	1000 nm
Near IR	1 µm
10^{14}	
Infra-red	10 µm
10^{13}	
Thermal IR	100 µm
10^{12}	
Far IR	1000 µm
	1 mm
10^{11}	
Microwaves	1 cm
10^{10}	
Radar	10 cm
10^{9}	
	1 m
10^{8}	
Radio, TV	10 m
10^{7}	
	100 m
10^{6}	
AM	1000 m
Long-waves	

400 nm
500 nm
600 nm
700 nm

1000 MHz
500 MHz
UHF
100 MHz
VHF 7-13
FM
VHF 2-6
50 MHz

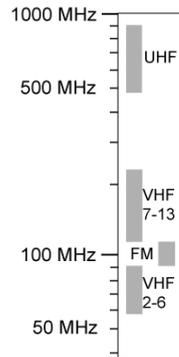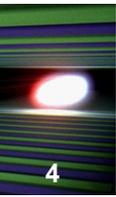XFELs   early 21th century

Quantum lasers

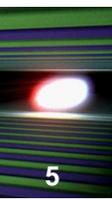Vacuum tube devices   early 20th century

X-ray FEL is the central subject to this talk, to be outlined in three separate parts as follows:

(I) FEL theory results

(II) Inventions

(III) Applications

A. Kondratenko and E. Saldin Part. Accel. 10, 207 (1980)

In this paper, for the first time the possibility was considered of using high gain regime of amplification, starting from spontaneous emission, to reach saturation in the single pass infrared FEL.

This paper opened up the possibility of using the same approach at shorter wavelengths and extend FEL to the X-ray region.

GENERATION OF COHERENT RADIATION BY A RELATIVISTIC ELECTRON BEAM IN AN ONDULATOR*

A. M. KONDRATENKO and E. L. SALDIN

*Institute of Nuclear Physics, 630090, Novosibirsk, USSR*
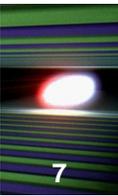
5. ON THE LEVEL OF BEAM MODULATION AT THE ENTRANCE OF AN ONDULATOR

To reveal the effect of self-modulation, a knowledge of the initial level of the harmonics of beam density is necessary. In a realistic situation, if the initial conditions are not prepared in a special manner, there exists a continuous spectrum of fluctuations of density harmonics that arise from the fact that there is a finite number of particles in the beam. Hence all the harmonics in a band of width $(\triangle K/K) \approx \lambdabar_0/l$ will become unstable and grow by a few times in the length l. After passage of a length $L \approx l \cdot \ln (\rho_0/\tilde{\rho}_i)$ all the harmonics achieve a size of the order of ρ_0.

The spectrum width $\triangle K \sim K\lambdabar_0/l$ corresponds to a correlation length of the order of $l/2\gamma_{\parallel}^2$. Hence the values of harmonics of density fluctuations for the narrow and wide beams respectively are

$$\tilde{\rho}_i/\rho_0 \approx (\dot{N}l/2\gamma_{\parallel}^2)^{-1/2}, \ \tilde{\rho}_i/\rho_0$$

$$\approx (\dot{N}l/2\gamma_{\parallel}^2)^{-1/2}(\sigma^2/\lambdabar l)^{1/2}.$$
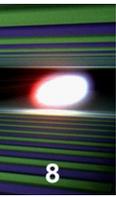
Ya. Derbenev, A. Kondratenko and E. Saldin Nucl. Instrum. and Methods 193 (1982)

In this paper, for the first time the possibility was considered of using high gain FEL amplifier starting from noise, inserted in storage ring, to produce soft X-rays

ON THE POSSIBILITY OF USING A FREE ELECTRON LASER FOR POLARIZATION OF ELECTRONS IN STORAGE RINGS

Ya.S. DERBENEV, A.M. KONDRATENKO and E.L. SALDIN

Institute of Nuclear Physics, 630090, Novosibirsk 90, U.S.S.R.

The possibility to polarize electrons (or positrons) by colliding with circularly polarized photons is discussed. For this purpose the coherent radiation of relativistic electron beams in the helical undulator is proposed. The possibility of polarizing by soft photons without beam loss in the storage ring is demonstrated. The cyclic version of the hard coherent radiation source (i.e. an X-ray laser) is proposed for polarization by the knock-out method. It has been shown that the use of a free electron laser enables the construction of an intense polarized positron beam source.

The density modulation increment is determined by the peak current $e\dot{N}$ in the FEL beam, its transverse area $2\pi\sigma^2$, the value of the transverse rotation velocity u driven by the undulator and by the energy of an electron source $\epsilon_s = \gamma_s mc^2$. For a wide beam, when

$$\sigma^2 \gg \sigma_0^2 = \frac{\lambda_{ph}^2}{u}\left[\frac{\gamma_s \gamma_{11}^2 c^3}{\dot{N} r_e}\right]^{1/2},$$

$(r_e = e^2/mc^2)$ the growth length is minimum at the exact resonance (3) and is equal to [5−11]:

$$l_g = \frac{2^{4/3}}{3^{1/2}}\frac{1}{\lambda_{ph}}(\sigma^2 \sigma_0^4)^{1/3}. \tag{4}$$

In the case of a narrow beam $(\sigma^2 \ll \sigma_0^2)$, the growth length is approximately equal to [10,11]:

$$l_g \simeq \frac{\sigma_0^2}{\lambda_{ph}}\left[\ln\frac{\sigma_0}{\sigma}\right]^{-1/2} \tag{5}$$

The beam, after its passage through the length $L = l_g \cdot \ln 1/a$, where (a) is the degree of initial beam modulation on the resonant harmonic, will have a modulation degree of the order of unity, and in this state it will radiate over a length of the order of l_g. The coherent radiation power W will have an order of magnitude,

$$W \simeq \dot{N}\epsilon_s \lambda_0/l_g. \tag{6}$$

The statistical fluctuations of beam density, which are caused by the finite number of particles, will play the role of an initial excitation of modulation. For example, for a narrow beam

$$a_{fl} \approx [2\gamma_{11}^2 c/\dot{N} l_g]^{1/2}.$$

In the development of the modulation from the spectrum of density fluctuations the angular divergence of the output radiation is approximately equal to $(\gamma_{11}\theta_{ph} \ll 1)$

$$\theta_{ph} \approx (\lambda_{ph}/l_g)^{1/2}, \qquad \sigma^2 \ll \sigma_0^2$$

$$\theta_{ph} \approx \max\left[\frac{\sigma}{L}, (\lambda_{ph}/l_g)^{1/2}\right], \qquad \sigma^2 \gg \sigma_0^2.$$

Radiation instability occurs if the particle shifts due to the spread of longitudinal velocities may be ingored over length of the order of l_g:

$$(\Delta\beta_{11}l_g)^2 \ll \lambda_{ph}^2.$$

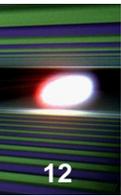The longitudinal velocity spread results from the energy and angular spreads:

$$(\Delta\beta_{11})^2 = \frac{1}{\gamma_{11}^4}\left(\frac{\Delta\epsilon_s}{\epsilon_s}\right)^2 + \tfrac{1}{4}(\Delta\theta)^4.$$

consider an electron beam with the following parameters: $\gamma \simeq 4 \times 10^4$, the number of particles in the beam $N_e \simeq 10^{13}$, the bunch length $l_b \simeq 3$ cm, the horizontal beam emittance $\sigma_x \Delta\theta_x \simeq 5 \times 10^{-7}$ cm, the beam size $\sigma_z \simeq 0.1\sigma_x$. Let this beam pass through an helical undulator with period $\lambda_0 = 7$ cm and magnetic field $H_0 = 20$ kG. In this case, the resonant wavelength of the coherent radiation is equal to $\lambda = (2\gamma_{11}^2)^{-1} \lambda_0 = 5 \times 10^{-7}$ cm. The characteristic growth length of the density modulation, with the transverse size in the undulator; $\sigma_x \sigma_z \simeq 10^{-5}$ cm^2, is calculated by eq. (4) and is equal to $l_g \simeq 200$ cm. To perform the beam self-modulaton it is necessary that the angular and energy spreads should satisfy the conditions

$$(\Delta\theta)^2 \lesssim 10^{-9}, \quad \Delta\gamma/\gamma \lesssim 0.5 \times 10^{-2}.$$

For a given phase space volume of the circulating beams, these conditions may be fulfilled if the value of the β-function in the undulator is of the order of 5 m. The required length of the undulator in the development of modulation from the spectrum of fluctuations is of the order of 15 m. The fraction of the beam energy converted into coherent radiation during one flight will amount to about 0.5%. The area of the radiated beam at its exit from the undulator is of the order of that of the circulating electron beam in the undulator and the radiated beam divergence angle is $\simeq 3 \times 10^{-5}$. The peak radiation power (on a wavelength of 5×10^{-7} cm and with the degree of monochromaticity $\Delta\lambda/\lambda \simeq 10^{-2}$) is approximately 10^{12} W.

In conclusion, we would like to mention that storage ring-generators are, in essence, X-ray lasers. In our opinion, the creation of such devices is within the scope of present-day acceleration technology.

Science fiction becomes reality

	XFEL (1982)	EXFEL(SASE3)
Electron energy	20 GeV	10-17.5 GeV
Undulator period	7 cm	7 cm
Photon energy	0.25 keV	0.25 -3 keV
Peak current	14 kA	5-10 kA
Field gain length	~ 2 m	~ 2 m *
Output peak power	~ 1 TW	~ 1 TW **

Review of x-ray free-electron laser theory
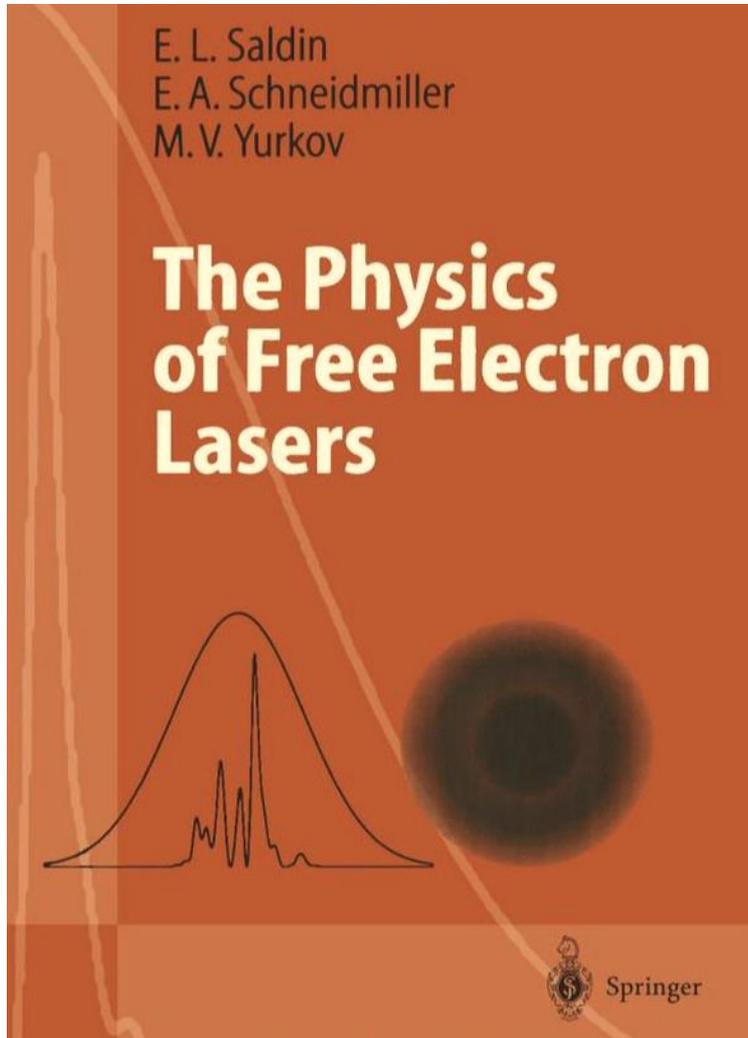
Zhirong Huang

Stanford Linear Accelerator Center, Stanford, California 94309, USA

Kwang-Je Kim

Argonne National Laboratory, Argonne, Illinois 60439, USA
(Received 25 August 2006; published 12 March 2007)

[1] J. Madey, J. Appl. Phys. **42**, 1906 (1971).
[2] D. A. G. Deacon, L. R. Elias, J. M. J. Madey, G. J. Ramian, H. A. Schwettman, and T. I. Smith, Phys. Rev. Lett. **38**, 892 (1977).
[3] A. Kondratenko and E. Saldin, Part. Accel. **10**, 207 (1980).
[4] Y. Derbenev, A. Kondratenko, and E. Saldin, Nucl. Instrum. Methods Phys. Res., Sect. A **193**, 415 (1982).
[5] R. Bonifacio, C. Pellegrini, and L. Narducci, Opt. Commun. **50**, 373 (1984).

E. L. Saldin
E. A. Schneidmiller
M. V. Yurkov

**The Physics
of Free Electron
Lasers**

Springer

The work of the period 1979 to 1999 is summarised in this monograph

- **Series: Advanced Texts in Physics**

- **Paperback: 470 pages**
- **Publisher: Springer; Softcover reprint of hardcover 1st ed. 2000 edition**
- **Language: English**
- **ISBN-10: 3642085555**
- **ISBN-13: 978-3642085550**

Theoretical computation of the polarization characteristics of an X-ray Free-Electron Laser with planar undulator

Gianluca Geloni[a] Vitali Kocharyan[b] Evgeni Saldin[b]

[a]European XFEL GmbH, Hamburg, Germany
[b]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

Exact inhomogeneous wave equation for electric field

$$c^2 \nabla^2 \vec{E} - \frac{\partial^2 \vec{E}}{\partial t^2} = 4\pi c^2 \vec{\nabla} \rho + 4\pi \frac{\partial \vec{j}}{\partial t}$$

The current source provides the main contribution to the radiation field in an FEL amplifier and the contribution of charge term is negligibly small

$$W_\pi / W_\sigma \simeq 1.5 \cdot 10^{-7}$$
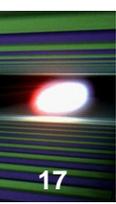
FEL literature is full of brilliant ideas that did not work…

…but self-seeding is an idea that does definitely work.

■ Self-seeding opened a route to XFEL with laser-like output characteristics

■ Self-seeding works best from 5 nm down to 0.1 nm

- First undulator generates SASE
- X-ray monochromator filters SASE and generates seed
- Chicane delays electrons and washes out SASE microbunching
- Second undulator amplifies seed to saturation
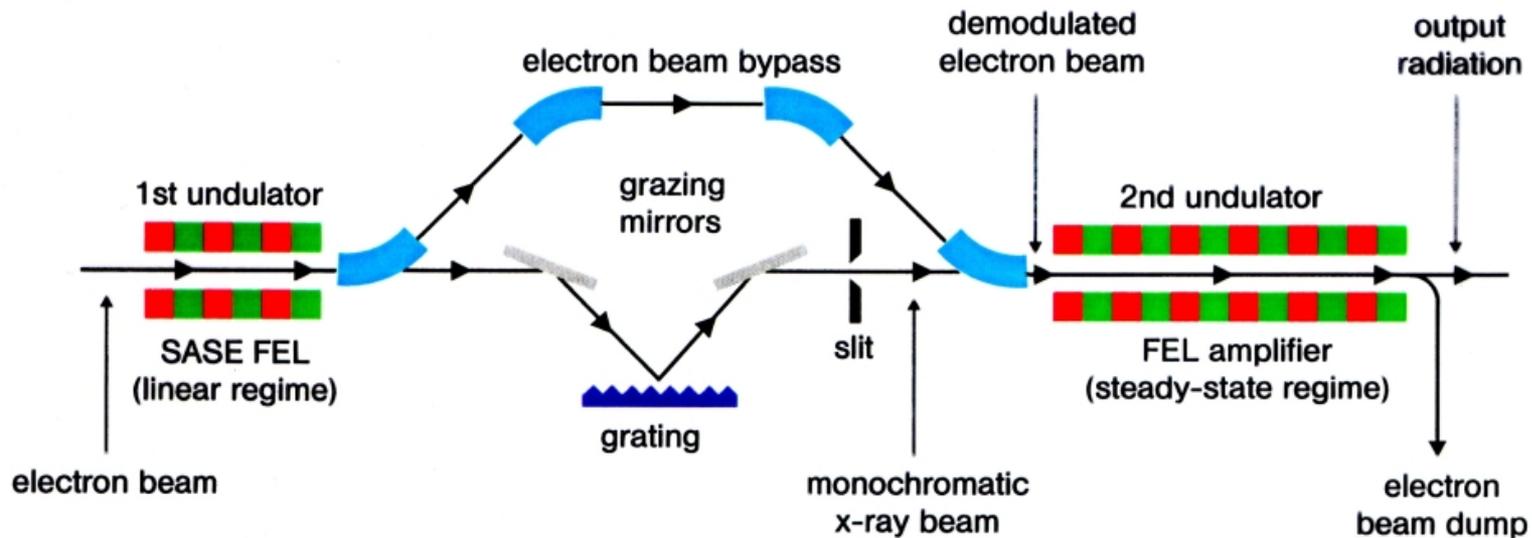
[1] *J. Feldhaus, E.L. Saldin, J.R. Schneider, E.A. Schneidmiller, M.V.Yurkov, Opt. Comm., V.140, p.341 (1997)*

Grating monochromator substituted by crystal monochromator for applications to hard x-rays
[E. Saldin, E. Schneidmiller, Yu. Shvyd'ko and M. Yurkov, NIM A 475 357 (2001)]

Extra x-rays path due to monochromator ~1cm. Long electron bypass (tens of meters) needed
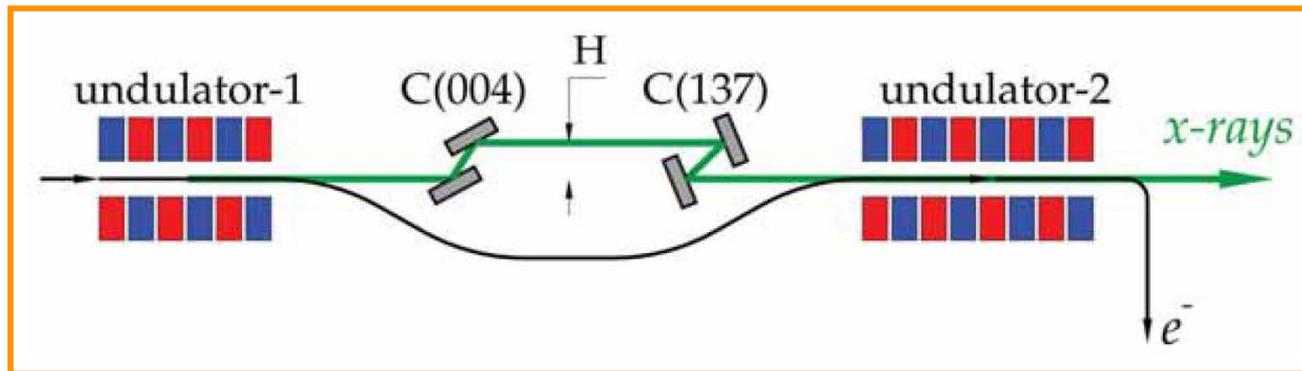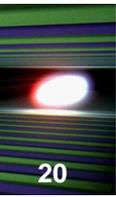
Quite surprisingly, monochromatization can be performed by an almost trivial setup of as few as two components:

- a short (3 m-long) chicane and
- a single crystal

HXRSS scheme with single-crystal monochromator:

*G. Geloni, V Kocharyan, E Saldin
J. Modern Opt. 2011; 58:1391-14303*

Working principle
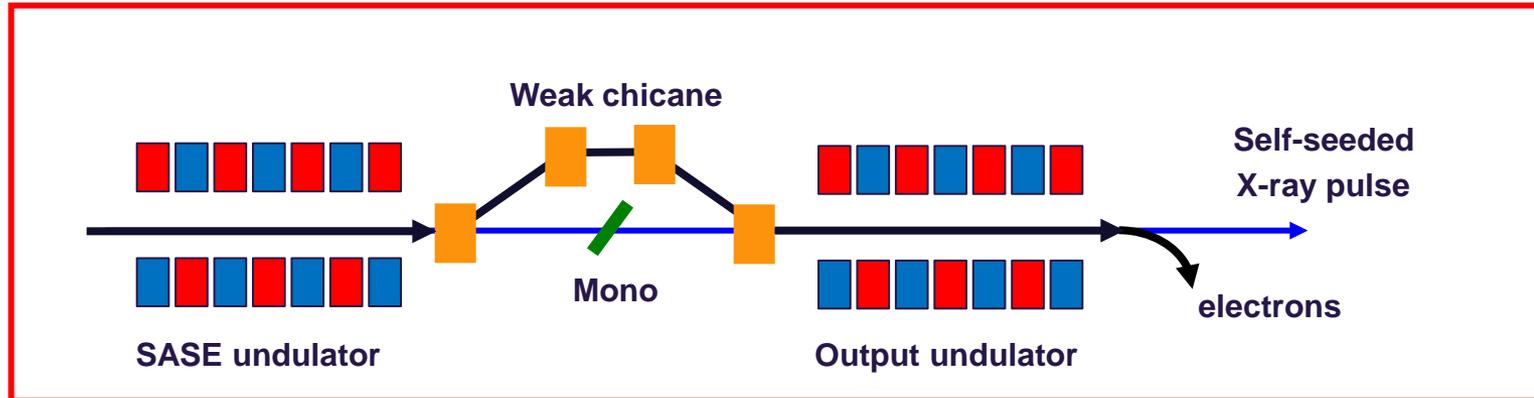
Monochromatization of X-rays using a single crystal in Bragg-transmission geometry.

Monochromator introduces no path delay of X-rays, thus avoiding the need for a long electron beam bypass, as required in schemes with the monochromator in Bragg reflection geometry

The scheme is extremely compact and based on the substitution of a single undulator module with a weak chicane and single crystal

2.0e9

After the Diamond crystal

5.0e6

After the Diamond crystal
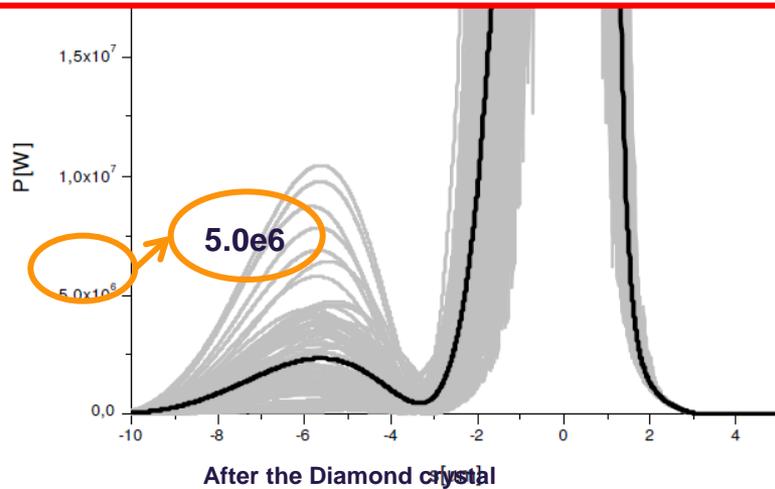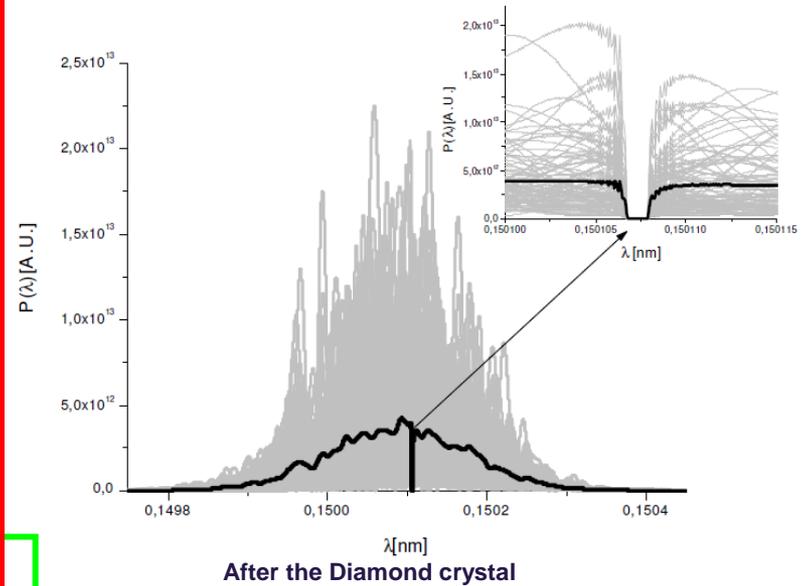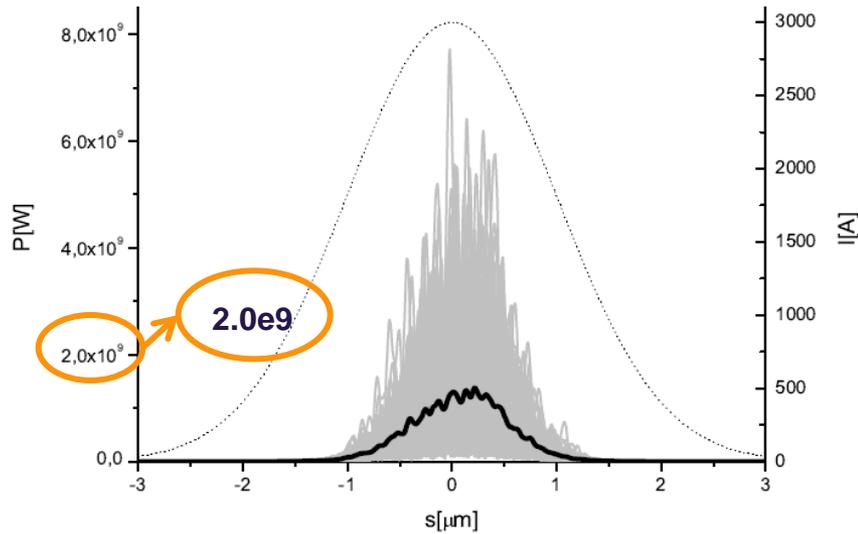
Efficient seeding mechanism (monochromatic tail much larger than shot noise) is achieved

G. Geloni, V. Kocharyan, E. Saldin
DESY 10-133

C(400) Bragg symmetric
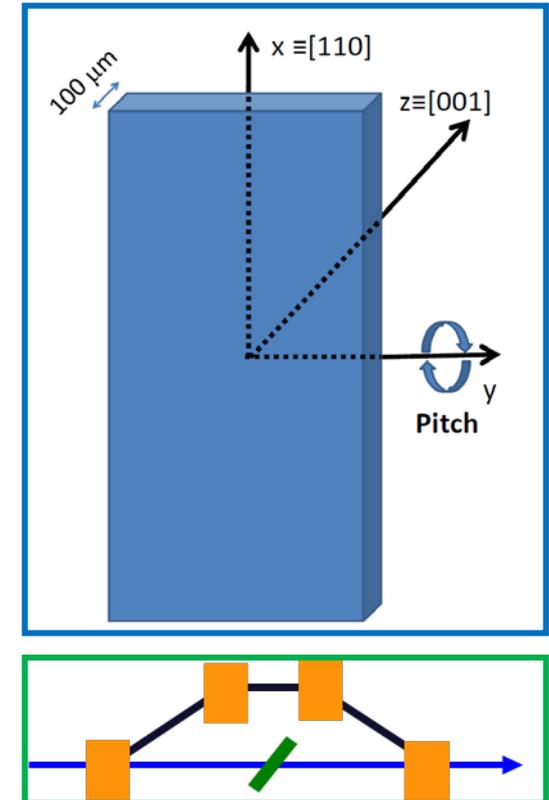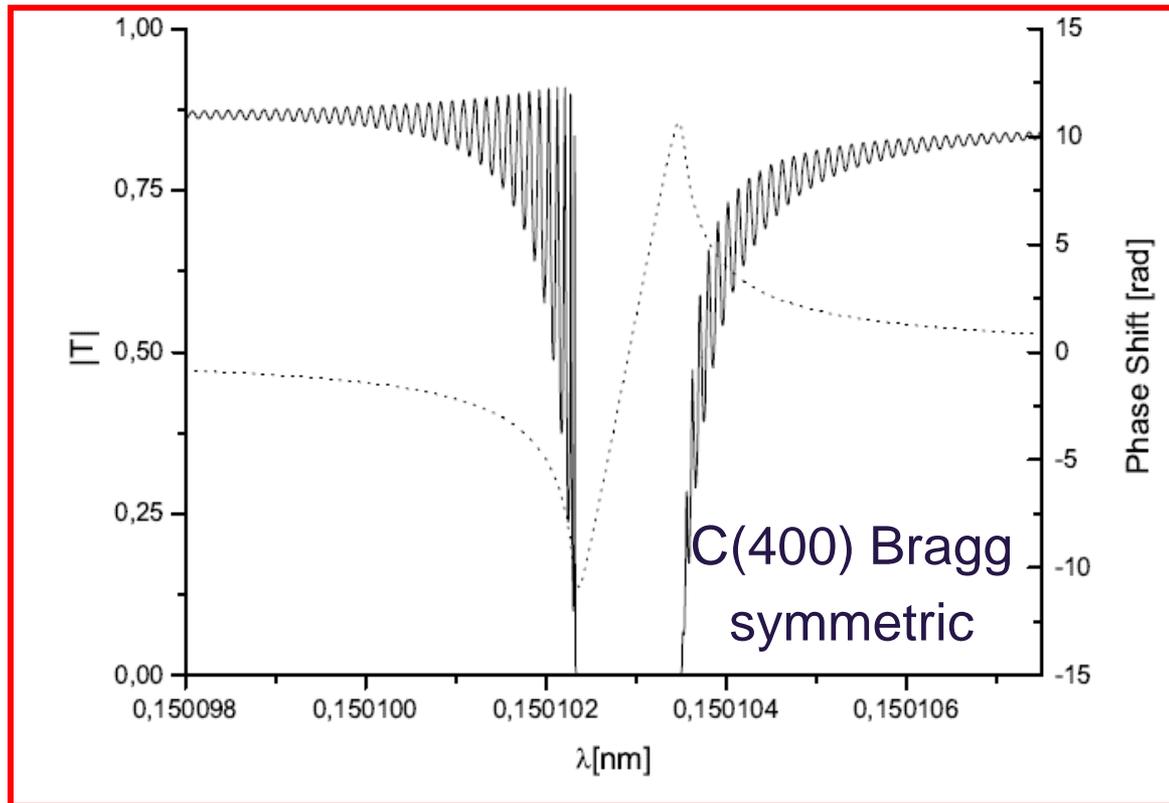
The monochromator hardware is constituted by a single crystal. The forward diffracted beam is considered. In the space-frequency domain, the crystal acts as a band stop filter (modulus and phase). Characterization of the filter needed.

This can be shown, proving directly that

$$T = T(\eta)$$

Has no zeros on the upper complex plane (so that ln[|T|] is not singular and we can recover the phase).

So, knowing |T| from e.g. XOP or other easily available programs, we use

$$\Phi(\omega) = -\frac{2\omega}{\pi}\mathcal{P}\int_0^\infty \frac{\ln[\|T(\omega')\|]}{\omega'^2 - \omega^2}d\omega'$$

Legend: Directly from dynamical theory / Using kK

Axes: Phase [rad] (vertical), Wavelength [m] (horizontal)
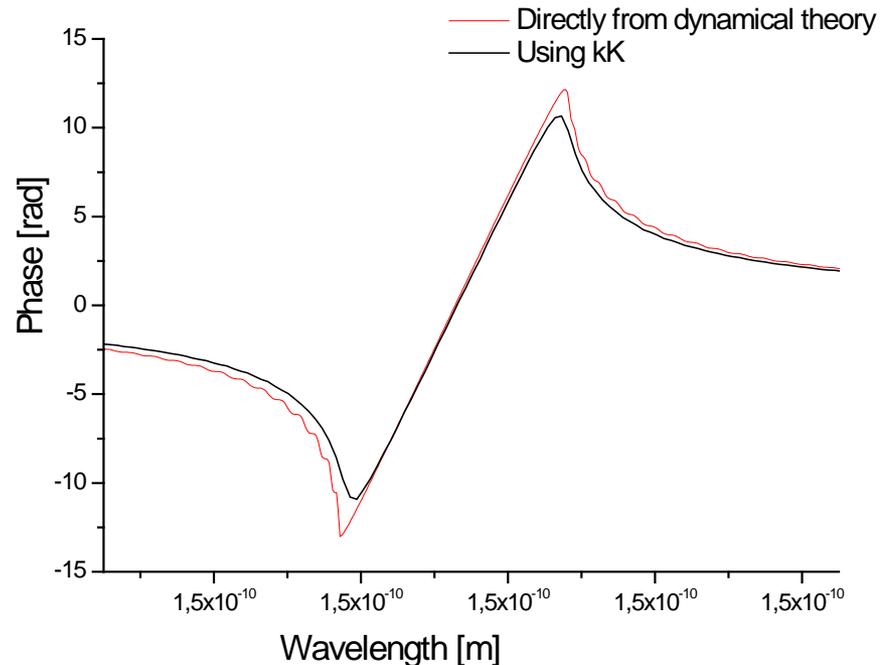
Demonstration of self-seeding in hard-X-ray free electron laser, Amman, et al.

Nature Photonics, DOI:10.1038/NPHOTON 2012.180

HXRSS
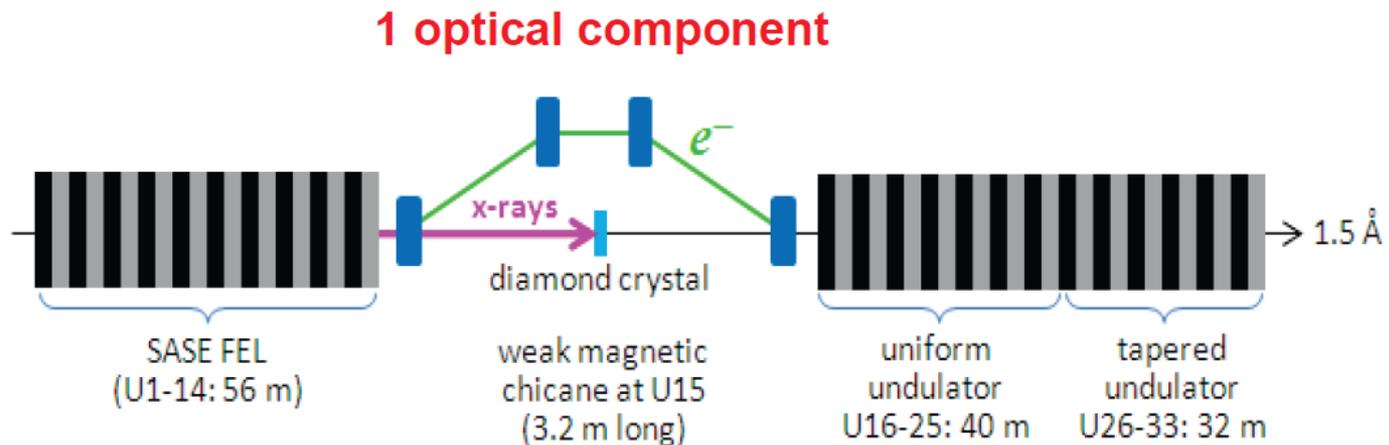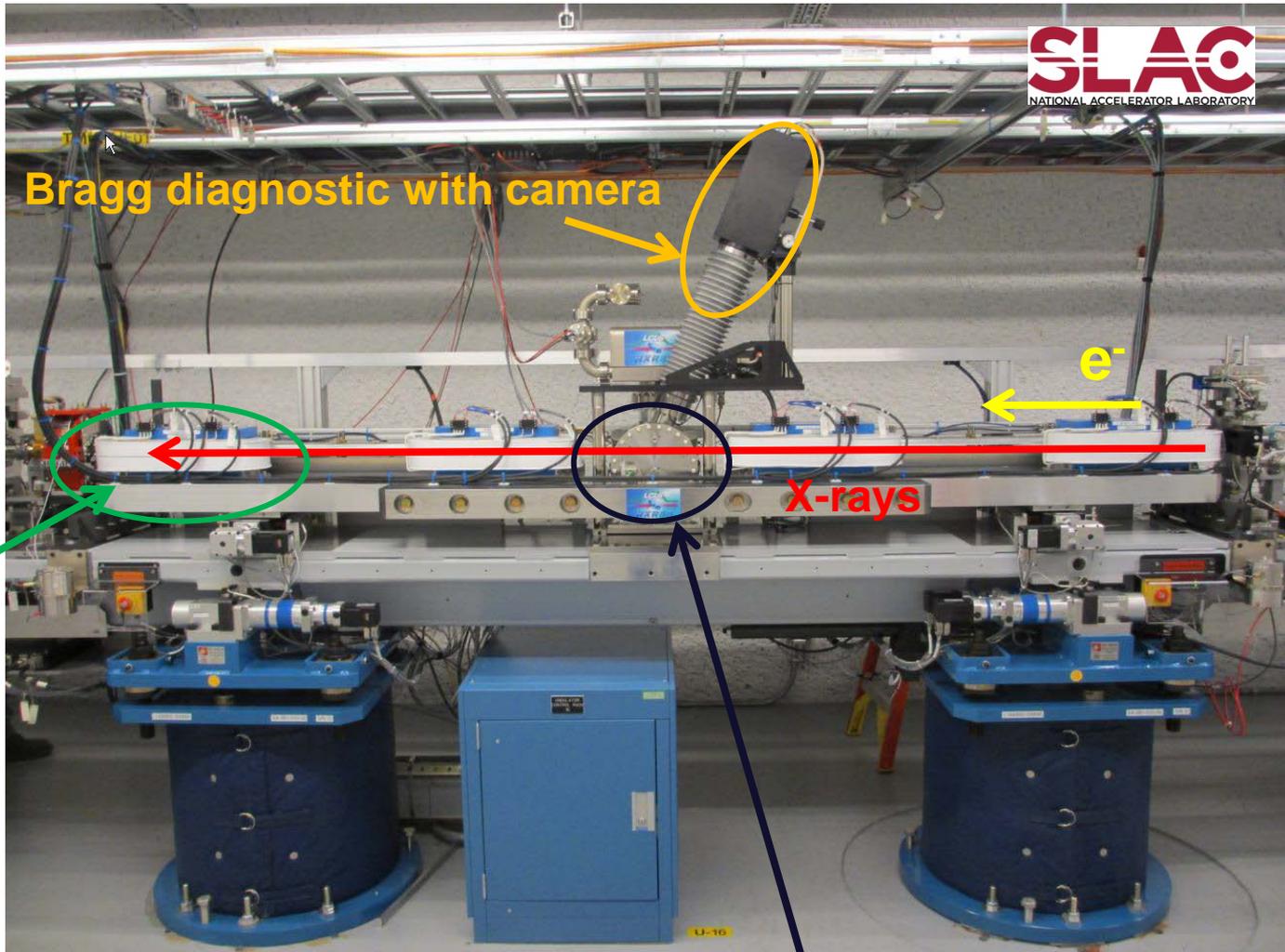
Bragg diagnostic with camera

e⁻

Chicane magnet

X-rays

Diamond mono chamber

a
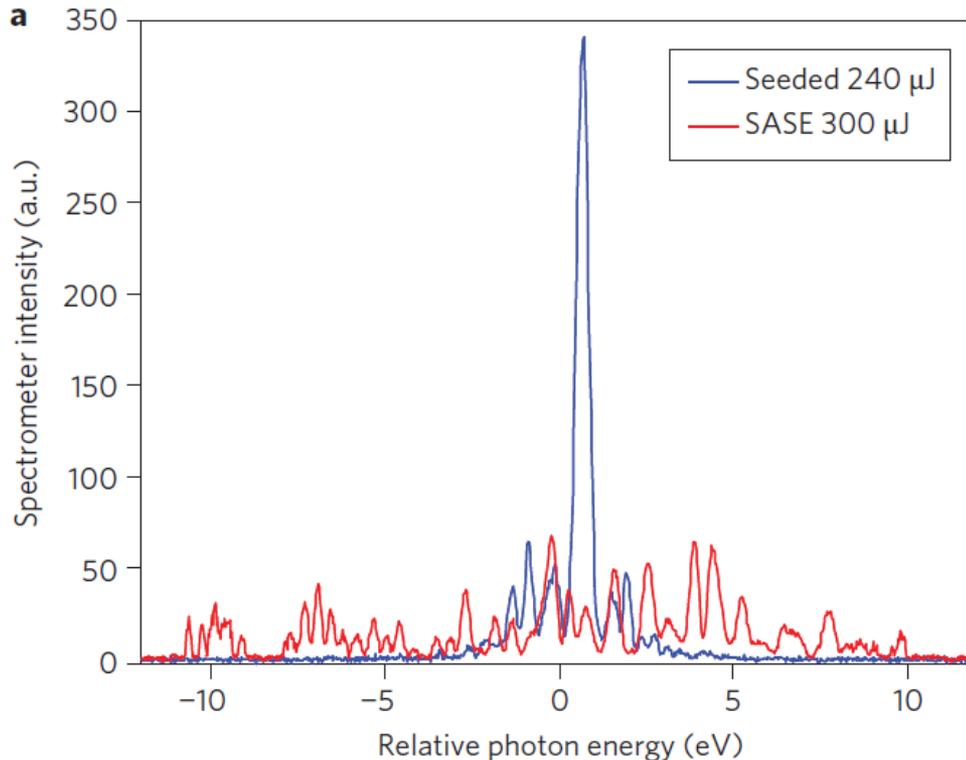
- Single-shot X-ray SASE spectrum compared with single-shot seeded spectrum at 0.15 nm for a 40pC electron bunch

- SASE spectrum includes all 28 undulators

- The seeding increases the spectral density of the FEL pulse.

J. Amann et al., Demonstration of self-seeding in a hard-X-ray free-electron laser, *NATURE PHOTONICS DOI: 10.1038/NPHOTON.2012.180 (2012)*

Profile Monitor XPP:OPAL1K:1 09-Jan-2012 19:36:24

Diamond OUT

FWHM BW ≈ 20 eV

(0.2%)
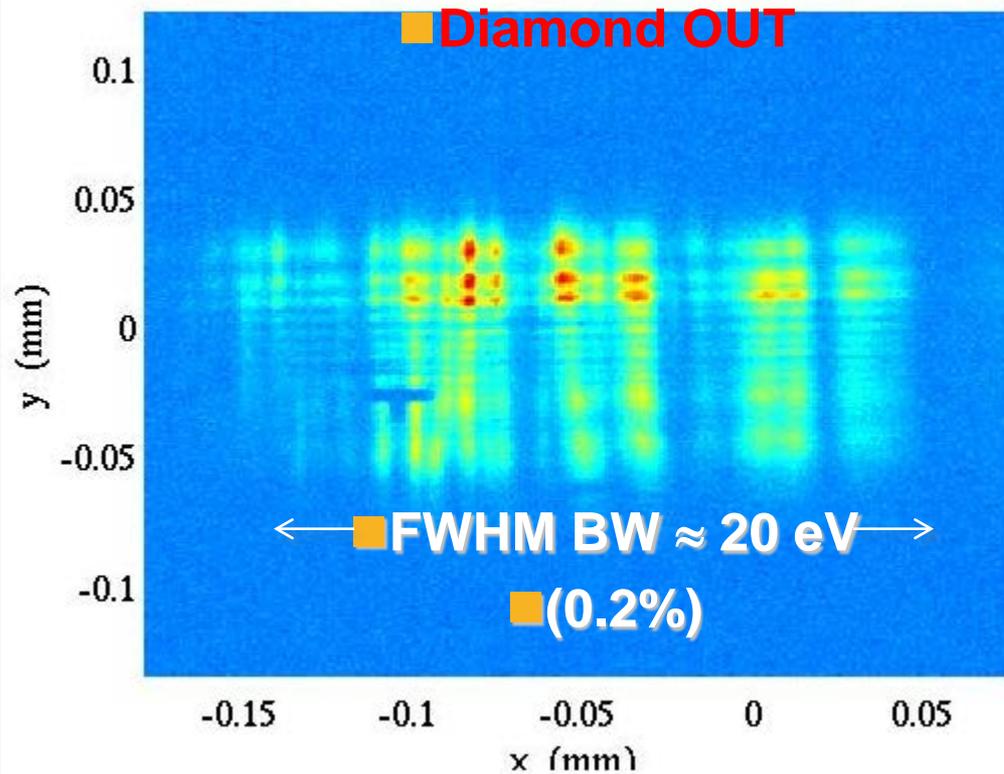
file Monitor XPP:OPAL1K:1 10-Jan-2012 01:45:53

Diamond IN

FWHM BW ≈ 0.5 eV

(0.005%)
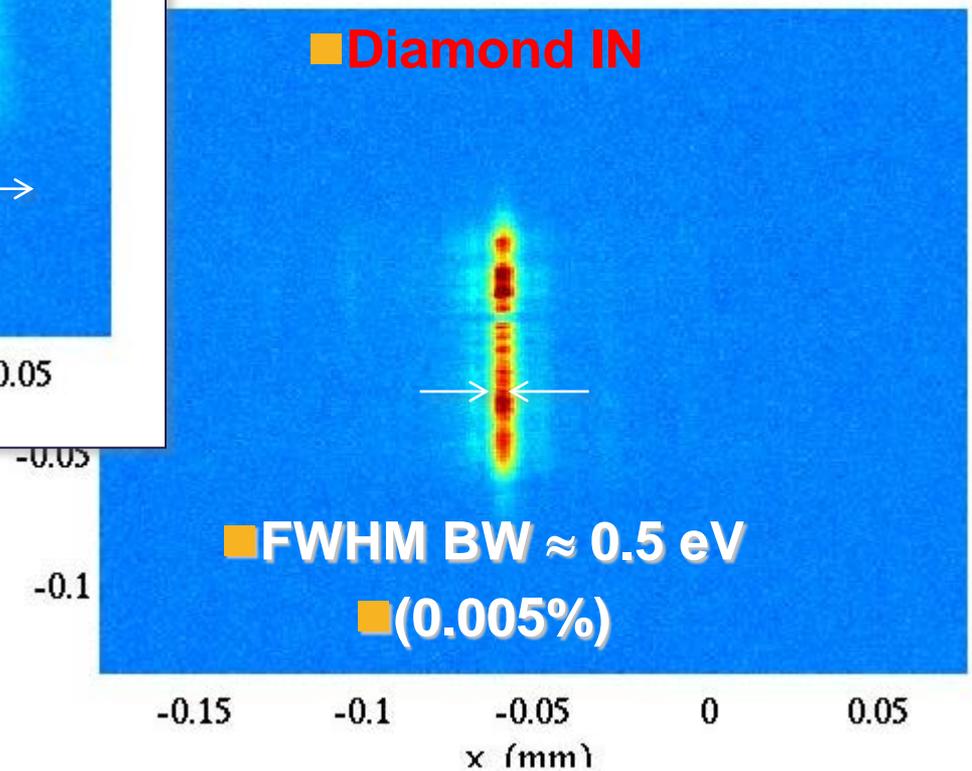
Chicane Delay Scan Shows X-Ray Wake Pulse

Power dist. after diamond crystal

Wide-band power

Monochromatic seed power

5 MW

20 fs
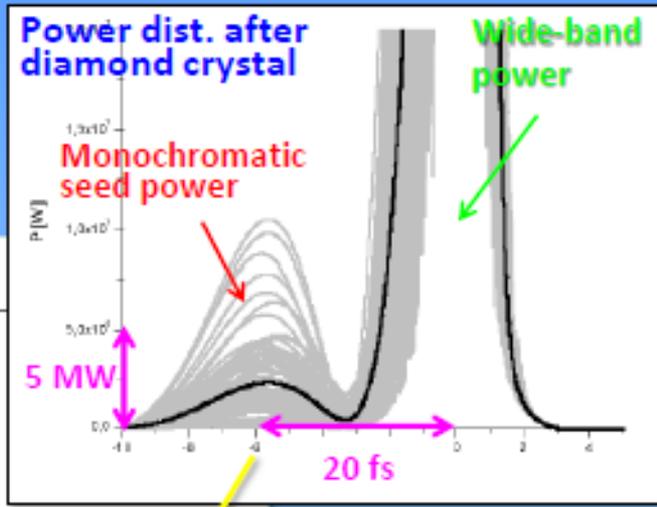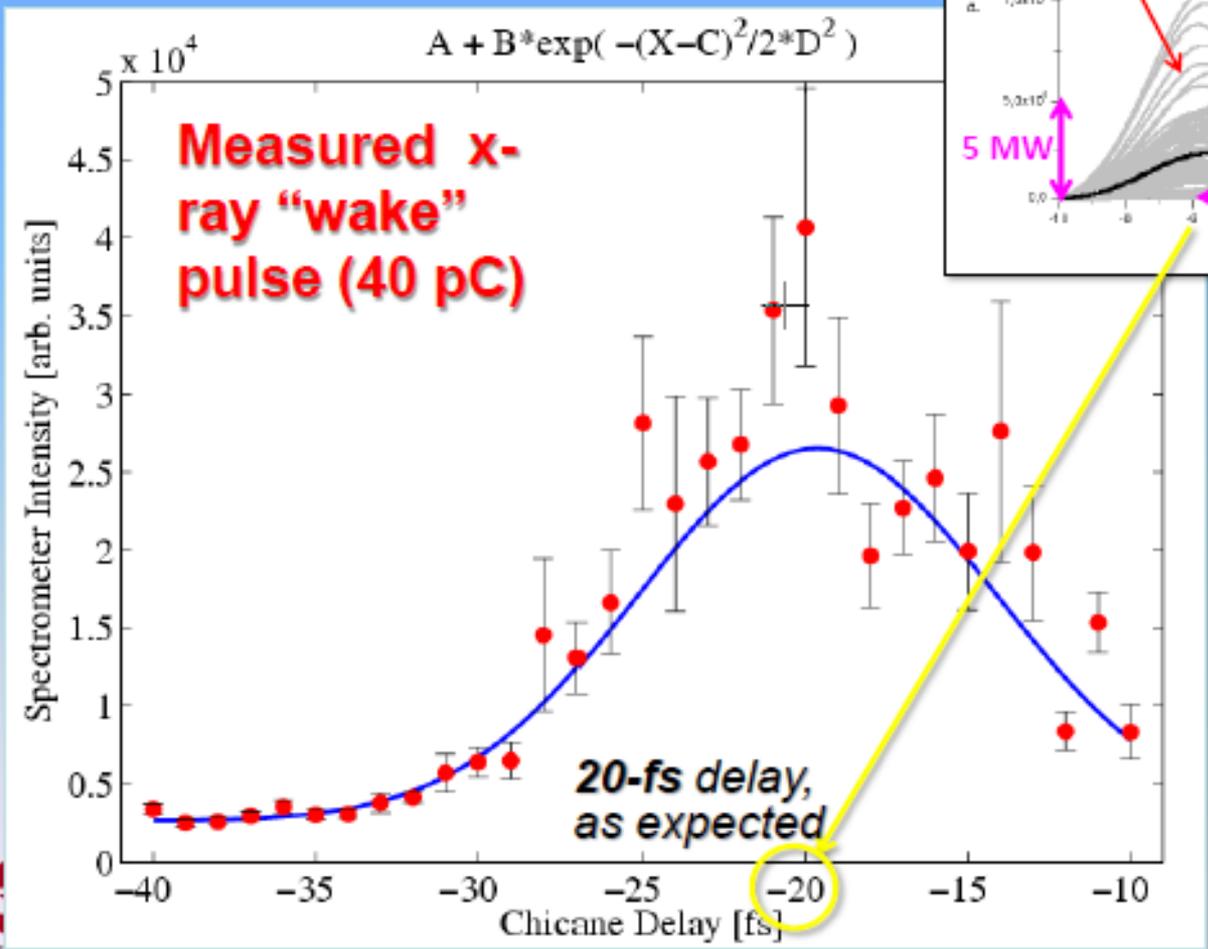
Geloni, Kocharyan, Saldin (*DESY 10-133*)

$$A + B*\exp(-(X-C)^2/2*D^2)$$

Measured x-ray "wake" pulse (40 pC)

20-fs delay, as expected

Demonstration of self-seeding in soft-X-ray free electron laser, D. Ratner, et al.

Phys. Rev. Lett, 114, 054801, 2015

SXRSS

5 optical components and 2 diagnostics
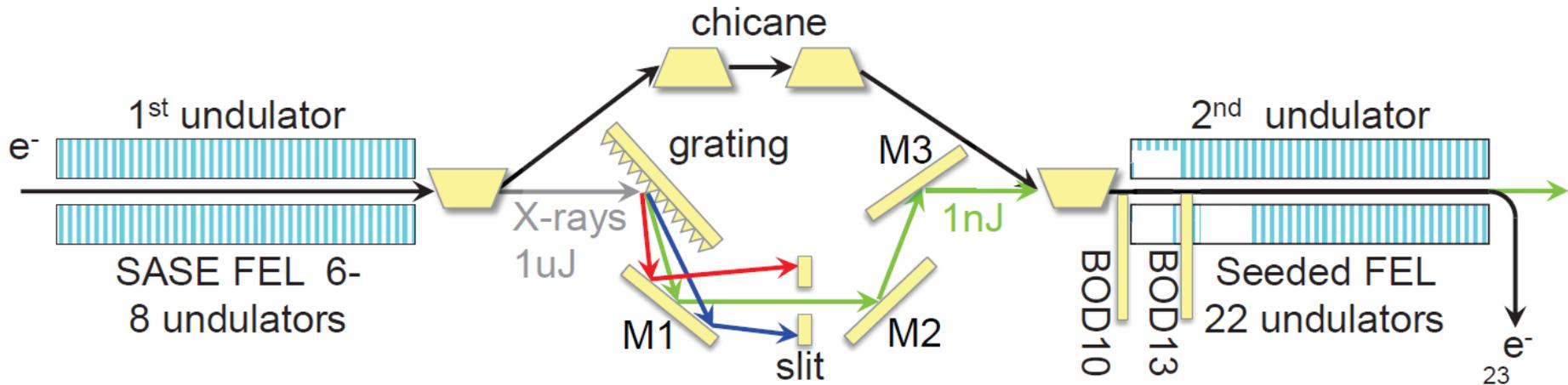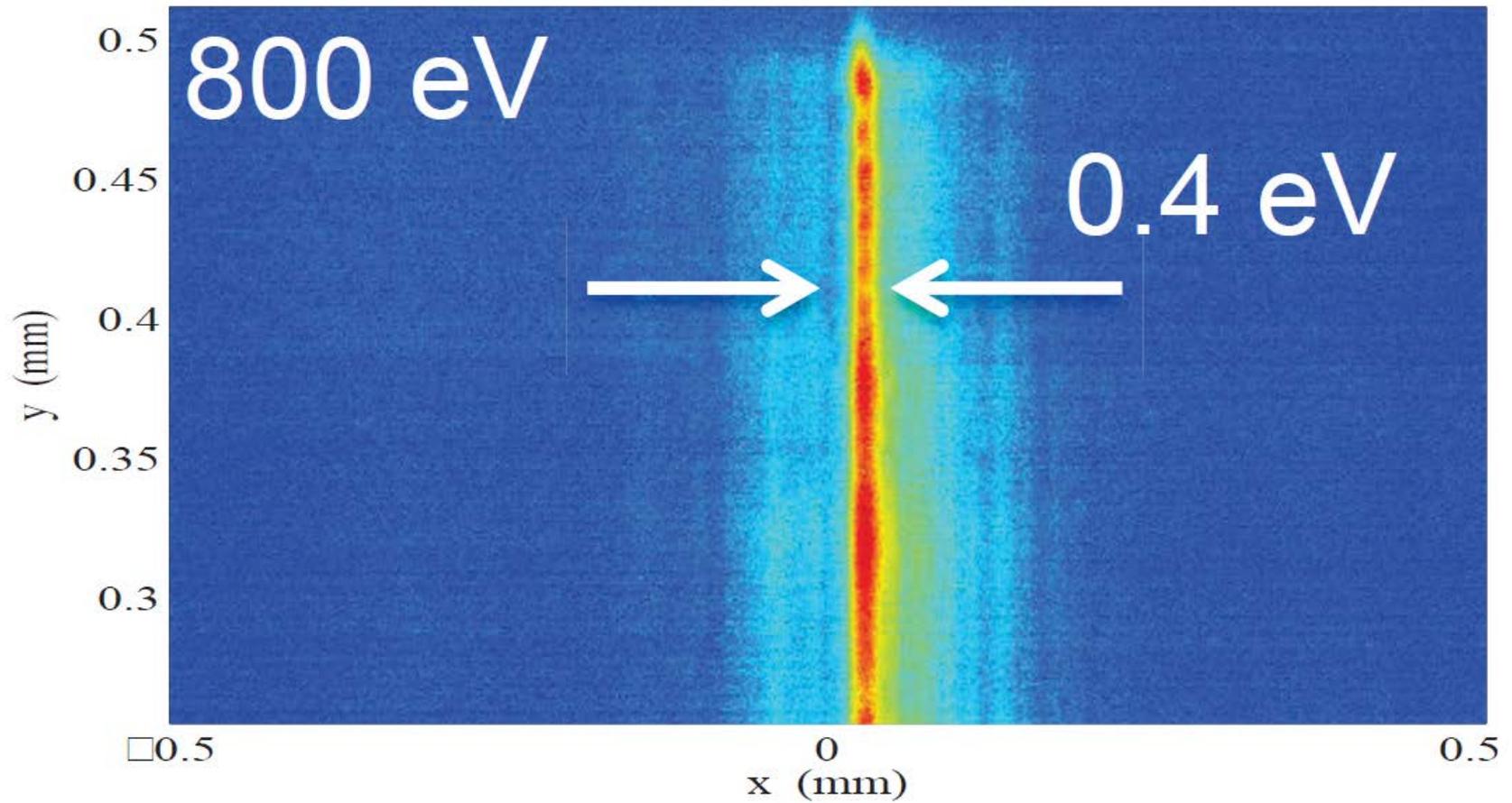
Self-seeding is sensitive to energy jitter of the electron beam at the LCLS
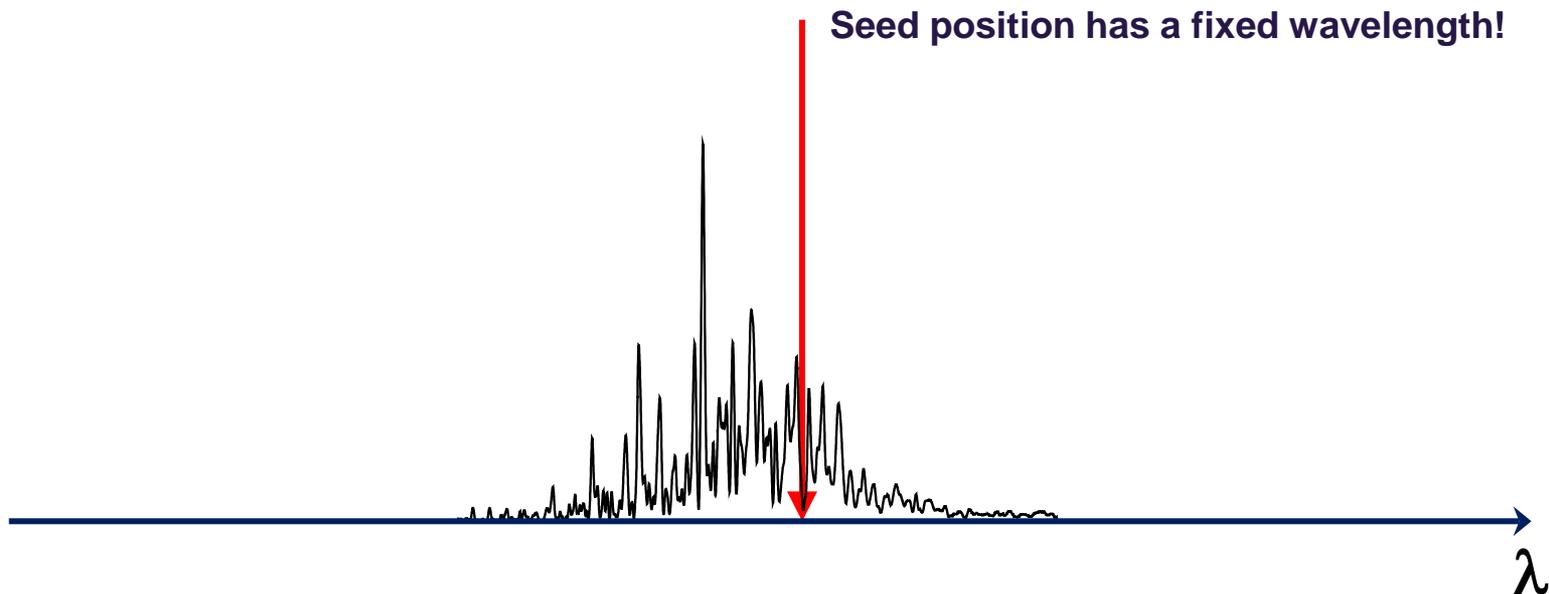
Seed position has a fixed wavelength!

λ

Self-seeding is sensitive to energy jitter of the electron beam at the LCLS

Seed position has a fixed wavelength!

No signal here!

λ
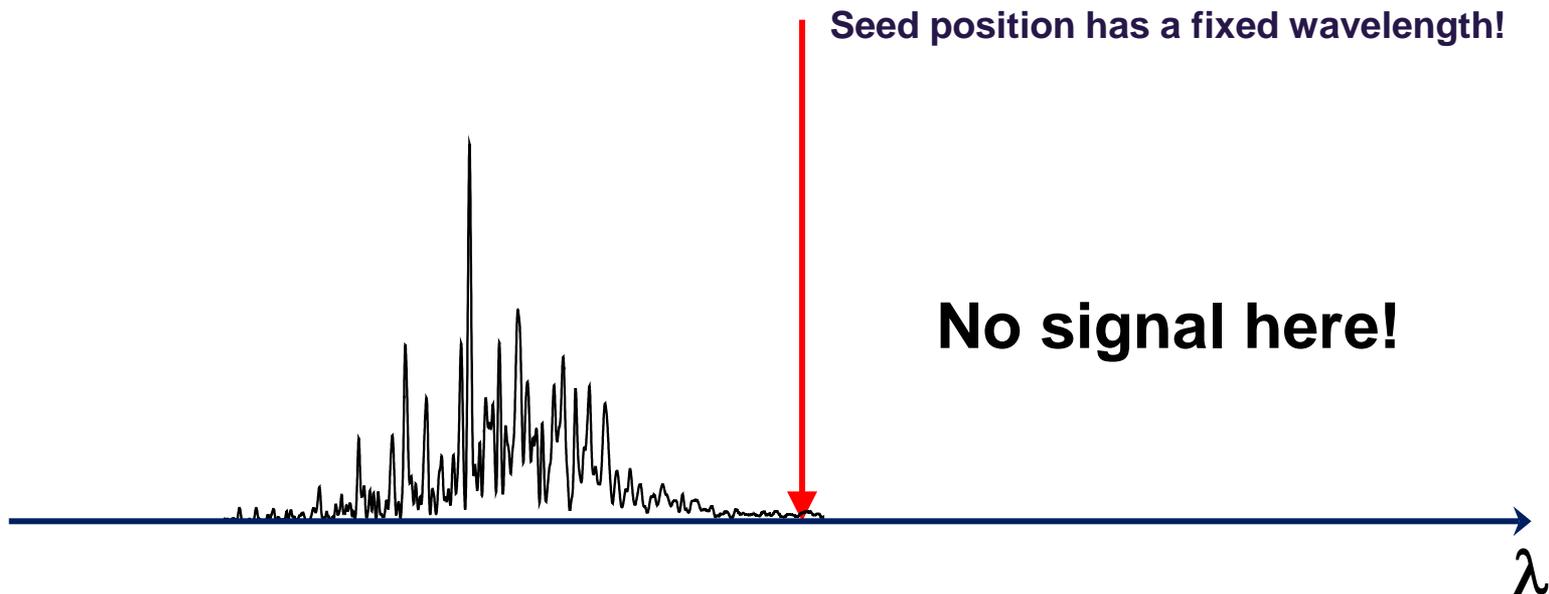
Self-seeding is sensitive to energy jitter of the electron beam at the LCLS

LCLS energy jitter: 0.04% ~ ρ!!

→ SASE spectral jitter ~ 0.08%

→ Need reduction to 0.02%

…it should not be a problem for the European XFEL (jitter 0.01%)

Amann et al., Nature Photonics DOI: 10.1038/NPHOTON.2012.180

1. Creation of transform-limited pulses through self-seeding at EXFEL

2. Generation of TW X-ray pulses

3. Schemes for variable X-ray polarization at EXFEL

4. Possible THz pump/X-ray probe option at EXFEL

European XFEL pulse repetition rate ~ 27000 Hz → compromise in the first undulator length (heat loading!)
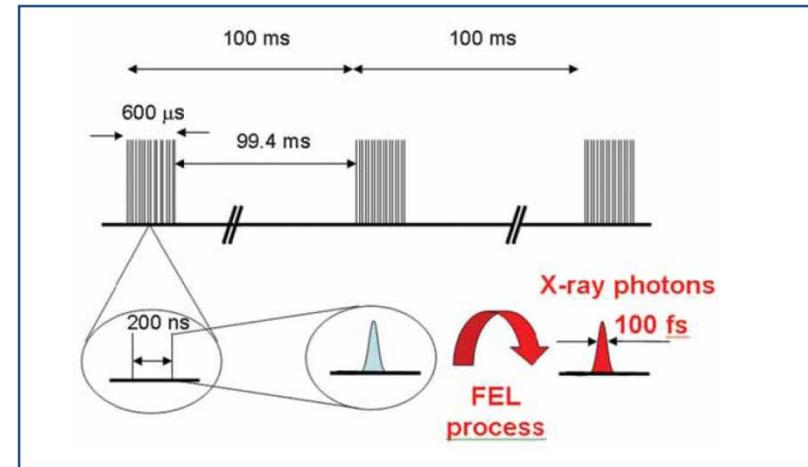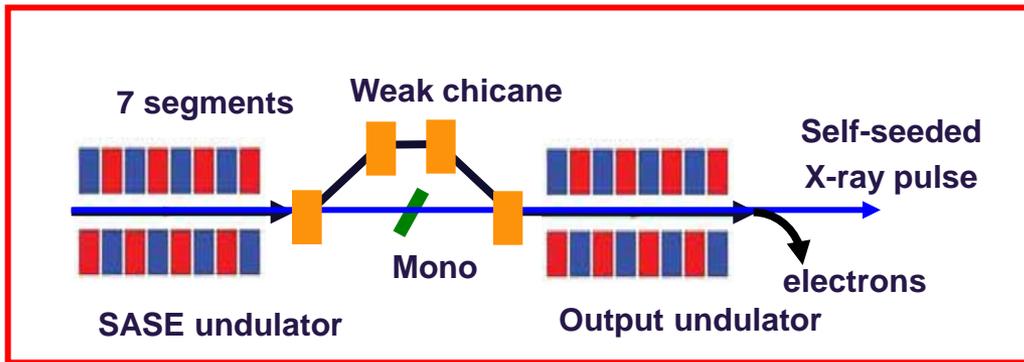
Energy per pulse 25pC/0.25nC bunch ~ **150-1500 nJ/pulse**

→**Average incident power density at normal incidence within a train:**
300 W/mm² (25pC) – 3000 W/mm² (0.25nC)

Three-undulator setup
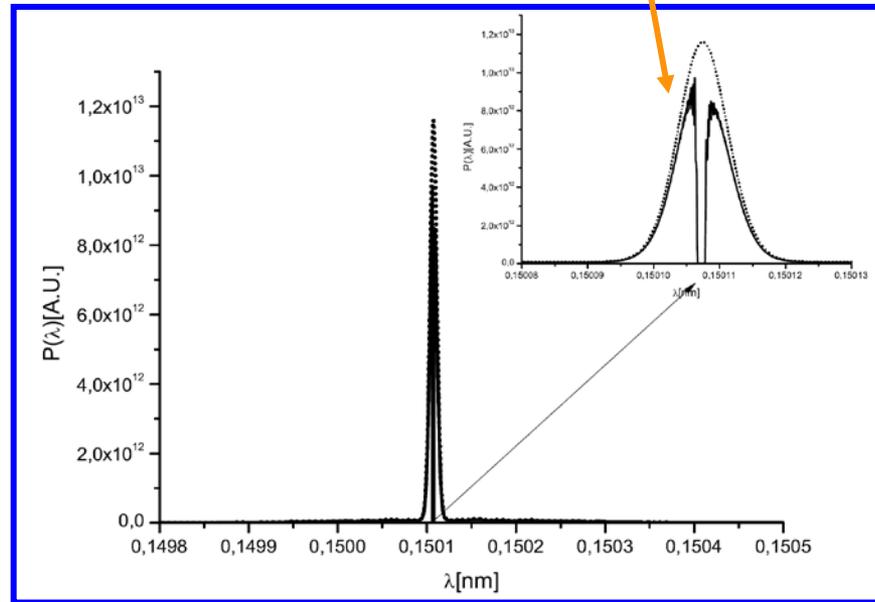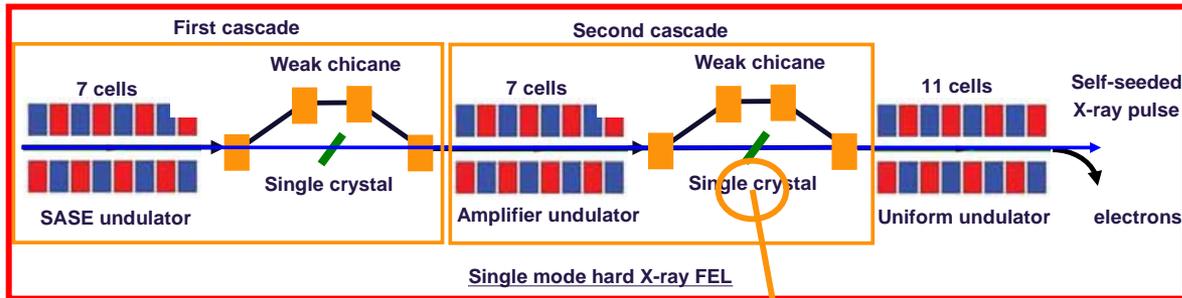
Small SASE contribution: at the second filter BW nearly Fourier limited already

First cascade

Second cascade

Output undulator

9 keV

Weak chicane

Weak chicane

TW-level
Self-seeded
X-ray pulse

5 cells

6 cells

6 cells

18 cells

Single crystal

Single crystal

electrons

SASE undulator

Amplifier undulator

Uniform undulator **Tapered undulator**

Single mode hard X-ray FEL

Self-Seeding and Undulator Tapering for Highest Spectral Flux from the European XFEL

5 cells (uniform) — Single crystal monochromator — 5 cells (uniform) — Single crystal monochromator — 22 cells (8 uniform, 14 tapered)

Pulse duration $\simeq$ 15 fs (FWHM)

Spectral width $\simeq$ 0.9 eV (FWHM)

G. Geloni, V. Kocharyan, E. Saldin et al.

Self-Seeding and Undulator Tapering for Highest Spectral Flux from the European XFEL

5 cells (uniform) — Single crystal monochromator — 5 cells (uniform) — Single crystal monochromator — 22 cells (8 uniform, 14 tapered)

Pulse energy $\simeq 10$ **mJ**

6.5×10^{12} ph/pulse @ 9.1 keV

Pulse duration $\simeq 15$ fs (FWHM)

Spectral width $\simeq 0.9$ eV (FWHM)

Beam diameter $\simeq 50$ μm (FWHM)

Beam divergence $\simeq 2$ μrad (FWHM)

Peak sp. flux 6×10^{9} **ph/meV/pulse**

Average sp. flux 2×10^{14} **ph/meV/s** $\simeq 10^{3} - 10^{4}$-times more than at synchrotrons

G. Geloni, V. Kocharyan, E. Saldin et al.

High-repetition-rate seeded XFELs

Features

$\simeq 10^4$ times more spectral flux than at storage ring sources

Science

ultra-high-resolution spectroscopies

Novel opportunities for sub-meV inelastic X-ray scattering experiments at the European XFEL

Oleg Chubar, [a] Gianluca Geloni, [b] Vitali Kocharyan, [c] Anders Madsen, [b] Evgeni Saldin, [c] Svitozar Serkez, [c] Yuri Shvid'ko [d] and John Sutter [e]

[a] Brookhaven National Laboratory, New York, United States
[b] European XFEL GmbH, Hamburg, Germany
[c] Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany
[d] Argonne National Laboratory, Argonne, United States
[e] Diamond Light Source Ltd, Didcot, Oxfordshire OX11 0DE, UK

IXS is challenging!

The smaller ΔE is required, the higher indexed Bragg reflection at higher photon energy E has to be used.

Example: $\Delta E = 0.1$ meV requires $E = 31$ keV

Low flux & countrates,

time-consuming experiments:

for $\simeq 10^9$ incident photons only $\simeq 1$ scattered photon in the detector

Angular Dispersion

An asymmetrically cut crystal behaves like a diffraction grating dispersing photons with different photon energies: **effect of angular dispersion.**
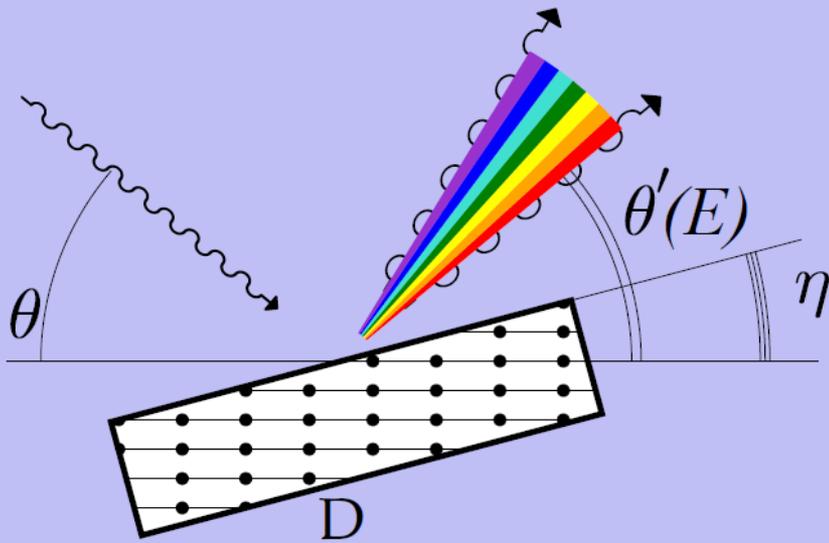
M. Kuriyama and W.J. Boettinger, *Acta Cryst.*, **A32** (1976) 511

T. Matsushita and U. Kaminaga, *J. Appl. Crystallogr.*, **13** (1980) 472

Yu. Shvyd'ko, *X-Ray Optics*, Springer-Verlag **(2004)**

Angular Dispersion

An asymmetrically cut crystal behaves like a diffraction grating dispersing photons with different photon energies: **effect of angular dispersion.**
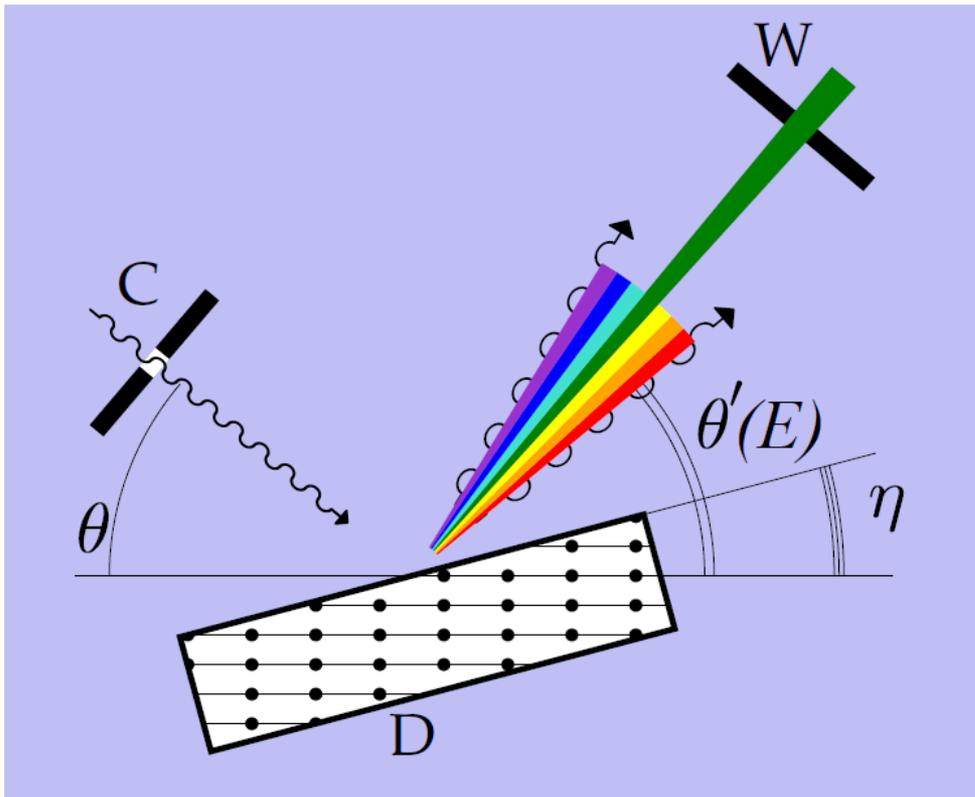
C - collimator

D - dispersing element

W - wavelength selector

Yu. Shvyd'ko, *X-Ray Optics*, Springer-Verlag (2004)

Angular dispersion: overcoming limitations set by the Darwin width.

A proof-of-principle x-ray spectrometer for ultra-high-resolution IXS applications (UHRIX) has been developed, built, and recently tested at the APS

The work is in progress to demonstrate an IXS spectrograph with 0.1 meV and $\lesssim 0.1$ nm^{-1} resolution.

UHRIX utilizes 9 keV x-ray photons. It is applicable therefore at XFEL facilities.

Wafront Propagation of the XFEL Pulse Through X-ray Optic to the Sample

$\Delta E \simeq 1$ eV

source point in the output undulator

$\simeq 33$ meV   0.1 meV   < 5 μm

CRL$_1$ offset mirror   HHLM   CDDW+W   CRL$_s$ sample

Fluence

$2.5 \times 5 \mu m^2$

Vertical Position / Horizontal Position

Spectral Energy

Spectral Energy [J/eV] vs Photon Energy
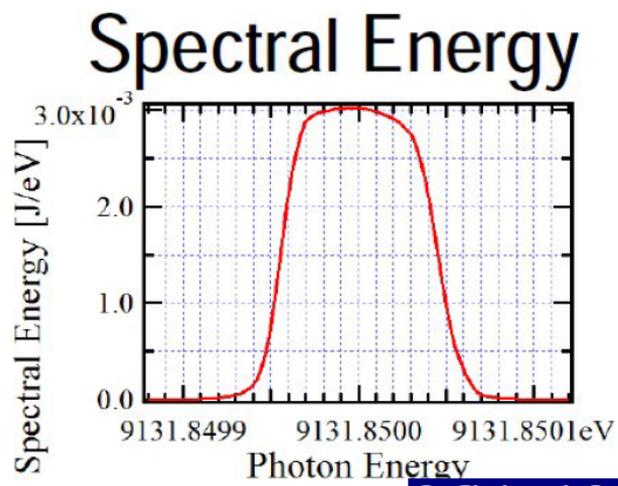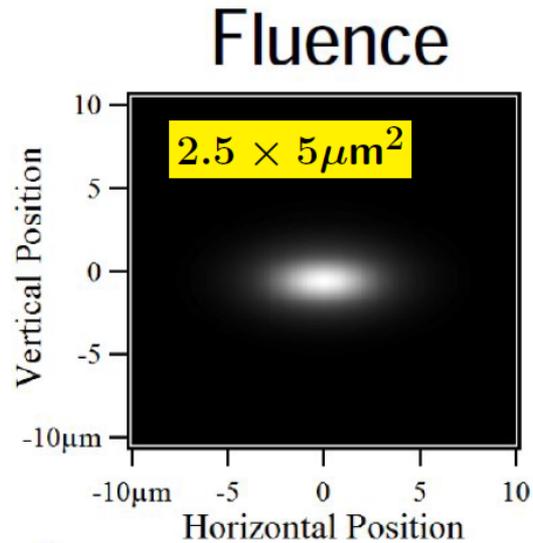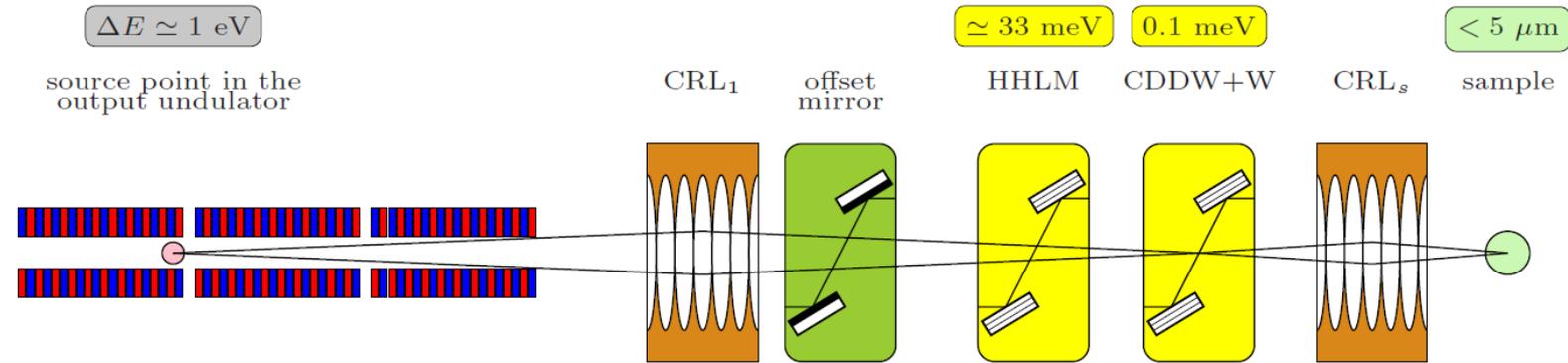
Energy: 0.27 μJ $\Rightarrow$ 2×10^8 ph/pulse

Bandwidth: 0.09 meV

Average sp. flux: 6×10^{13} ph/meV/s

$> 10^3$ than at the APS

O. Chubar, J. Sutter et al.

THEORY predicts XFELs may allow high resolution imaging of single particles / molecules

Neutze, Wouts, van der Spoel, Weckert, Hajdu *Nature* 406, 752-757 (2000)

X-ray free-electron lasers may enable atomic-resolution imaging of biological macromolecules

One pulse, one measurement

Particle injection

10-fs pulse

Noisy diffraction pattern

H. Chapman
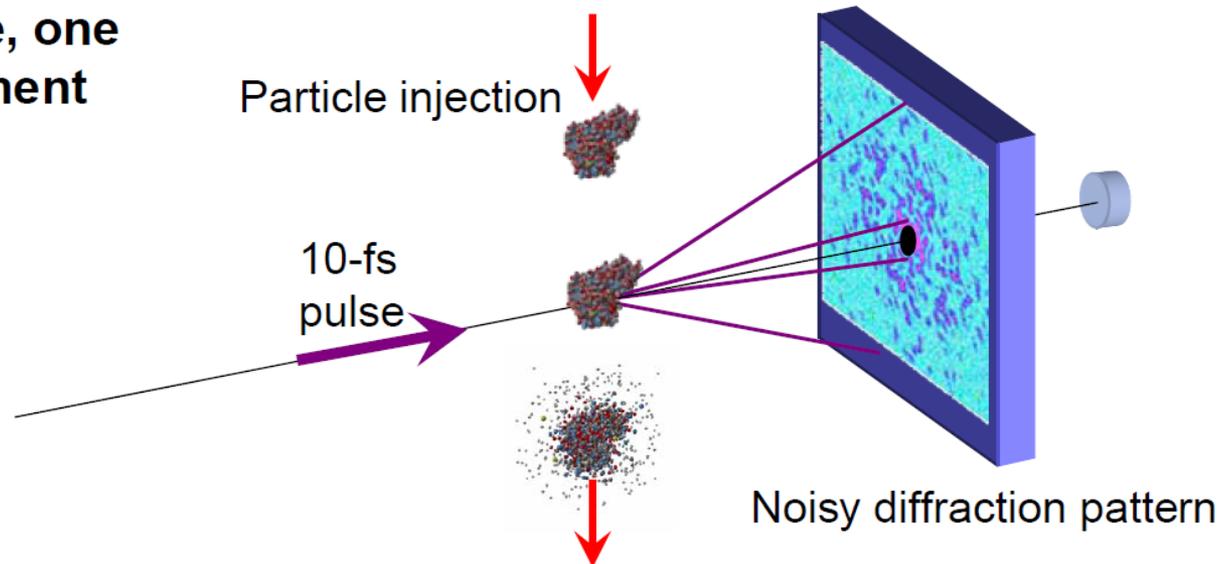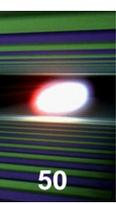
Imaging of a single protein molecule…

…can we solve this problem at European XFEL in its baseline configuration?

Perspectives for Imaging Single Protein Molecules with the Present Design of the European XFEL

Kartik Ayyer,[1] Gianluca Geloni,[2] Vitali Kocharyan,[3] Evgeni Saldin,[3] Svitozar Serkez,[3] Oleksandr Yefanov,[1] and Igor Zagorodnov[3]

[1] *Center for Free-Electron Laser Science, Hamburg, Germany*
[2] *European XFEL GmbH, Hamburg, Germany*
[3] *Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*

Simulations Flowchart

Electron source

| Injector -ASTRA- | → | ACC1 -ASTRA- | → | ACC39 -ASTRA- | → | Laser Heater -CSRtrack- | → | Straight section -ASTRA- | → | Dogleg -CSRtrack- |

| BC0 -CSRtrack- | → | Linac1 -ASTRA- | → | BC1 -CSRtrack- | → | Linac2 -ASTRA- | → | BC2 (+slotted foil) -Elegant- | → | Linac3 -ASTRA- |

X-ray source

| SASE1 undulator (first part) -Genesis- | → | Self-seeding setup -SCRYM- | → | SASE1 undulator (second part) -Genesis- | → | SPB X-ray optics -SRW- |

X-ray/ sample interaction

| Atomic structure factor determination -MOLTRANS- | **Detector effects** | Noise and quantum efficiency -CORREL- | **Data analysis** | 3D reciprocal space orientation -EMC- |

In this talk: consider one case study
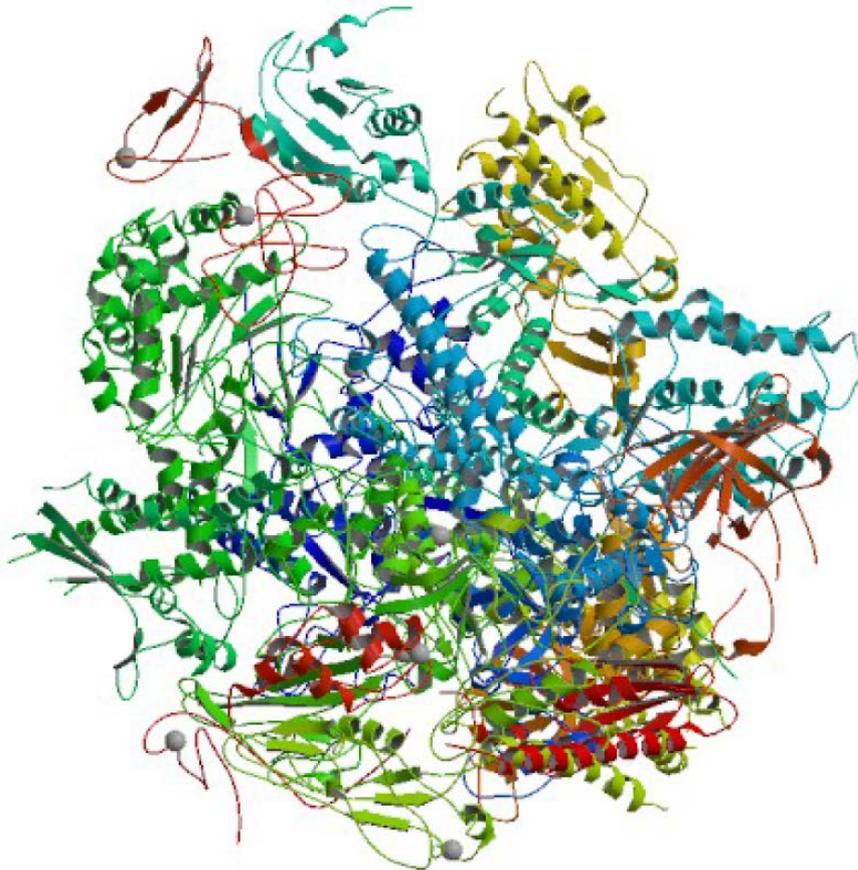
- RNA Pol II   size w ~ 15 nm
- 30000 atoms
- Wanted resolution : 0.4 nm
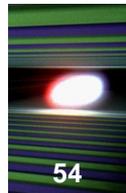
- Object with width w → speckles of minimal size $2\pi/w$

- Shannon interval $\Delta q_s = \pi/w$

- Average #photons per $\Omega_p \sim \lambda^2/(2\pi)^2(\Delta q_s)^2 = \lambda^2/(2w)^2$:

$$\langle N_p \rangle = F \cdot P \cdot r_e^2 N_{\text{atom}} |f|^2 \frac{\lambda^2}{4w^2}$$

- For our molecule: F=10^{13} ph/(100 nm)^2 → $\langle N_p \rangle \sim 1.5$ per Shannon pixel at 4 keV

- To avoid damage: ~ < 5 fs long. Here we assume 4fs

- F=10^{13} ph/(100 nm)^2, 4fs pulse, 4keV → 6mJ → 1.5 TW

- **Note: 1TW at 4keV gives the same #ph as 27 TW at 12 keV!**

- Available with baseline SASE FELs: order of 100 GW vs. needed: 1.5 TW → **Self-seeding + Tapering?**
- Also, we need to transport and focus:

B$_4$C 50 nm on Si at 4100 eV
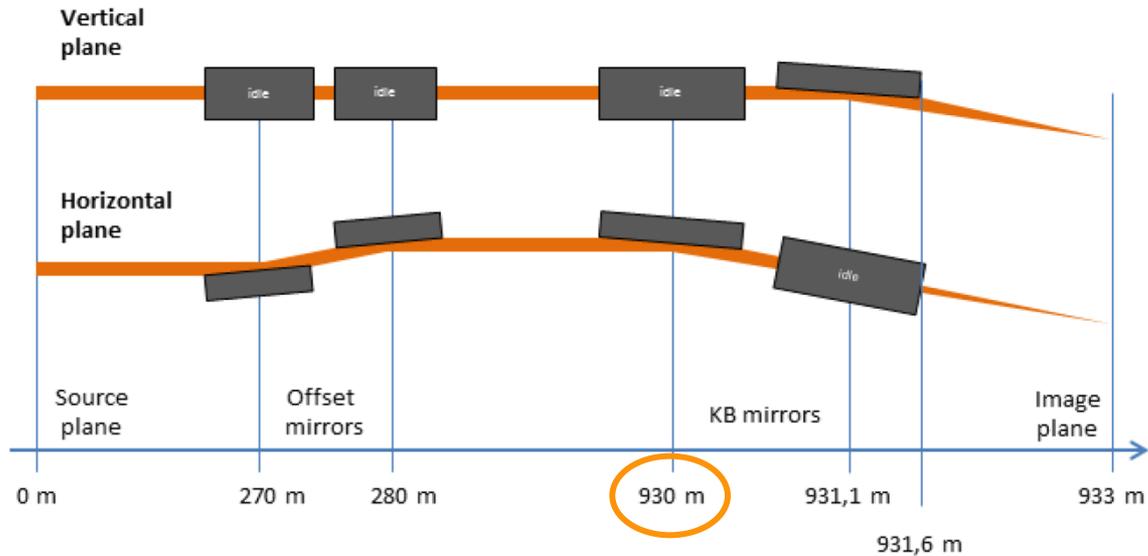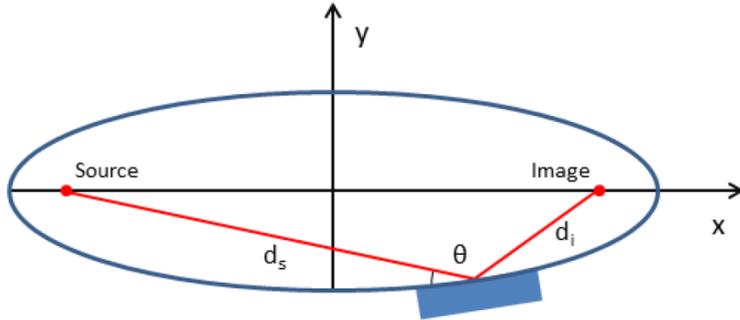
KB system: 100nm spot size (ok for w ~ 15nm)

Elliptical mirror → only one working angle without aberrations

- Selected angle: 3.5 mrad

    B$_4$C coating between 3keV and 7keV

    Ru   coating between 7keV and 16 keV

- 950mm clear aperture @ 3.5mrad

    → 3.3 mm available lateral aperture
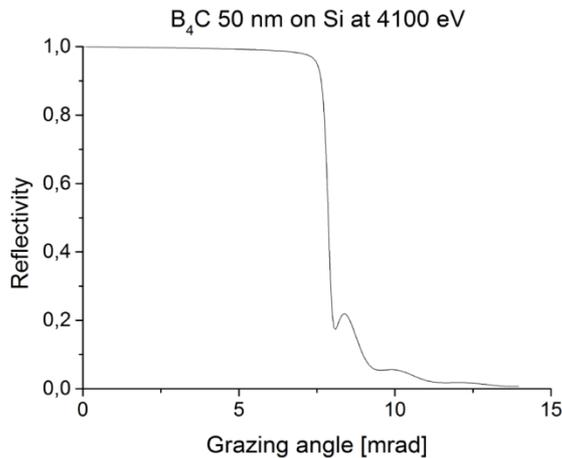
BUT

4fs photon pulse pulse length → 20pC charge → lowest emittance →shortest gain length → largest divergence ~ 5μrad FWHM @ 4keV

900m x 5μrad x 1.7~8mm required lateral aperture

HXRSS with special accelerator mode of operation
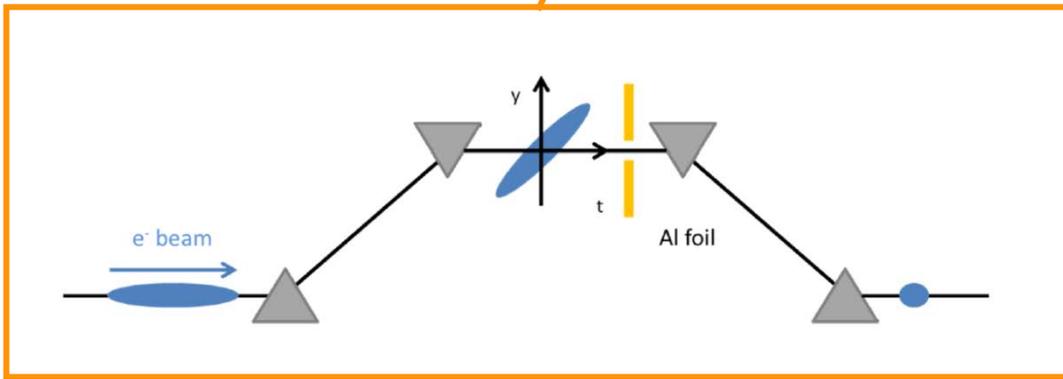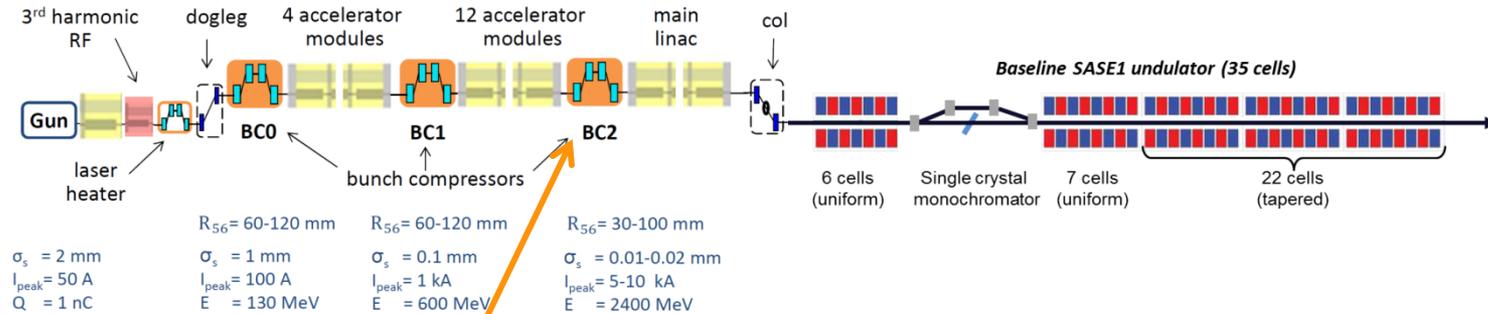
Insert a slotted foil in the last chicane (method invented and experimentally proven at the LCLS)

- **PRL 92, 074801 (2004).**
- **P. Emma, M. Cornacchia, K. Bane, Z. Huang, H. Schlarb, G. Stupakov, D. Walz (SLAC)**
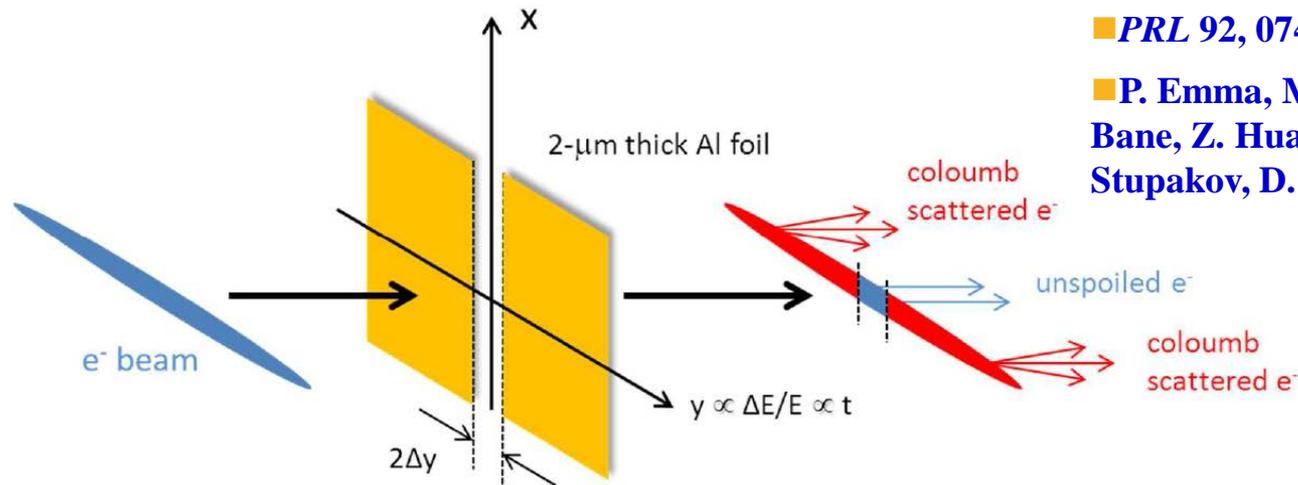
PRL 92, 074801 (2004).

P. Emma, M. Cornacchia, K. Bane, Z. Huang, H. Schlarb, G. Stupakov, D. Walz (SLAC)

2-μm thick Al foil

coloumb scattered e⁻

unspoiled e⁻

coloumb scattered e⁻

e⁻ beam

$y \propto \Delta E/E \propto t$

$2\Delta y$

1 nC
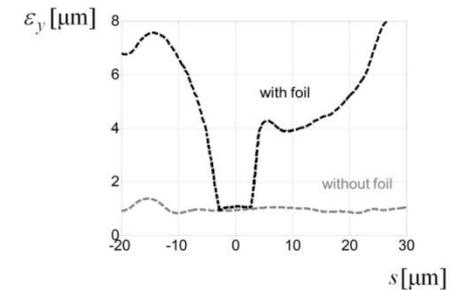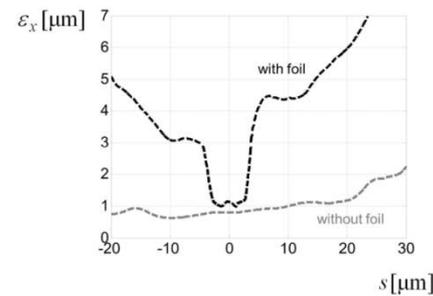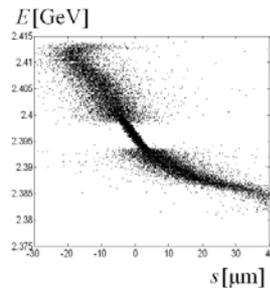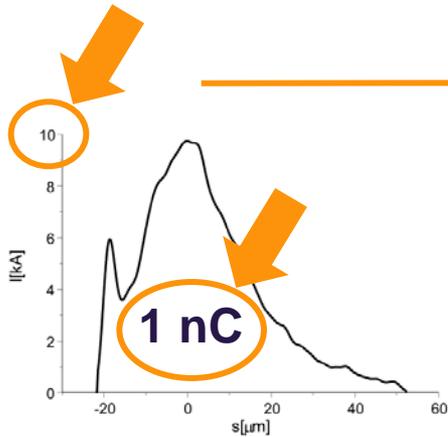
Advantage: pulse duration tunable decoupled from charge and hence from divergence. Here: 4fs and 12fs radiation pulse length

Baseline SASE1 undulator (35 cells)

| | 6 cells (uniform) | Single crystal monochromator | 7 cells (uniform) | 22 cells (tapered) |
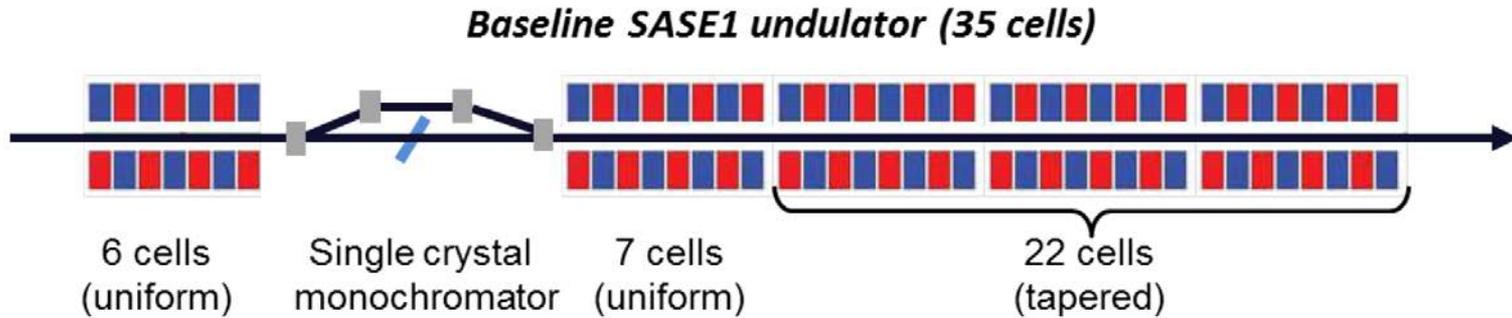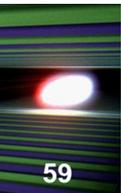
	Units	
Undulator period	mm	40
Periods per cell	-	125
Total number of cells	-	35
K parameter (rms)	-	3.217
Intersection length	m	1.1
Wavelength	nm	0.302
Energy	GeV	14
Charge	nC	1

Baseline SASE1 undulator (35 cells)

6 cells (uniform) — Single crystal monochromator — 7 cells (uniform) — 22 cells (tapered)

$x \equiv [110]$
$z = [001]$
$100\ \mu m$
y
Pitch
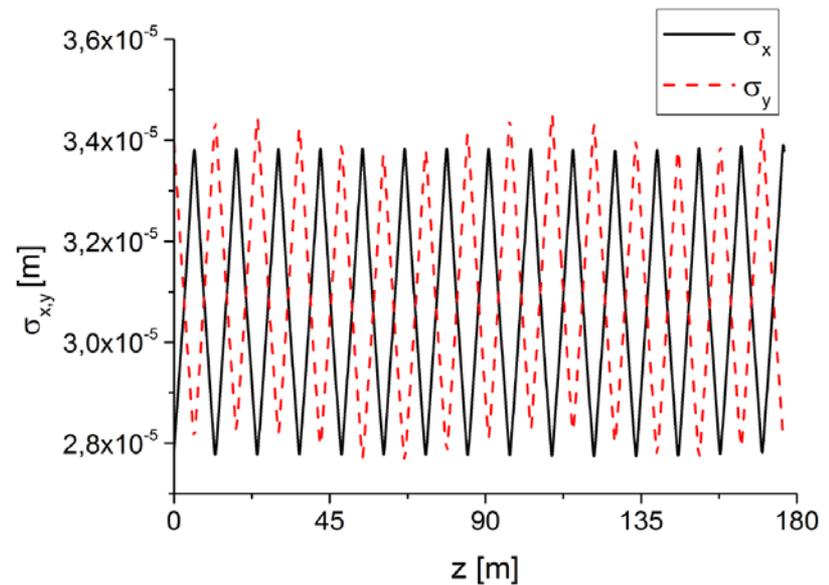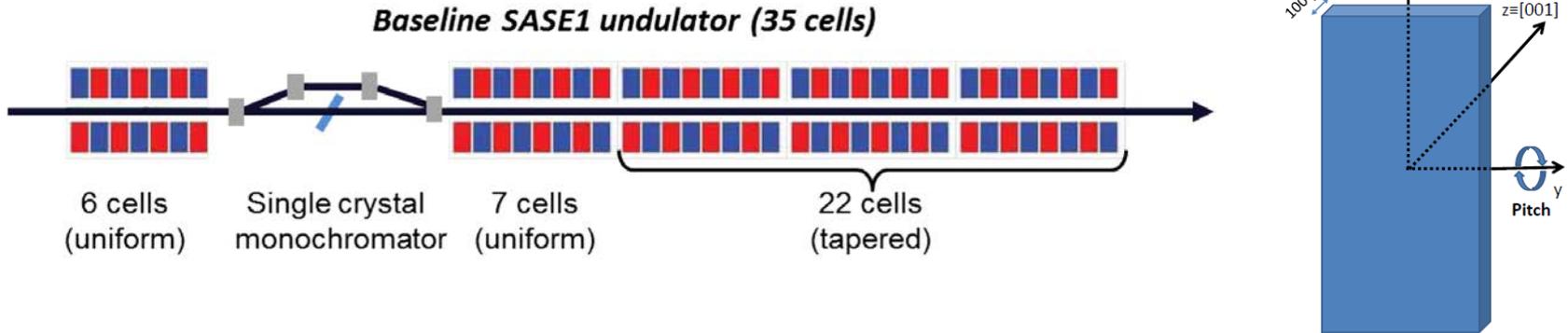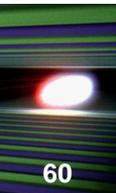
Assumes a crystal arrangement similar to that at the LCLS

Bragg planes
$\psi_0 = 11.9°$ $\psi_n = -35.3°$ $\psi_h = -82.5°$
$\theta_B = 47.2°$ $\theta_B = 47.2°$
s_h
Crystal surface
Diffracted direction
Incident direction
C(111) at 4.1keV
Laue geometry
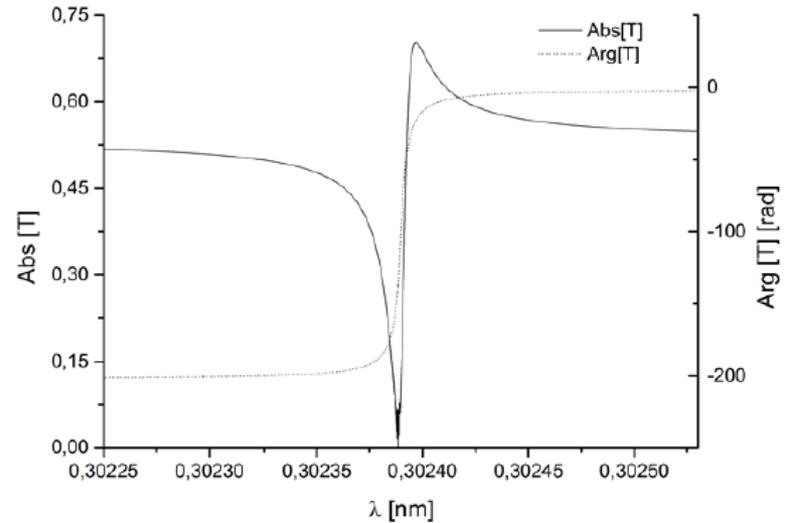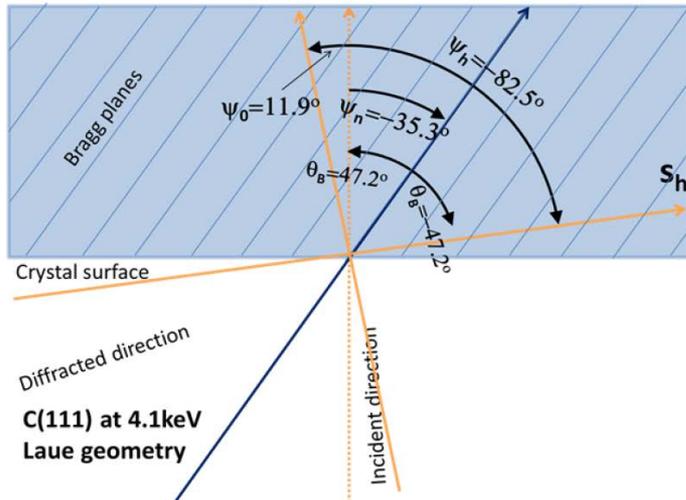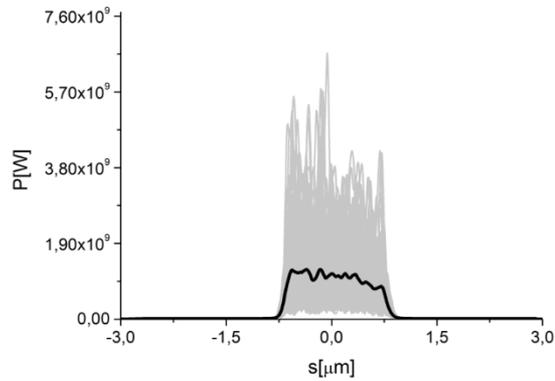
At the crystal

Tapering law
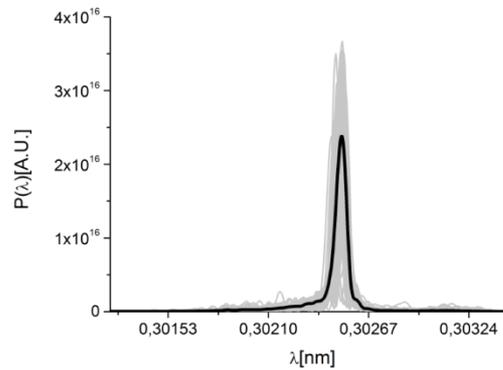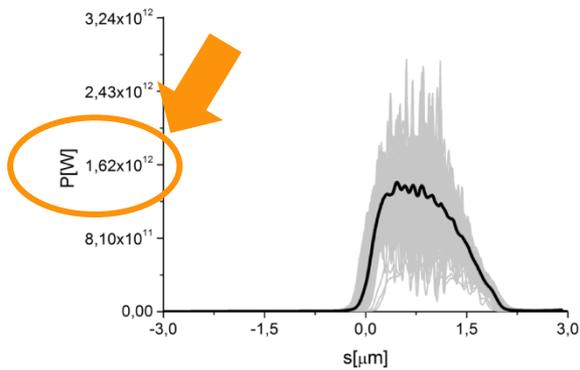
Output
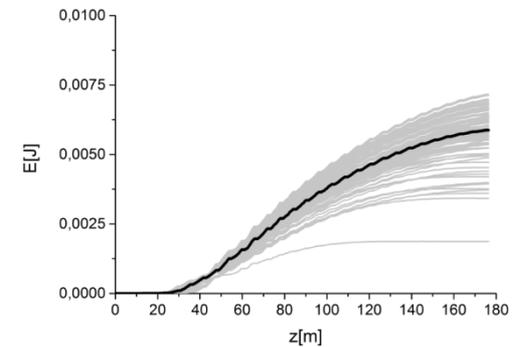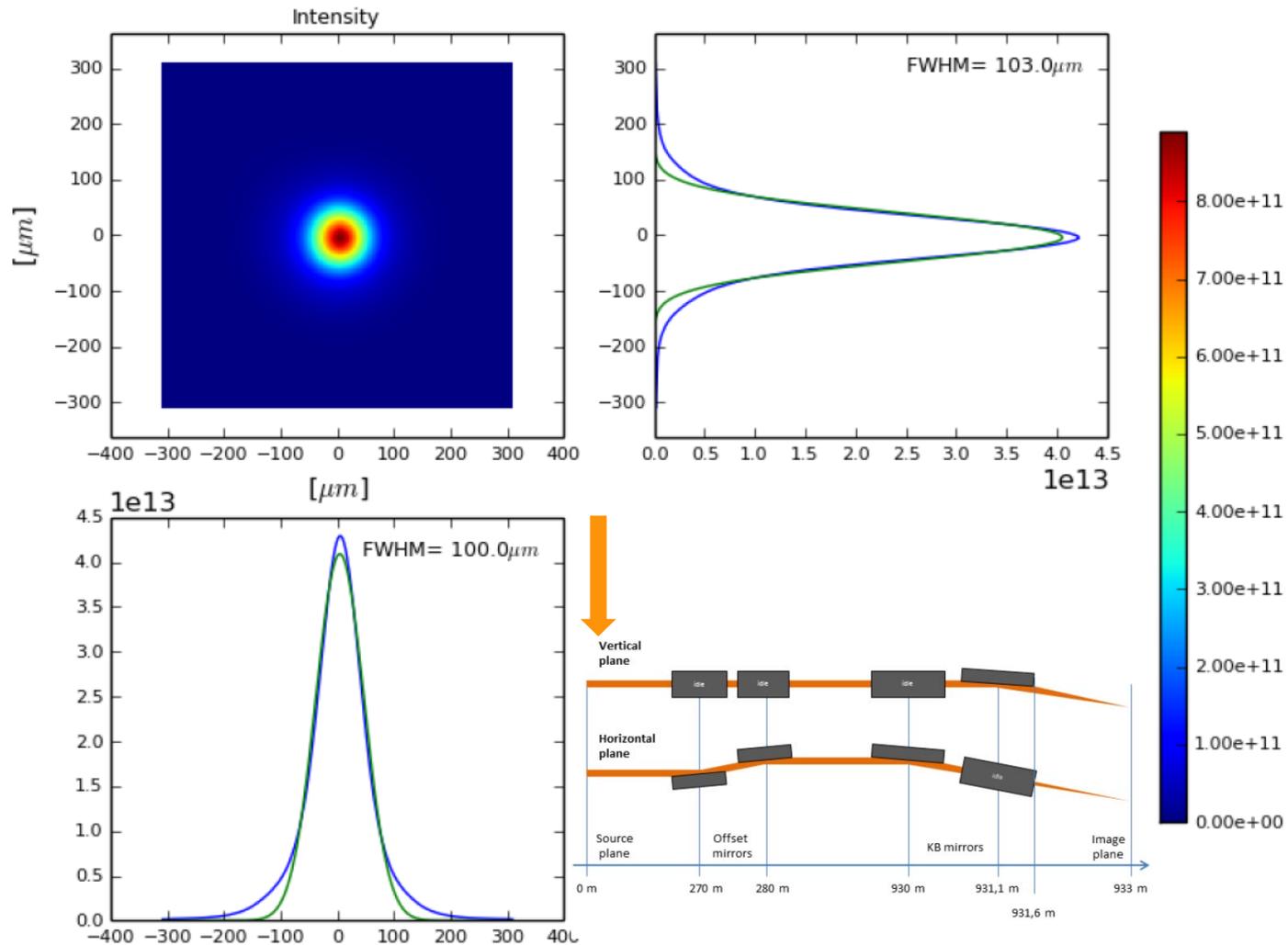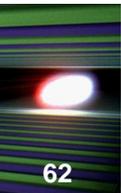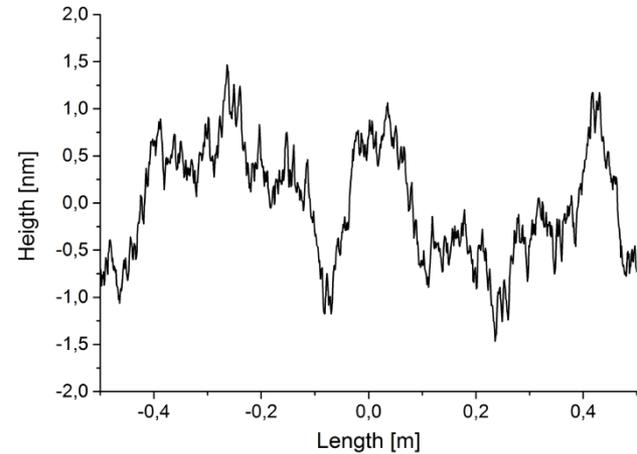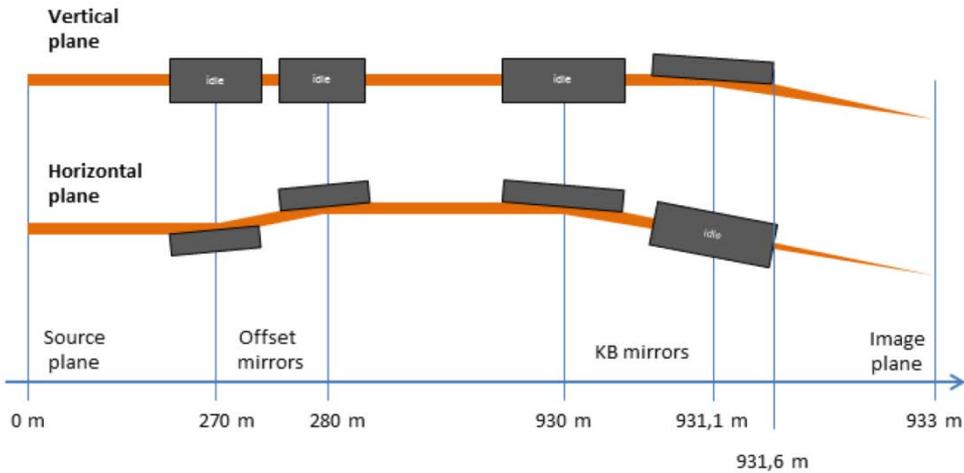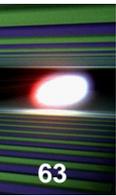
$$2h_{\mathrm{rms}}\theta_i \sqrt{N} < \lambda/14$$ → **rms height ~ 1nm**

$$\Delta\varphi = 2kh\sin\theta$$

Incident wavefront

Reflected wavefront

θ

$h(x,z)$
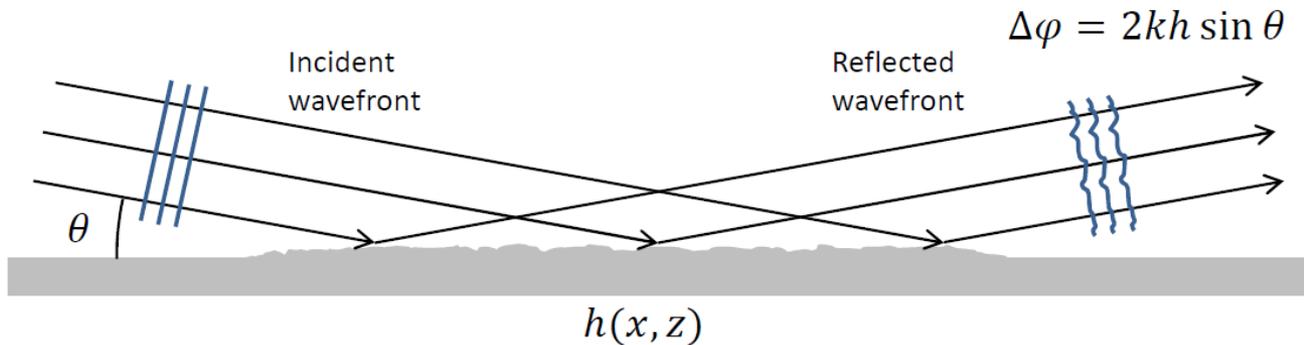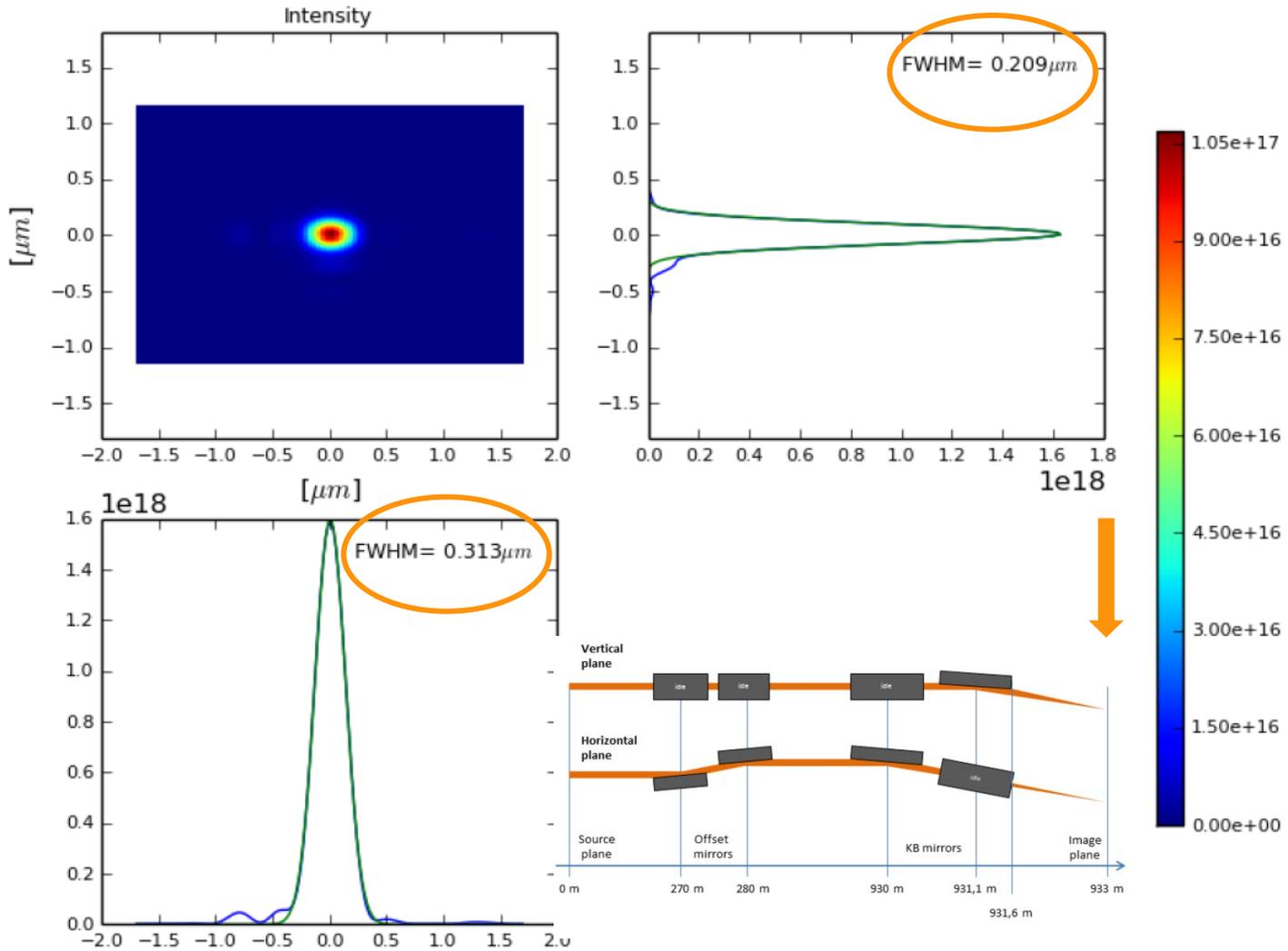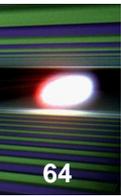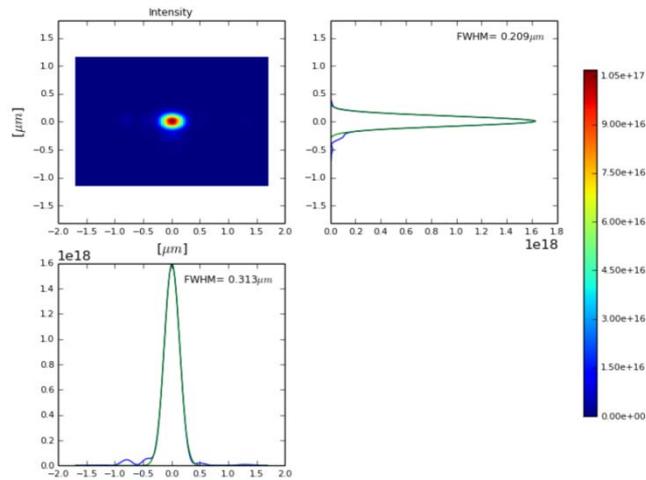
$$F = N_p/S$$

$$N_p \sim 10^{13}$$

$$\frac{1}{S} = \frac{\max(W)}{\int W(x,y)\,dxdy} \sim 1.5 \cdot 10^9 \text{ cm}^{-2}$$

→ At present design

→ F~ $1.5 \cdot 10^{22}$ ph/cm^2

This fluence we used in our simulations
of data processing
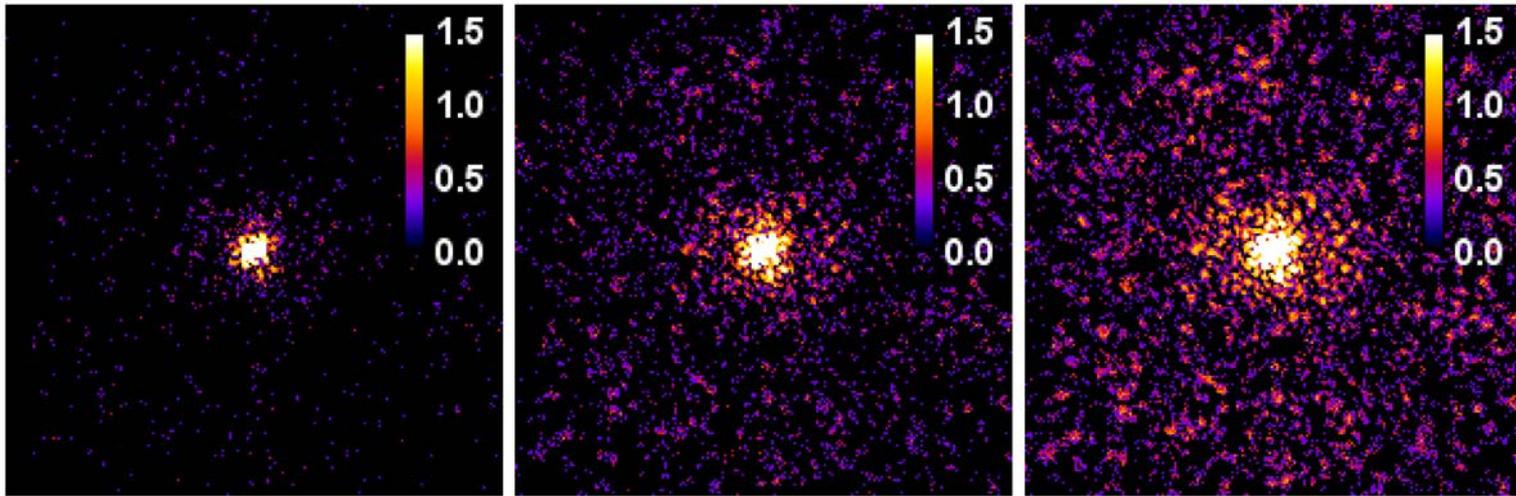
F~ $1.5 \cdot 10^{22}$ ph/cm^2 F~ $0.5 \cdot 10^{23}$ ph/cm^2 F~ $1.0 \cdot 10^{23}$ ph/cm^2

E photons = 4.1 keV.

Detector: 200 mm by 200 mm in size

Detector location: 100 mm from sample.

Detector rim → 0.39 nm resolution (100 mm from sample).

Shannon pixel size → 2 mm.

Physical Pixel array dimensions: 200 μm x 200 μm → 1 Mpix

Simulated pixel array: 200x200 (pixel size = 1mm) → s=2; b=5

Active (blue), Dead (grey), free (green)
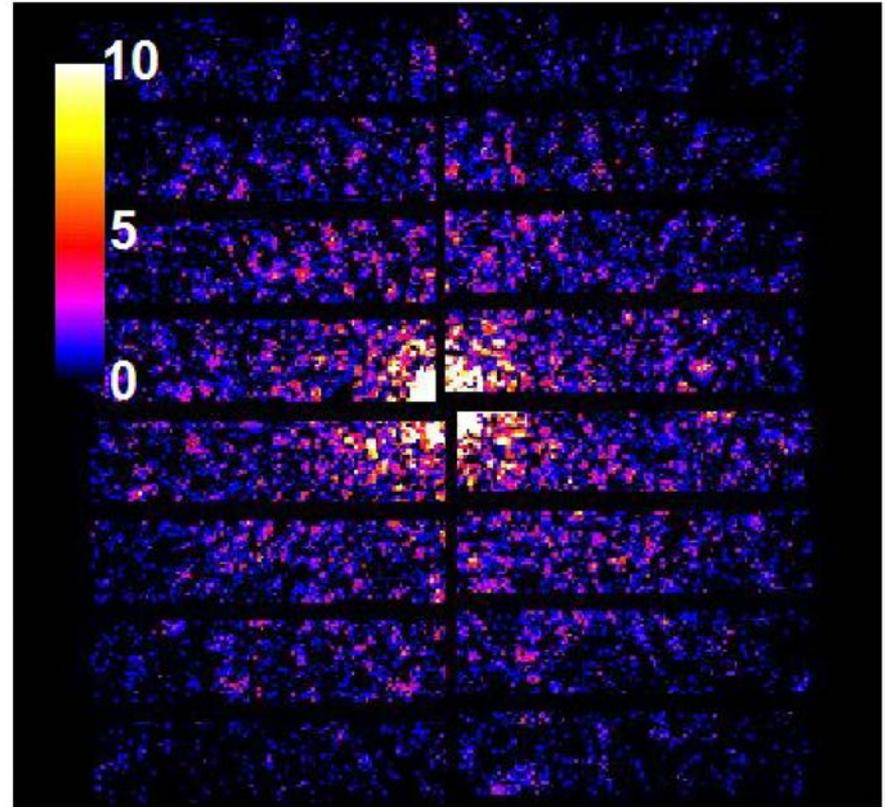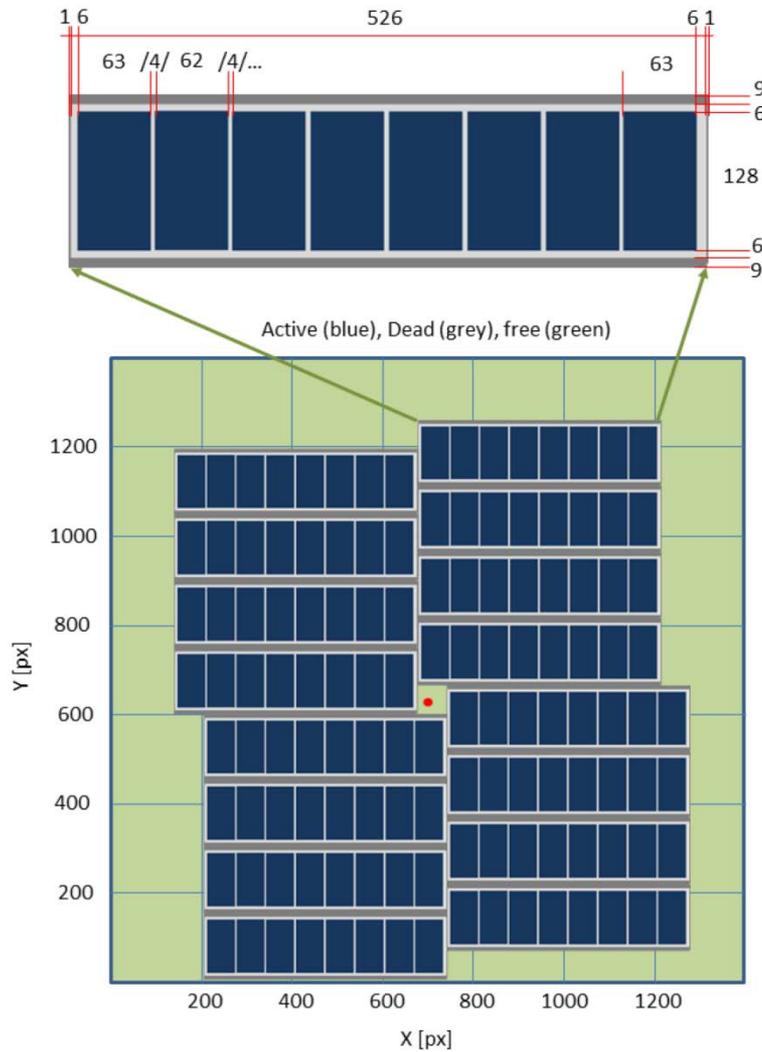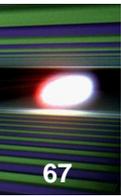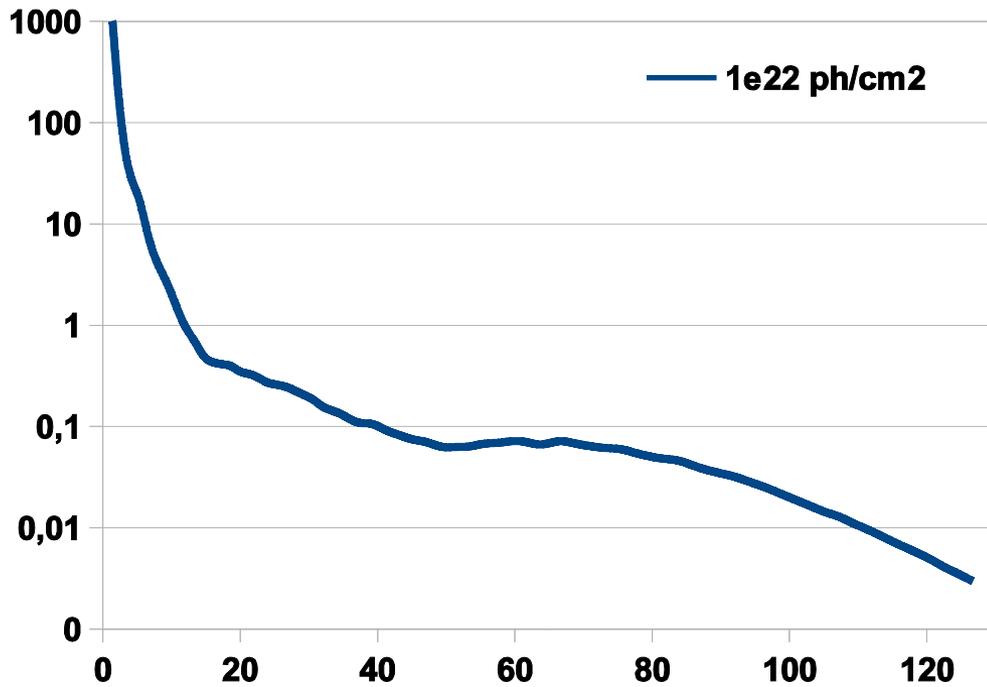
■ Radial average of the photon counts per pixel vs. position along the detector in mm, starting from the center of the detector.
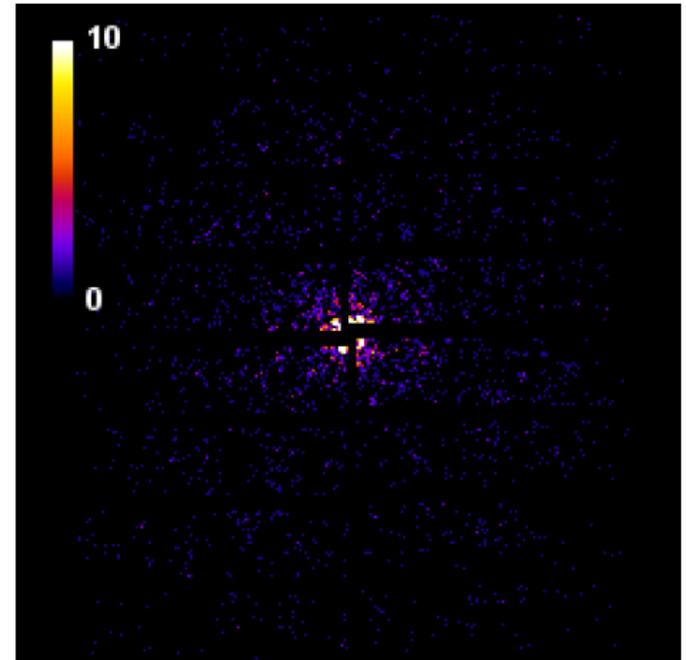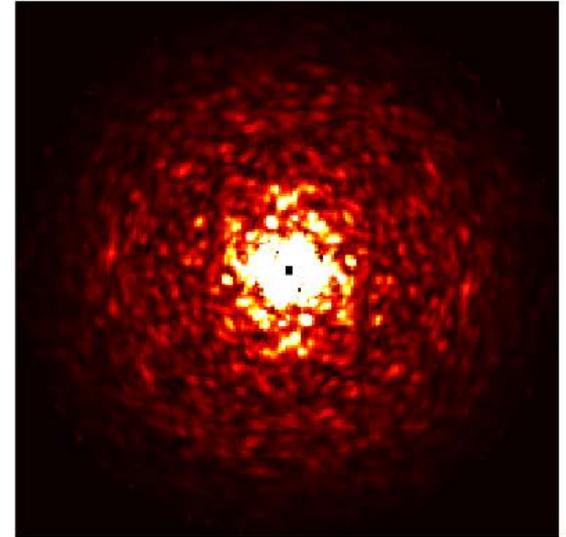
■ Simulated diffraction pattern from the RNA pol II test objectas seen by AGIPD detector at a fluence of 10^{22} photons/cm^2
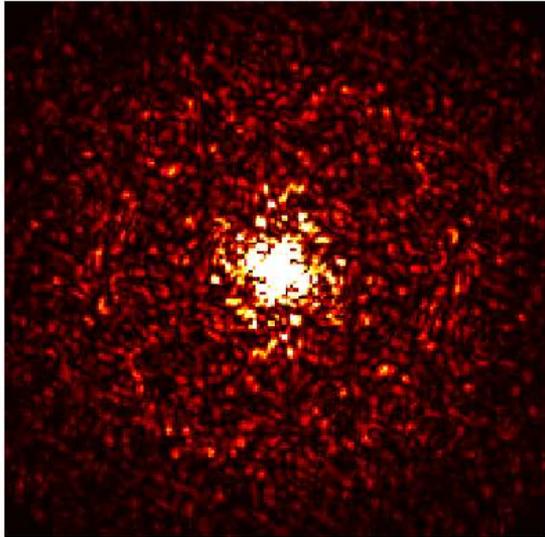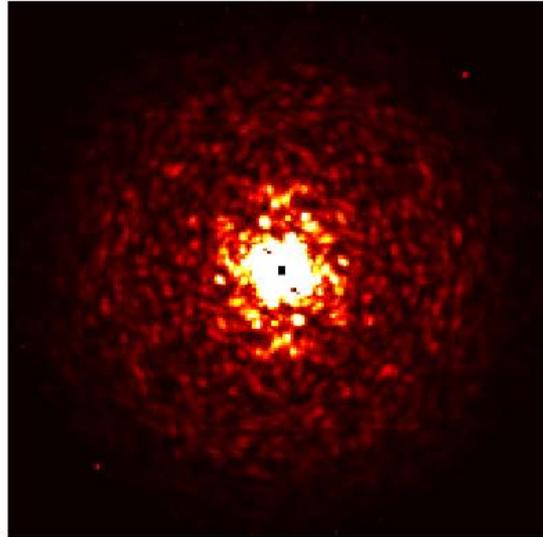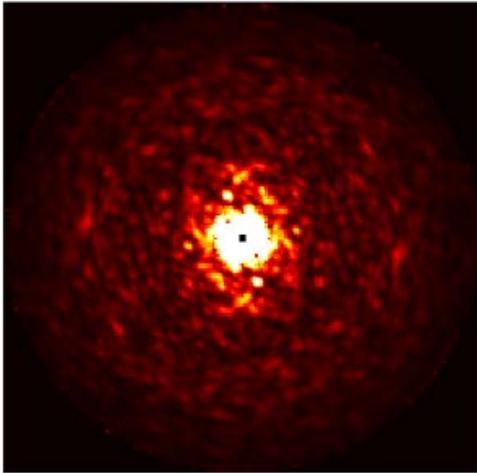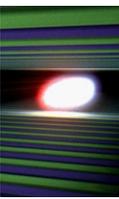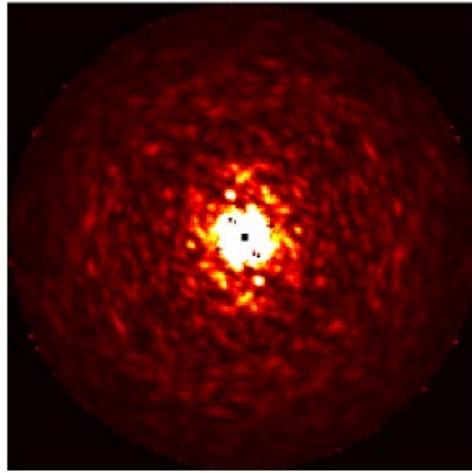
(a) Central slice through the ideal intensity distribution of the RNA Pol II distribution.
(b) Reconstructed intensities using 30,000 patterns with 4000 ph/pattern.
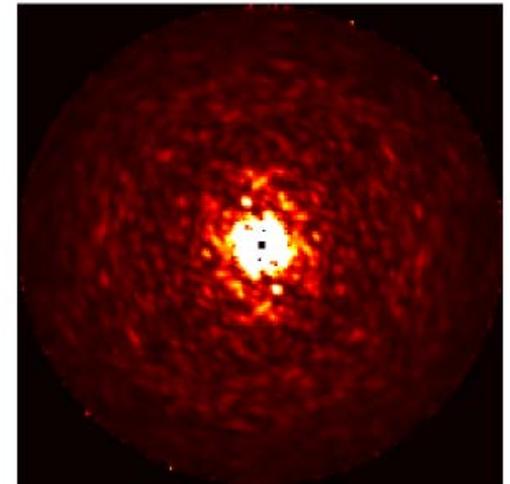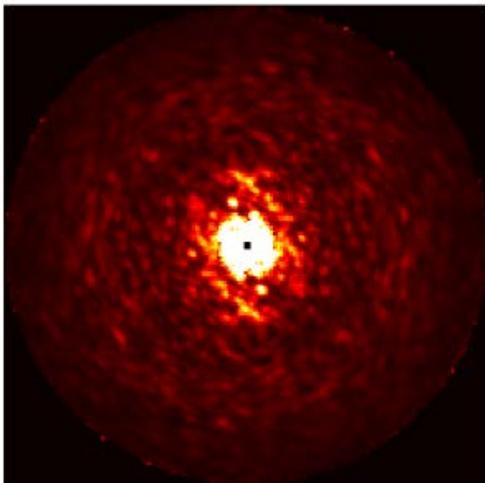(c) Same, using 300,000 patterns with 400 ph/pattern.
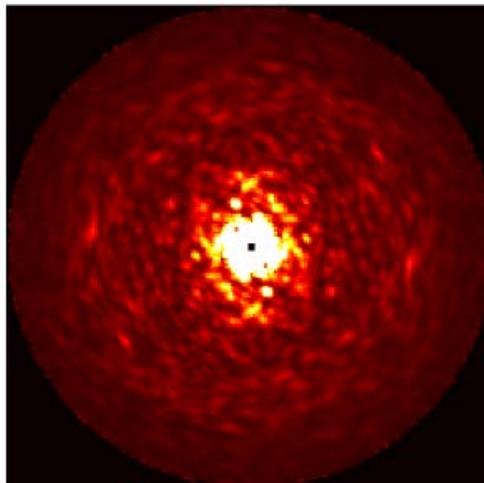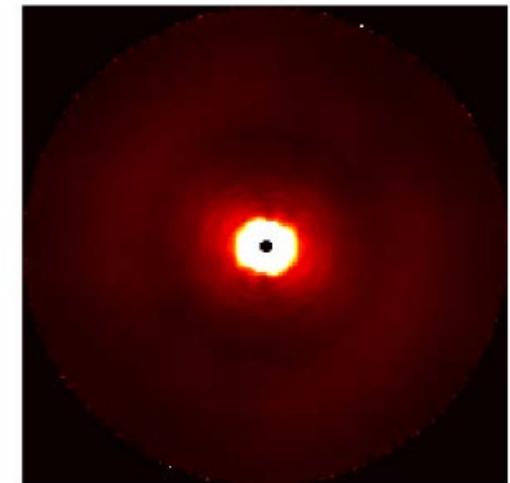
(a) 40 ph/pattern

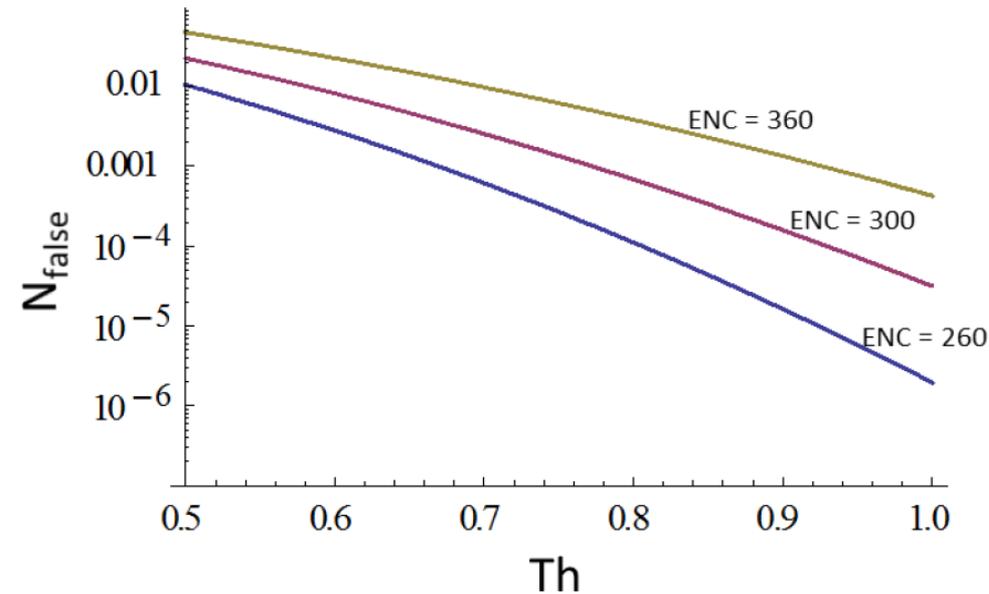(b) 120 ph/pattern

(c) 160 ph/pattern

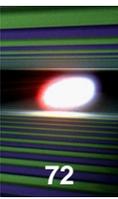(d) 200 ph/pattern

(e) 400 ph/pattern

(f) 600 ph/pattern

- Charge amplification in detectors → Noise

- Equivalent noise charge: for AGIPD less than 300 electrons (ENC)

- 1ph@4keV → 1200 electrons

- Assuming Gaussian-distribution random noise in a pix:

$$N_{\text{false}} = \frac{1}{2}\text{erfc}\left(\frac{\text{Th} \cdot N_e}{\sqrt{2}\text{ENC}}\right)$$

Detector noise (intrinsic) negligible

Our results indicate that one can achieve diffraction without destruction with about 0.1 phonons per Shannon pixel per shot at 0.4 nm resolution with 10^{13} photons in a 4 fs pulse at 4 keV photon energy and 300 nm focus, corresponding to fluence 10^{22} ph/cm^2 .

At signal level of 4000 ph/pattern (corresponding to incident fluence 10^{22} ph/cm^2) background level should be < 2000 ph/pattern

At this signal and background level one needs only about 30,000 diffraction patterns to recover full 3D information.

At highest repetition rate manageable by detector at European XFEL (~3000 per second), one is able to accumulate these data within a fraction of an hour, even assuming a relatively low hit probability of about one percent

1. Self-seeded European XFEL offers a unique opportunity for single-biomolecule imaging with high-rate of protein structure determination.

2. High-repetition rates of self-seeded European XFEL offer a unique opportunity for sub-millivolt inelastic X-ray scattering for nano- and mesoscale science

Yaroslav Derbenev, a member of Jlab's Center for Advanced Studies of Accelerators

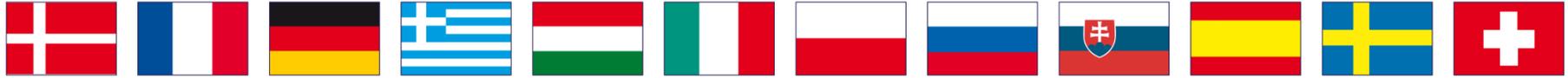Anatoly Kondratenko, Director of laser company (Russia)

I would like to express my gratitude to Yaroslav Derbenev and Anatoly Kondratenko, who have been teachers and colleagues to me. I feel extremely lucky to have worked for five years alongside such fantastic and dedicated scientists and researchers

BUDKER INSTITUTE OF NUCLEAR PHYSICS

NOVOSIBIRSK, RUSSIA

35 years ago XFELs were not even dreamt of.

Now they are real and this revolution has begun with FLASH, LCLS, SACLA, FERMI...

and will be continued with Swiss FEL, PAL, European XFEL

Thank you for your attention.
Any questions?