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X-ray free-electron lasers and ultrafast science at the atomic and molecular scale.

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Outline



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1. Introduction
2. Free-Electron Laser (FEL) physics and basic properties of the radiation
3. Present FEL experimental state of the art.
4. Directions of development and challenges
5. Conclusions

Introduction: X-Ray FELs



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The interest in X-ray FELs is motivated by their characteristics of tunability, coherence, high peak power, short pulse length. They can explore matter at the length **and** time scale typical of atomic and molecular phenomena, the Bohr atomic radius, about 1 Å, and the Bohr period of a valence electron, about 1 fs.

The large number of coherent photons/pulse and short pulse duration of X-ray FELs opens the door to do:

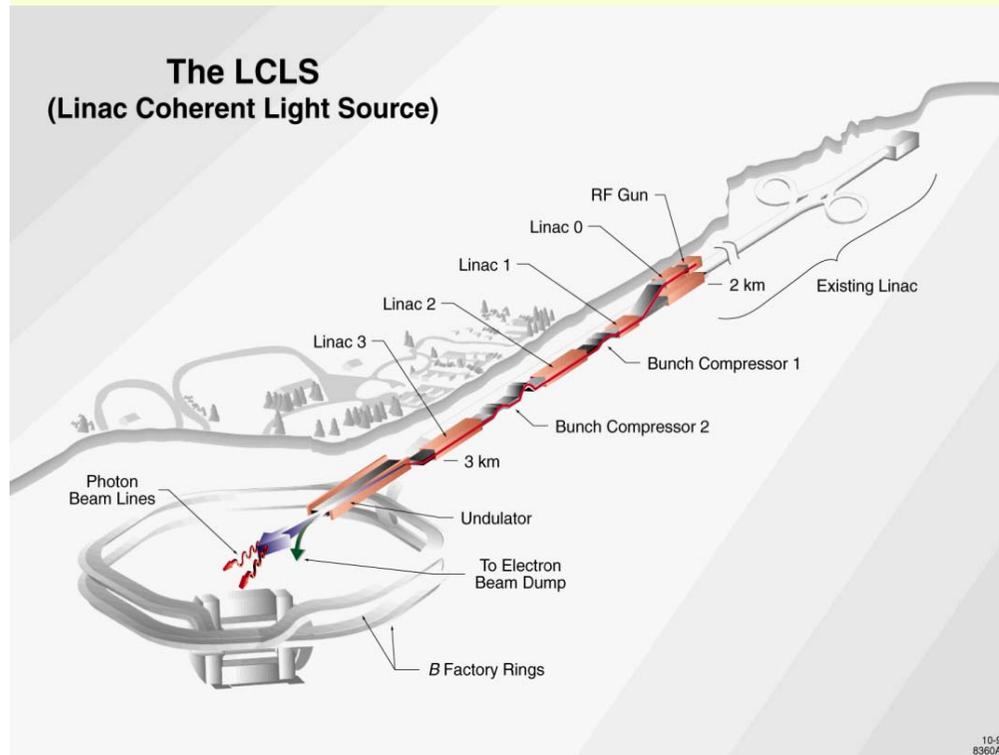
- a. single shot measurements of the structure of complex molecules, like proteins, and nanoscale systems;
- b. study of non linear phenomena;
- c. study of high energy density systems.

Using all these properties matter can be explored with X-ray FELs at an unprecedented time-space resolution.

Status of X-Ray FELs Projects



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After many years of research and development, going as far back as the 1980s, the first X-ray free-electron laser (X-FEL) operating in the 0.15 to 1.5 nm wavelength range, the LCLS, that I first proposed in 1992, is now being built and will be completed by 2009.

LCLS uses 1 km of the SLAC linac: beam energy ~ 15 GeV, $I_{\text{peak}} \sim 3.4$ kA, normalized emittance ~ 1.2 mm mrad, pulse duration ~ 100 fs.

The LCLS electron beam will be the brightest ever produced.

LCLS radiation characteristics



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Wavelength (fundamental)	1.5	0.15	nm
Undulator period/parameter	3/3.4		cm
Undulator length	130		m
Peak saturation power	4	8	GW
Pulse length, FWHM	140	76	μm
Photons per pulse	10.6	1.1	$\times 10^{12}$
Peak brightness	0.28	15	$\times 10^{32*}$

The brightness and peak power are about 10 orders of magnitude above any other source in its wavelength region.

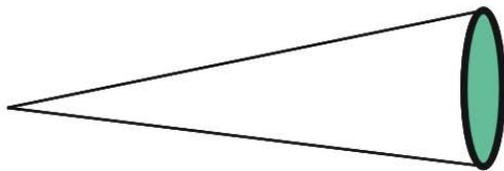
X-rays coherence properties



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The LCLS radiation has unprecedented coherence, about 10^9 photons in a coherence volume. The energy of coherent photons can be pooled to create multi-photons excitations and carry out non-linear X-ray experiments, a largely unexplored area of science.

3rd gen. beam line



coherence volume $1 \times 5 \times 50\mu\text{m}$

contains < 1 photon

LCLS source



coherence volume $0.1 \times 100 \times 100\mu\text{m}$

contains 10^9 photons

World wide Status of X-Ray FELs Projects



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X-ray FELs in Japan and Korea will follow shortly after LCLS. An X-ray FEL is being developed as a European project with a target date of 2012.

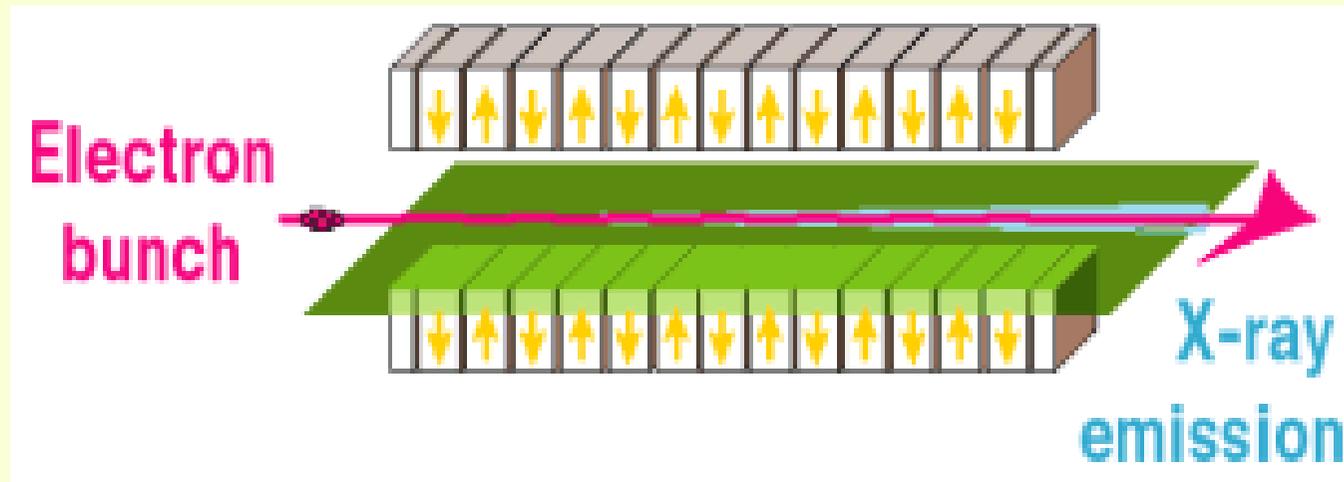
Radiation characteristics are similar to those of LCLS.

More FELs operating from the few to 100 nanometer region, are being designed and built in Asia, Europe and the US.

FEL Physics

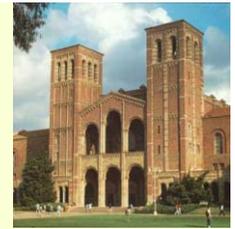


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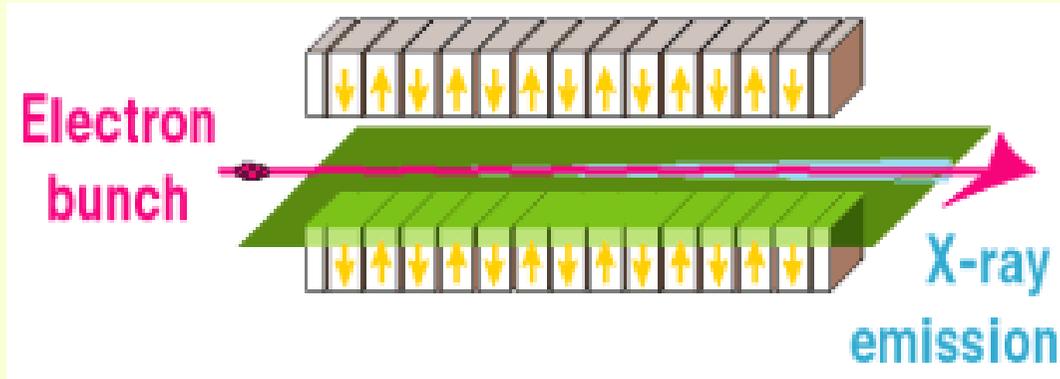


An electron beam executes an oscillation transverse to the direction of propagation in an undulator magnet. An electromagnetic wave co-propagates with the beam and modulates its energy. The electron beam itself radiates a field, which is added to the initial field, and acts on other electrons, establishing a collective interaction. The interaction produces a transition of the beam to a novel state, consisting of micro-bunches separated by the radiation wavelength, and emitting coherent radiation with larger intensity.

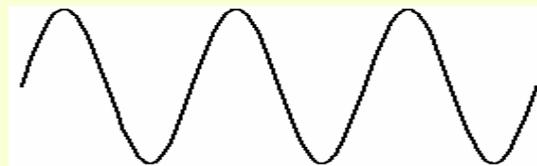
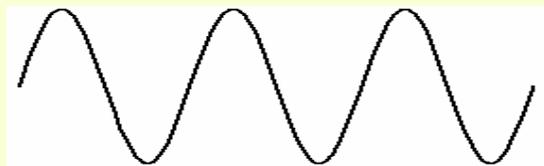
FEL physics: radiation from one electron



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Undulator with N_w periods.



$$\Delta\lambda/\lambda = 1/N_w$$



$$N_w \lambda$$



Each electron emits a wave train with N_w waves. The wavelength is:

$$\lambda = \lambda_w (1 + K^2/2 + \gamma^2 \theta^2) / 2\gamma^2$$

$$K = eB_w \lambda_w / 2\pi mc^2$$

For $\gamma = 3 \cdot 10^4$, $\lambda_w = 3$ cm, $K = 3$, $N_w \sim 3300$., $\lambda \sim 0.1$ nm, $\Delta\lambda/\lambda \sim 3 \cdot 10^{-4}$.

Wave train length $N_w \lambda \sim 0.3$ $\mu\text{m} \sim 1$ fs.

FEL physics: radiation from one electron



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Because of the angular dependence of the wavelength the “coherent angle”, corresponding to $\Delta\lambda/\lambda < 1/N_w$, is

$$\theta_c = (\lambda/N_w \lambda_w)^{1/2}$$

And the effective, diffraction limited, source radius

$$a_c = (\lambda N_w \lambda_w)^{1/2}/4\pi$$

with $a_c \theta_c = \lambda/4\pi$. For the X-ray FEL $\theta_c \sim 1 \mu\text{ rad}$, $a_c \sim 10 \mu\text{m}$.

The average number of coherent photons/electron in $\Delta\Omega = \pi\theta_c^2/2$,

$\Delta\lambda/\lambda = 1/N_w$ is

$$N_{ph} = \pi\alpha K^2/(1 + K^2) \sim 0.01,$$

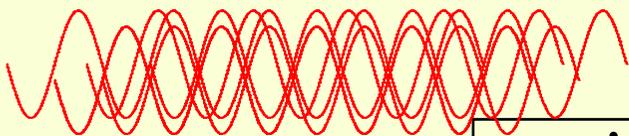
a small number, inefficient process.

FEL collective instability: beam self-organization

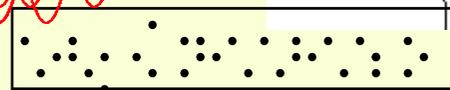


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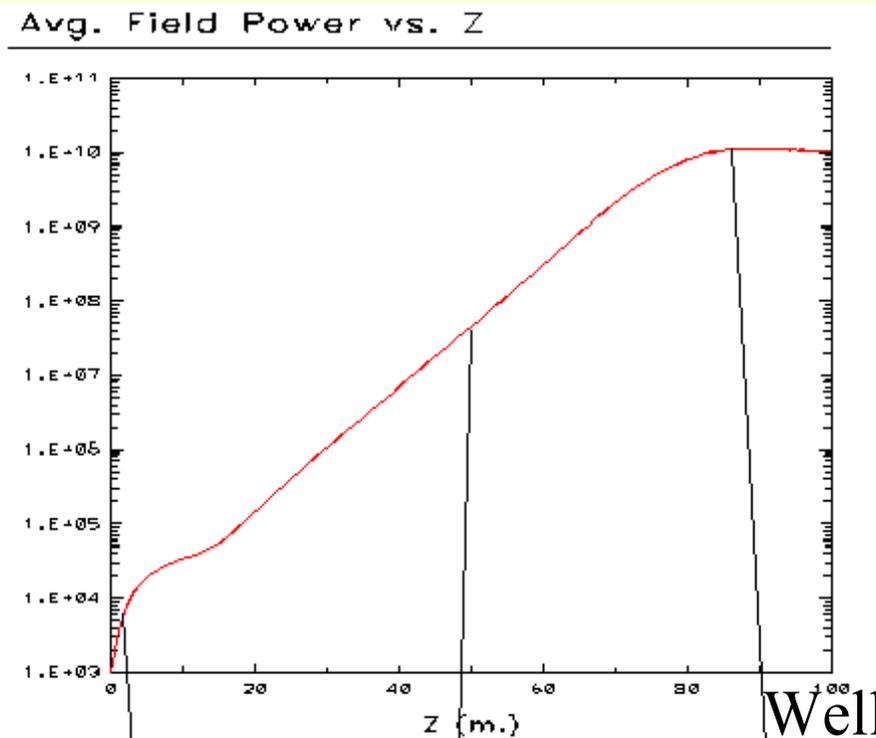
In the initial state the electrons have a random longitudinal position. The wave trains from each electron superimpose with random phases (spontaneous radiation).



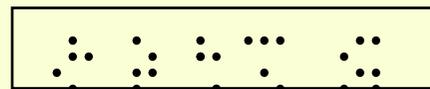
Intensity $\sim N_e$



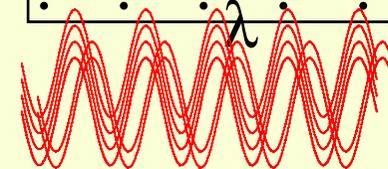
Random



Semi-bunched



Well bunched



In the final state the beam is like a 1-D relativistic crystal.

Final state \rightarrow Intensity $\sim N_e^{4/3} - N_e^2$

FEL collective instability



All key characteristics are given by one universal FEL

Parameter (Bonifacio & Pellegrini): $\rho = \left\{ (K/4\gamma)(\Omega_p/\omega_w) \right\}^{2/3}$

($\omega_w = 2\pi c/\lambda_w$, Ω_p = beam plasma frequency).

- Gain Length: $L_G = \lambda_w / 4\pi\rho$,
- Saturation power: $P \sim \rho I_{\text{beam}} E$
- Saturation length: $L_{\text{sat}} \sim 10L_G \sim \lambda_w / \rho$
- Line width: $1/N_w \sim \rho$

Photons/electron at saturation: $N_{\text{ph}} \sim \rho E/E_{\text{ph}}$. For $E_{\text{ph}} = 10\text{keV}$, $E = 15\text{ GeV}$, $\rho = 10^{-3}$, $N_{\text{ph}} \sim 10^3$, a gain of 5 orders of magnitude. There is still room for increasing the number of photons going beyond saturation by a factor of about 10^4 .

FEL Collective Instability



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The exponential growth occurs if

$\sigma_E < \rho$ (cold beam)

$\varepsilon \sim \lambda/4\pi$ (Phase-space matching) To satisfy this condition we use a large beam energy.

$Z_R/L_G > 1$ Optical guiding (Sessler, Moore, et al.)

These conditions require very high brightness, high peak current beams. X-ray FELs are pushing the science of beam generation, acceleration and control to a new level of sophistication.

Slippage, Cooperation Length, Time Structure



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- The radiation propagates faster than the electron (it “slips” by λ per undulator period); thus electrons communicate with the ones in front; total slippage $S=N_w\lambda$ is also the wave train length.
- The cooperation length (slippage in one gain length)

$$L_c = \lambda / 4\pi\rho$$

(R. Bonifacio, C. Pellegrini, et al., Phys. Rev. Lett. 73, 70 (1994))
defines the longitudinal coherence.

When the FEL starts from spontaneous radiation, noise, the radiation is “spiky”, and the number of “spikes” is the bunch length/ $2\pi L_c$. This is called a SASE-FEL.

SASE-FEL: LCLS pulse time structure



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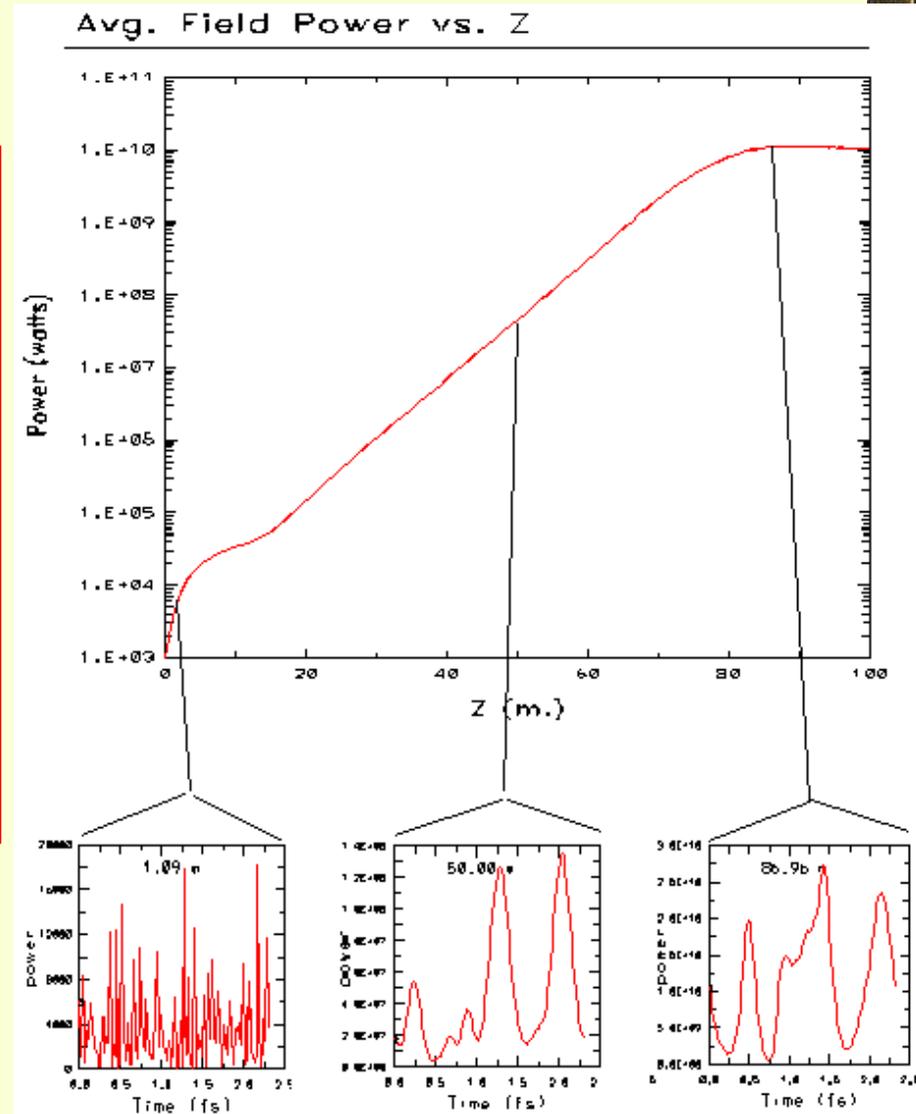
LCLS

$$L_c = 0.04 \mu\text{m}$$

Spike length $\sim 0.3 \mu\text{m}$ (1 fs)

$$\Delta\lambda/\lambda \sim 3 \times 10^{-4}$$

Spike number ~ 200 .



Reduction of line width: seeding/self seeding

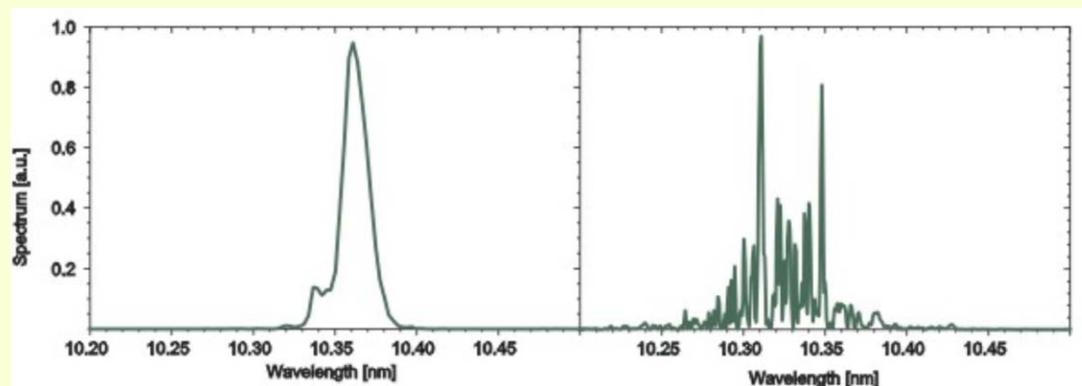


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Instead of starting from noise, as in SASE, the FEL can be seeded by an external laser field, at the FEL wavelength or a multiple.

If the laser field produces a beam energy modulation larger than that due to the spontaneous radiation, and the laser pulse is longer than the electron pulse and has a transform limited line width, then one can expect the FEL pulse to be also transform limited and have a smaller line width than in the case of SASE. In the LCLS case this would give, for the same bunch length, a line-width which is smaller by a factor given by the number of spikes in the SASE pulse, or $\Delta\lambda/\lambda \sim 4 \cdot 10^{-6}$.

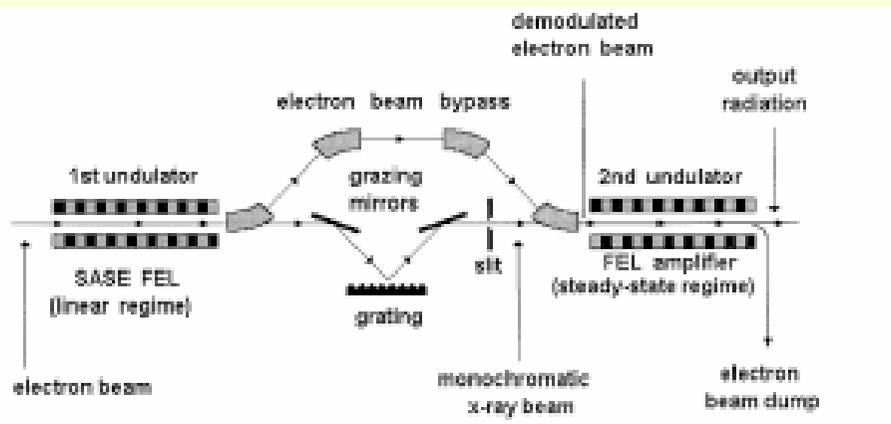
Seeded FEL
and SASE
spectra.



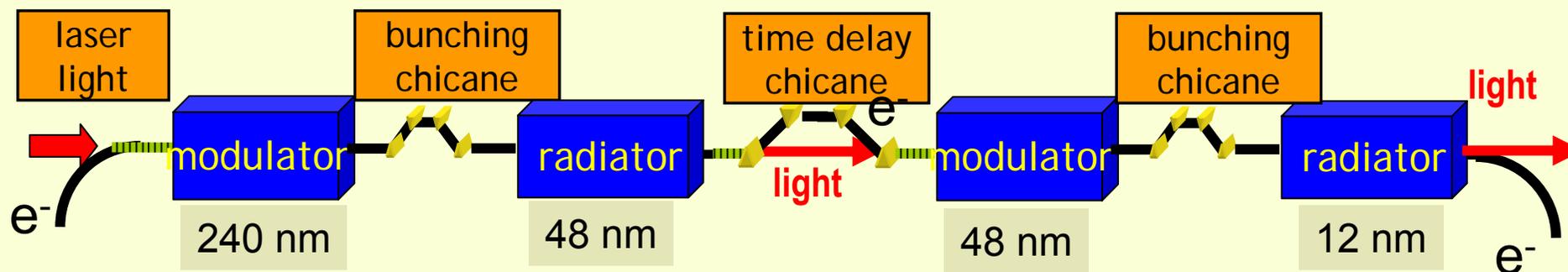
Self-seeding and high gain harmonic cascade



If there is no external laser pulse available another option is self seeding, using an additional undulator followed by a monochromator to produce the input radiation field (Saldin and al., 1997).



Another option is the harmonic cascade. (Csonka 1980; Kincaid 1980; Bonifacio 1990; L.-H. Yu 1990) Example: Fermi FEL in Trieste.



(Courtesy Zholents et al.)

Atomic laser sources at short wavelength



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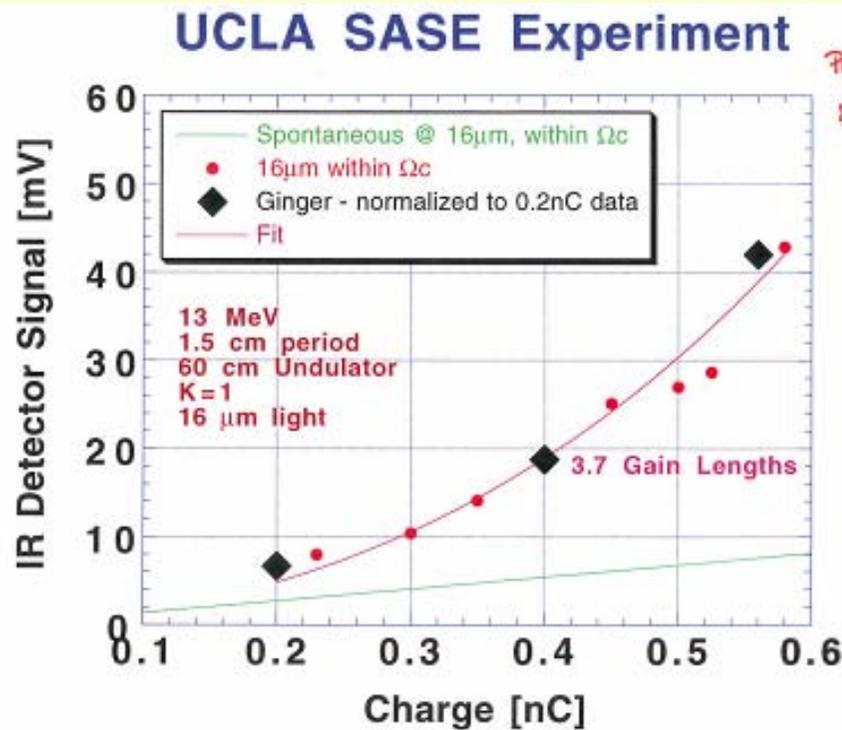
High harmonic generation (HHG) in a gas driven by a high power, multi-terawatt IR laser, is at present a source of femtosecond long, high intensity, laser pulses down to about 10 nm. These lasers are a competition to FELs in the 10 to 100 nm wavelength region. They can also be used as input seeding signals to be amplified by an FEL, or in a harmonic cascade scheme, after selection of the radiation in frequency and angular distribution to match the FEL radiation, assuming that the power they provide is larger than the FEL spontaneous radiation signal.

Experimental verifications of theory



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First demonstration in the microwave region at LLNL and MIT, in the 1980s.



First demonstration of SASE in the IR, by a UCLA/Kurchatov group, had to wait the development of higher brightness electron beams, using a photoinjector.

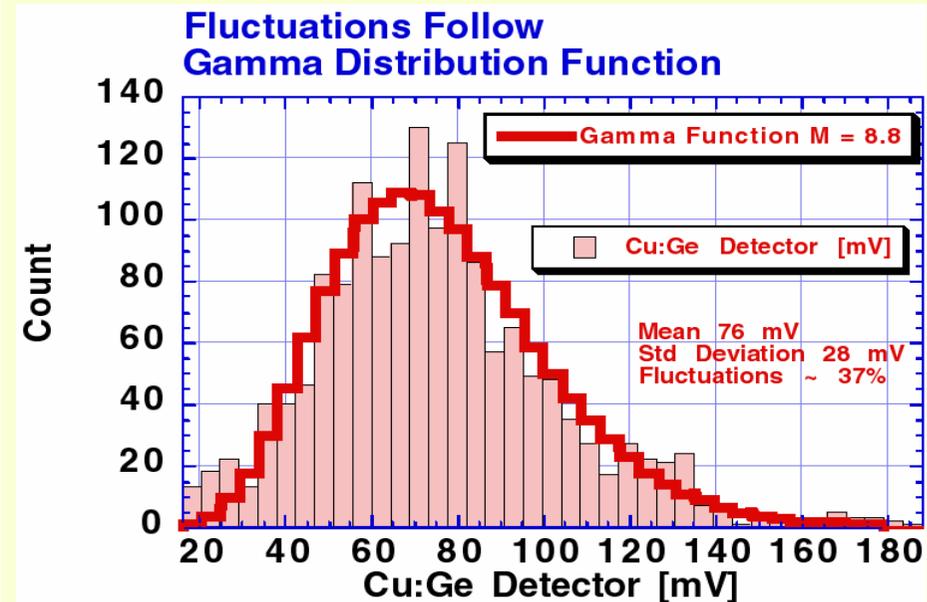
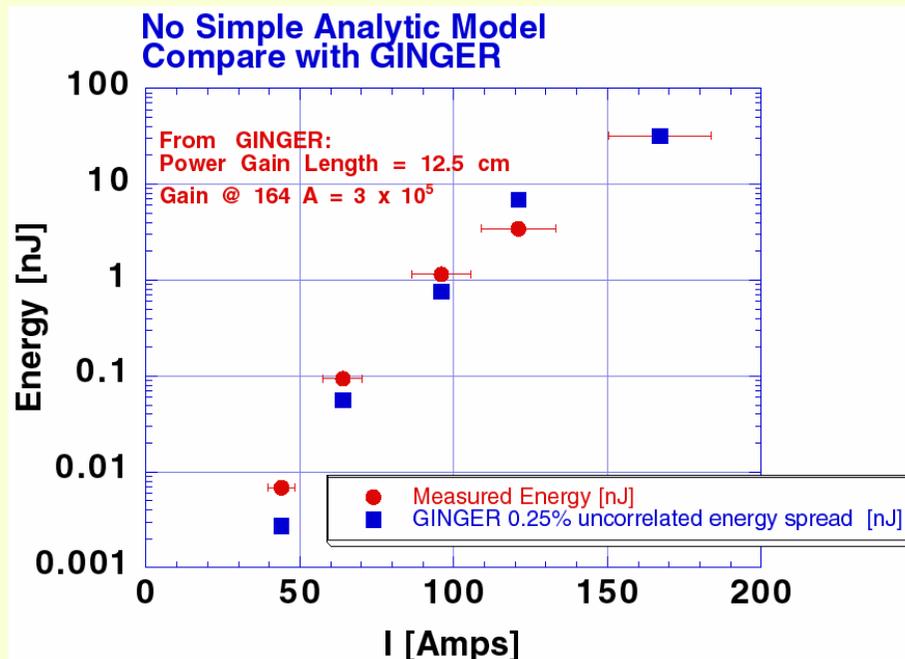
M. Hogan et al. Phys. Rev. Lett. 80, 289 (1998).

Experimental verifications of theory



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UCLA/Kurchatov/LANL/SSRL , SASE, gain of 3×10^5 at 12 μm . Demonstration of fluctuations and spikes, good agreement with theory. M. Hogan et al. Phys. Rev. Lett. 81, 4897 (1998).



Experimental verifications of theory



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UCLA/Kurchatov/LANL/SSRL

Direct measurement of microbunching using coherent transition radiation.

A. Tremaine et al., Phys. Rev. Lett. 81, 5816 (1998).

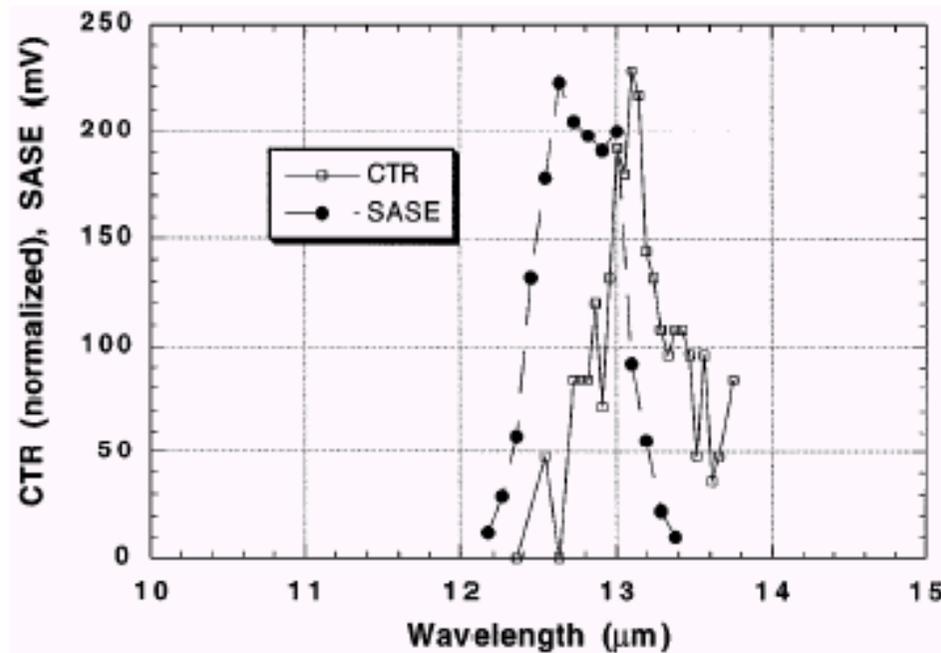
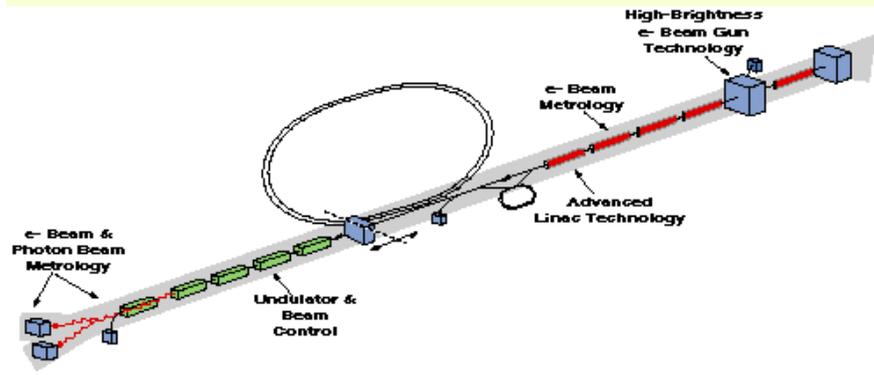


FIG. 3. SASE and CTR signals as a function of wavelength, with CTR scaled to SASE amplitude.

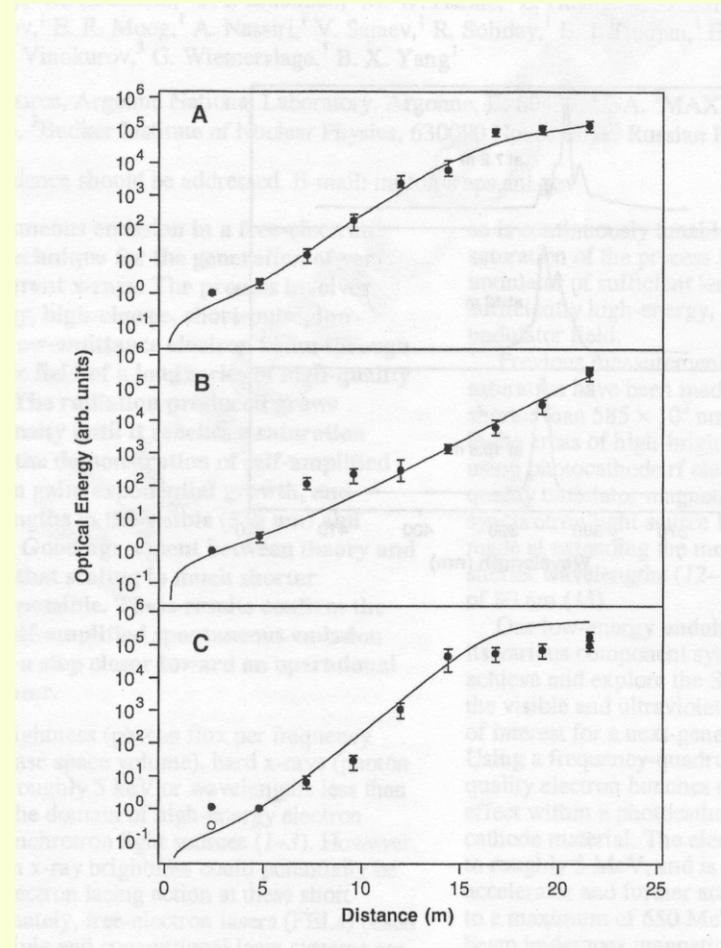
LEUTL, APS



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LEUTL exponential gain and saturation at 530 nm, A & B, and 385 nm, C. The gain reduction for case B was obtained by reducing the peak current.



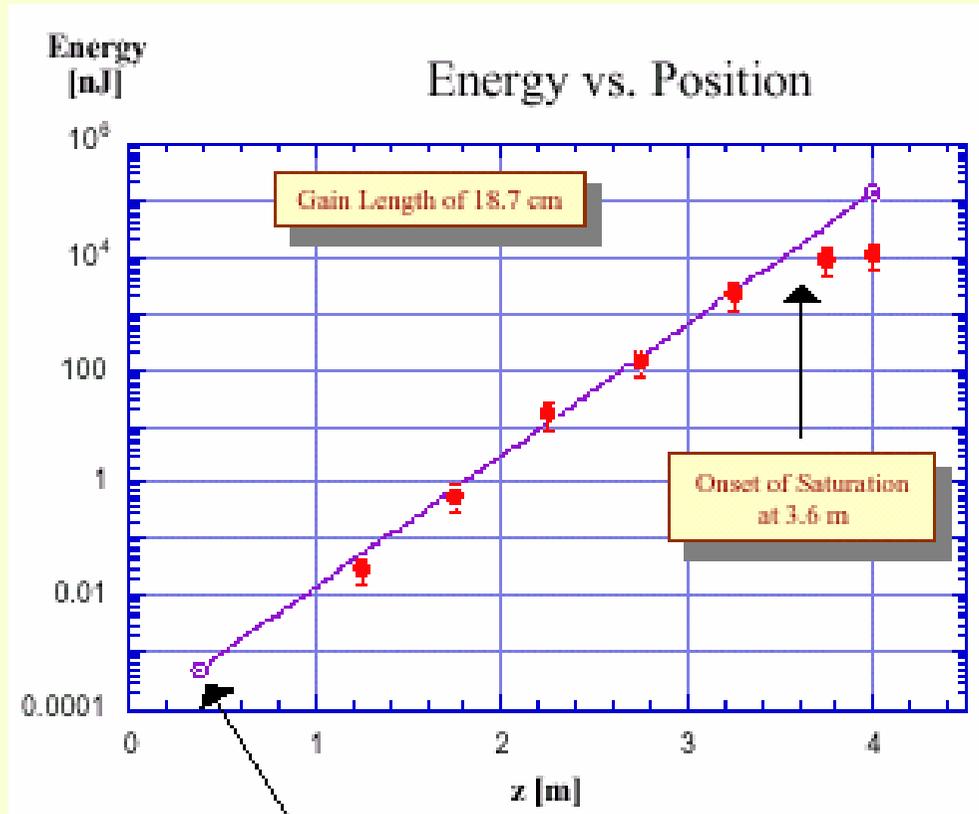
Milton et al., *Scienceexpress*, May 17, 2001.

VISA:Visible to Infrared SASE Amplifier



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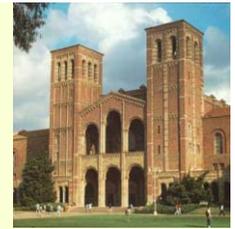
BNL-SLAC-LLNL-UCLA



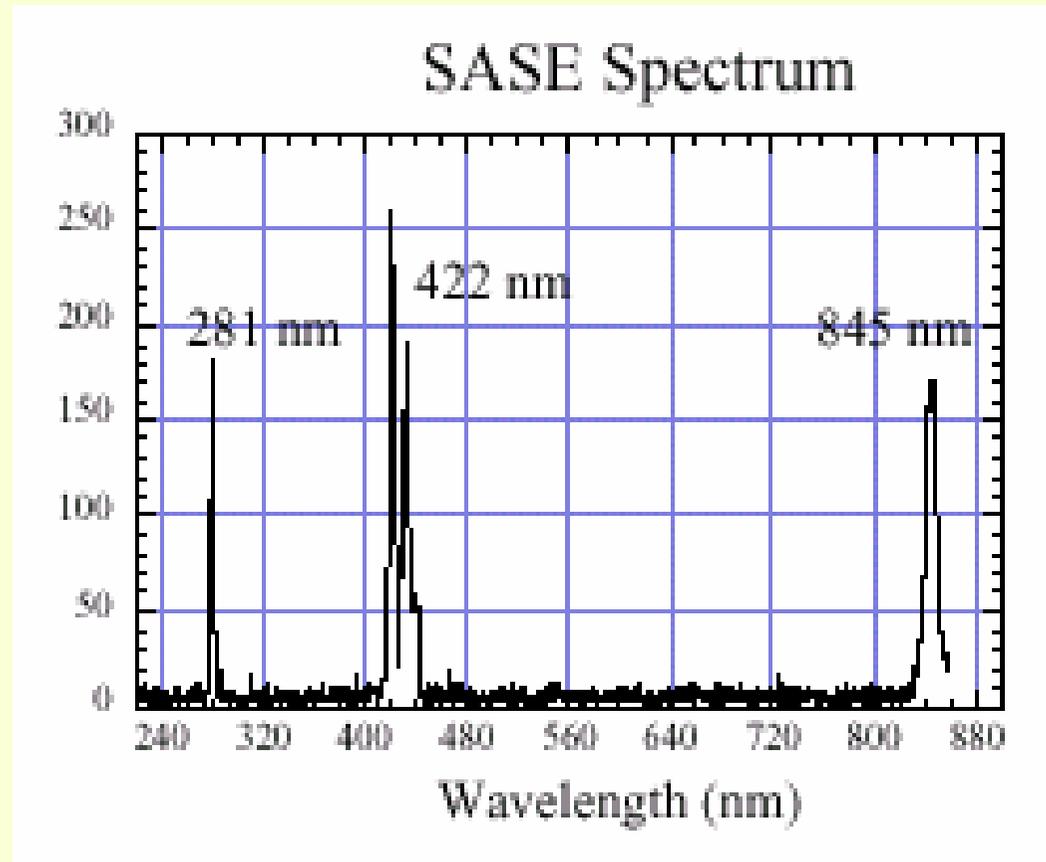
Saturation reached in 2001.

Wavelength 830nm
Average Charge:170 pC
Gain Length 18.5 cm
Equivalent Spontaneous
Energy: 5 pJ
Peak SASE Energy:10 μ J
Total Gain: 2×10^7

VISA: harmonic generation



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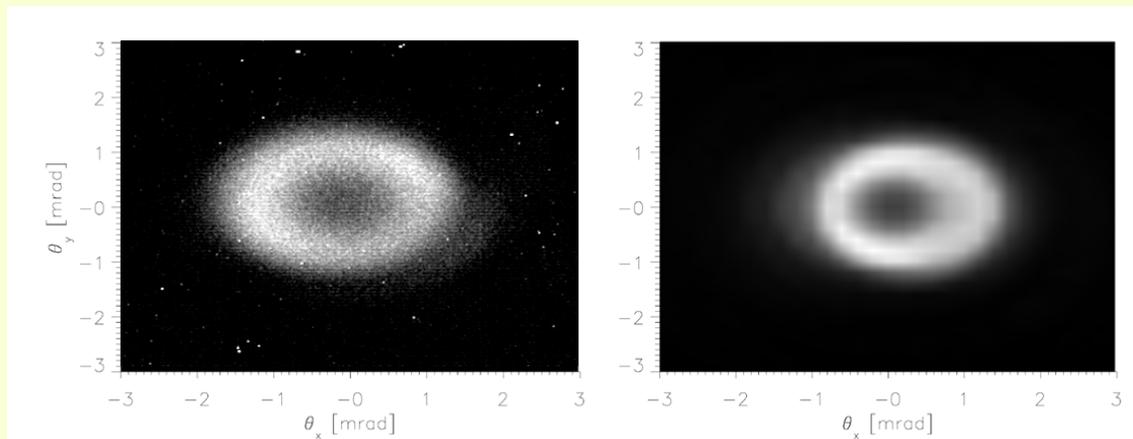
The LCLS 3rd harmonic at 0.5 Å is expected to have about 100 MW peak power.

VISA: angular distribution



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Effects of correlated transverse-longitudinal electron distribution on radiation angular distribution.



Measured
(left) and
simulated
(right)
angular
distribution
at saturation
in VISA

Simulation done with Genesis use the Parmela-Elegant output.

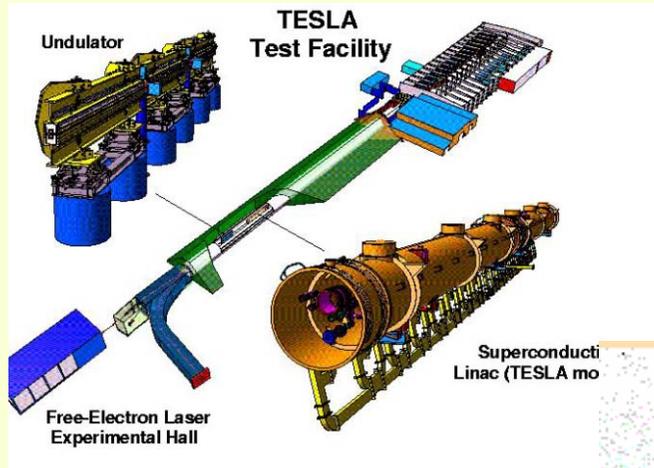
Courtesy Sven Reiche.

The present theories and codes can reproduce results even for unusual conditions due to non-linear bunch compression and wake fields.

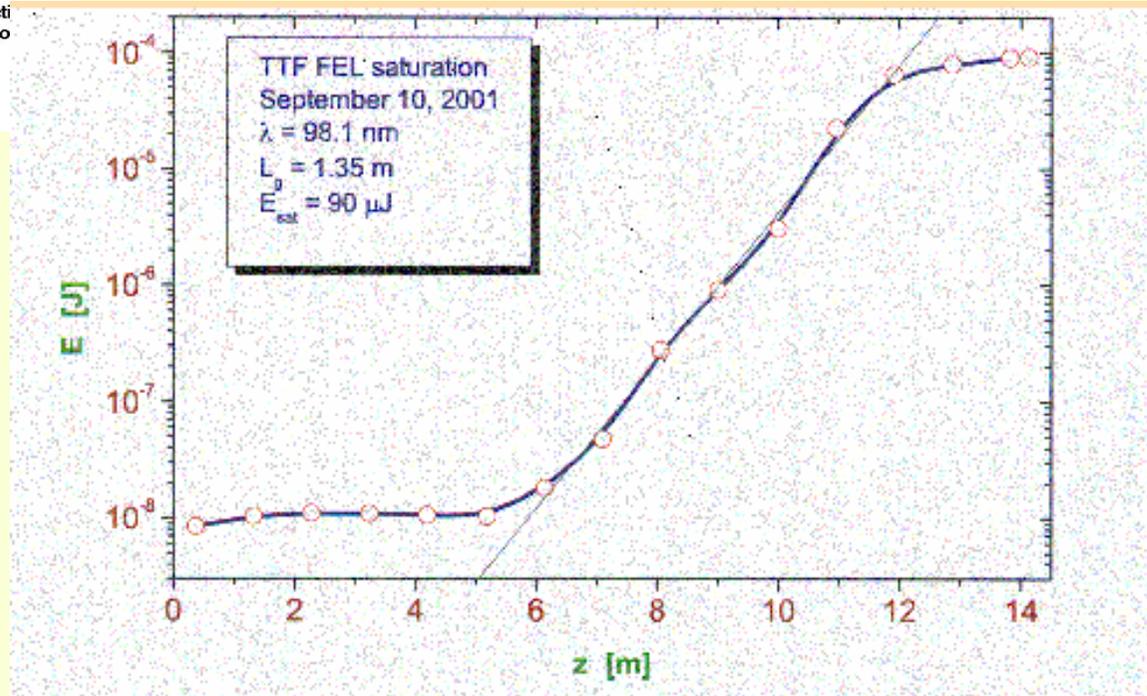
TTF VUV-FEL (Flash)



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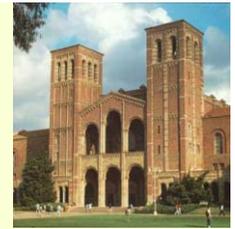


1 GeV – 6 nm
Norm. emittance: 2 mrad mm
FWHM FEL pulse length: ca. 100 fs
Peak current 2500 A
Linac rep. rate 10 Hz
Max. pulse rate 72 000

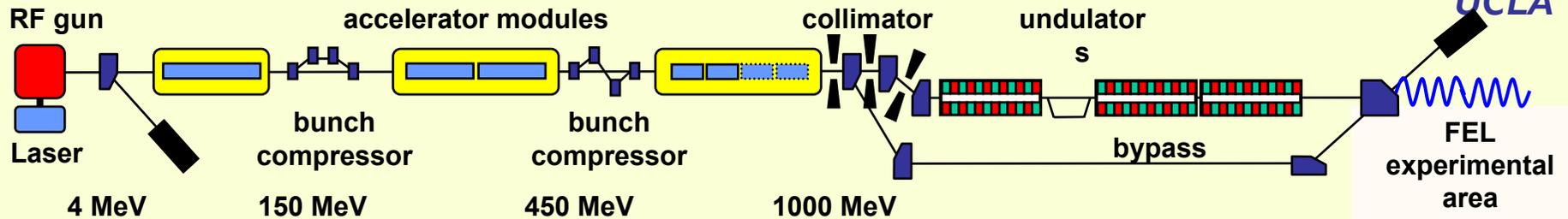


Courtesy J. Rossbach

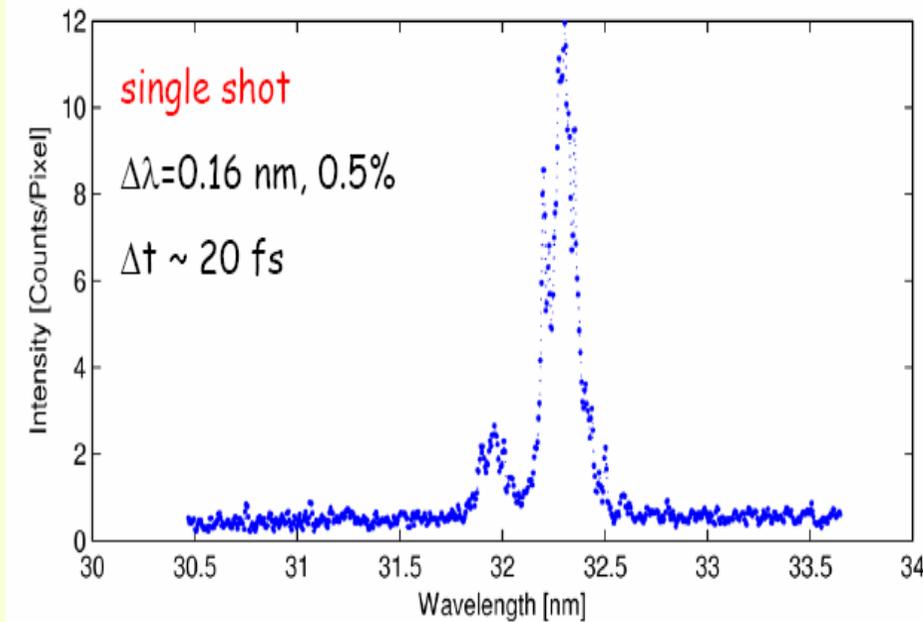
VUV-FEL → FLASH



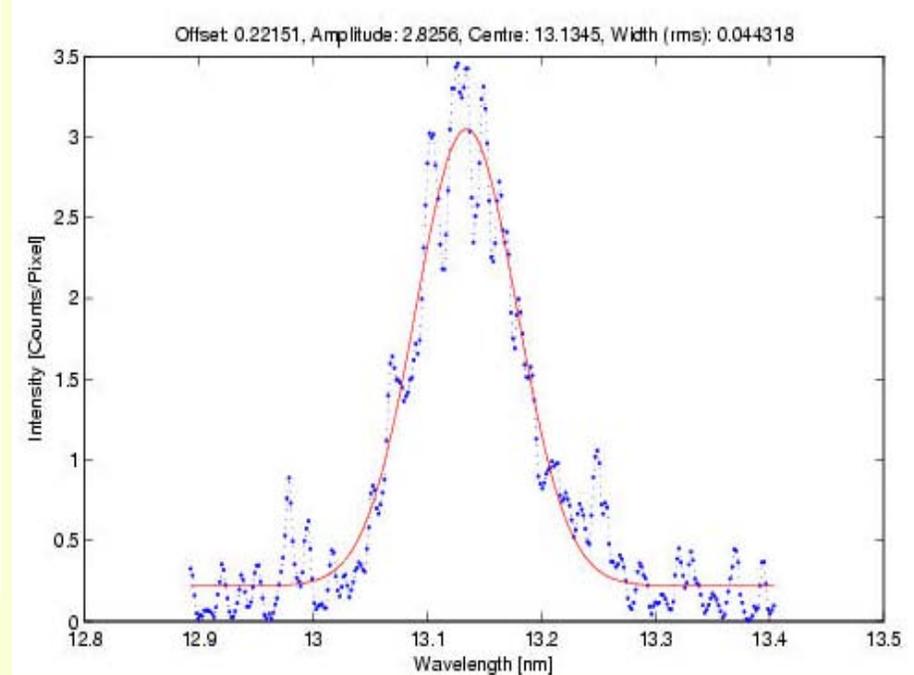
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Jan. 14, 2005: lasing at 32 nm



Latest wavelength record for SASE FELs: Apr. 26, 2006: lasing at 13 nm



Courtesy J. Rossbach, Desy

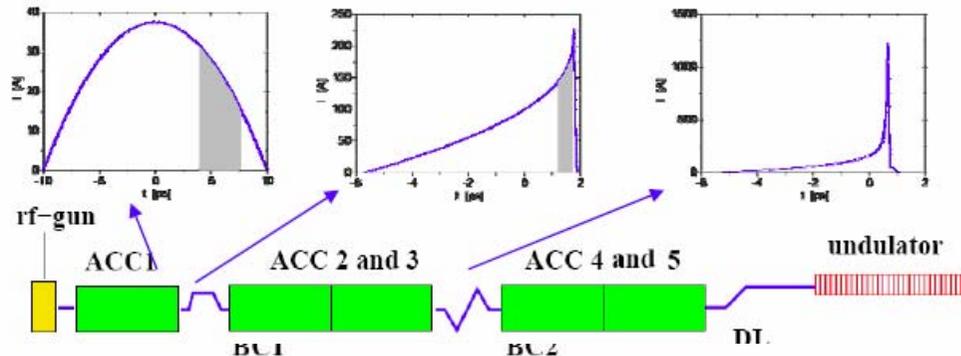


Production of ultra-short radiation pulses in the VUV FEL

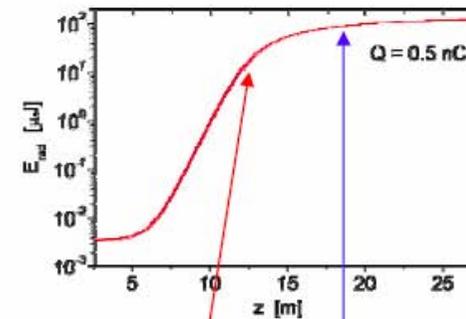
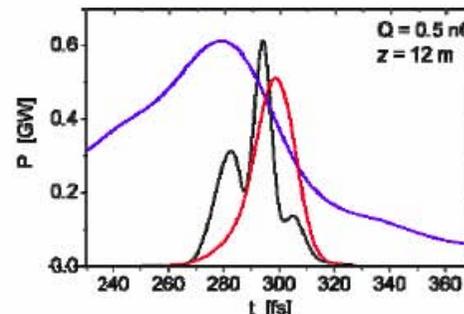


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An ultra-short current spike (50-100 fs FWHM) with peak current 1-2 kA is formed in the nonlinear bunch formation system of the VUV FEL



Strong energy chirp along current spike leads to significant shortening of the radiation pulse. Minimum pulse length occurs in the end of the linear regime.

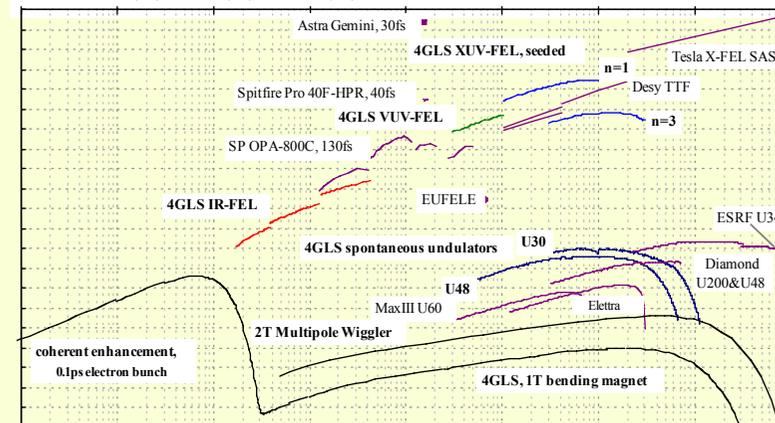
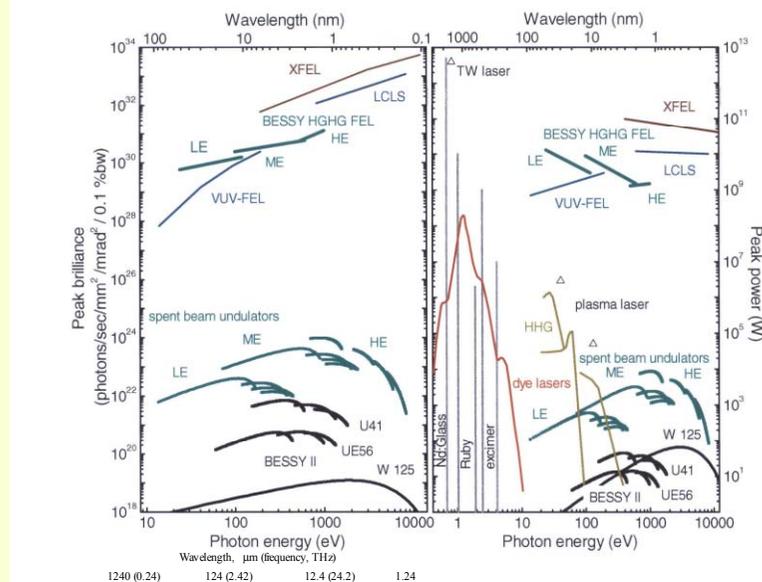
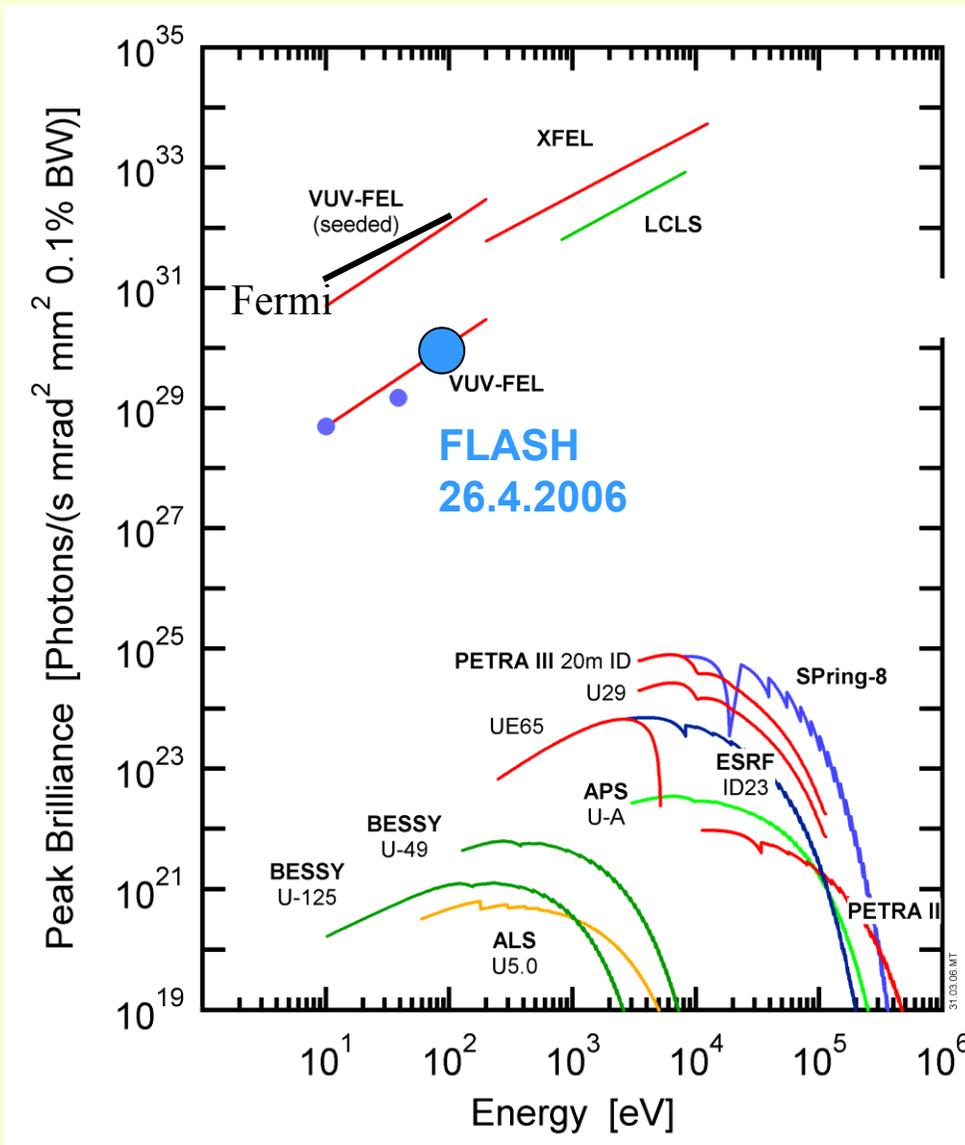


The VUV FEL is capable to produce short, down to 20 fs radiation pulses with GW-level peak power and degree of contrast 80 %:

$$C(\tau) = \frac{\int_{-\tau/2}^{\tau/2} P(t) dt}{\int_{-\infty}^{\infty} P(t) dt} \cdot$$

See J. Rossbach,
MOZBPA01

Soft X-ray and X-ray sources



Transverse coherence measurement at DESY

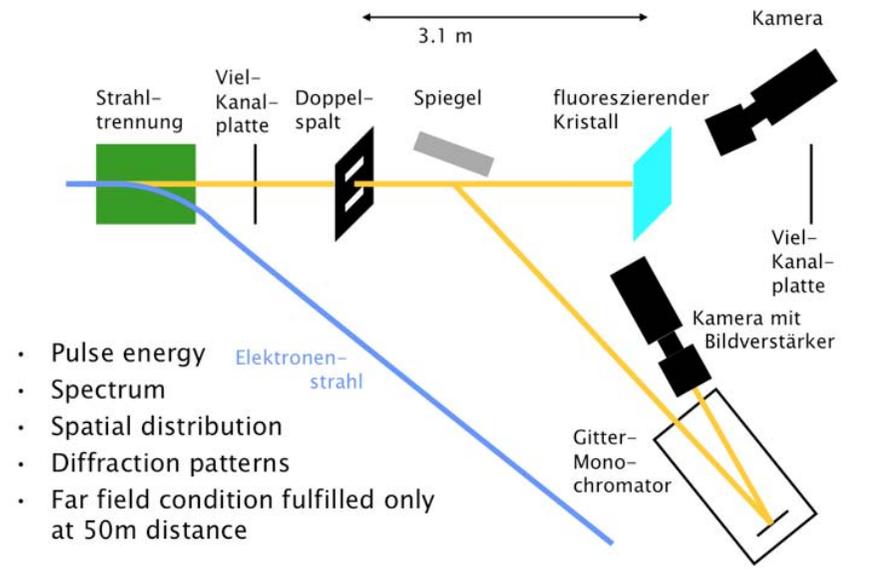


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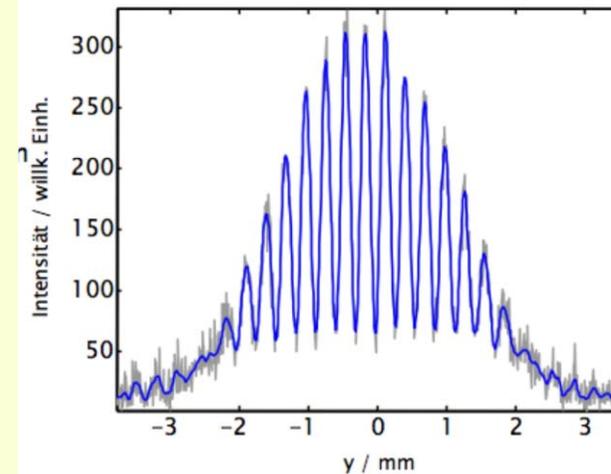
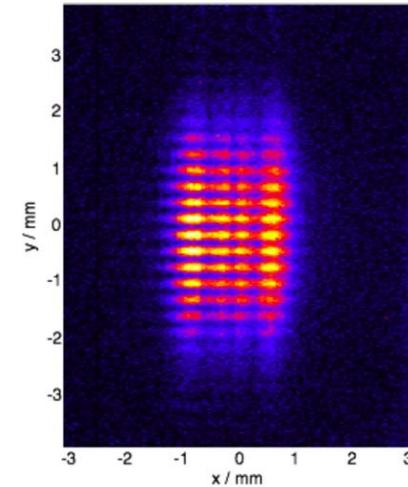
Courtesy of R. Ishebek et al.

$\lambda=100$ nm

Experimental Setup Photon Diagnostics at the TTF FEL



• Average of 100 images

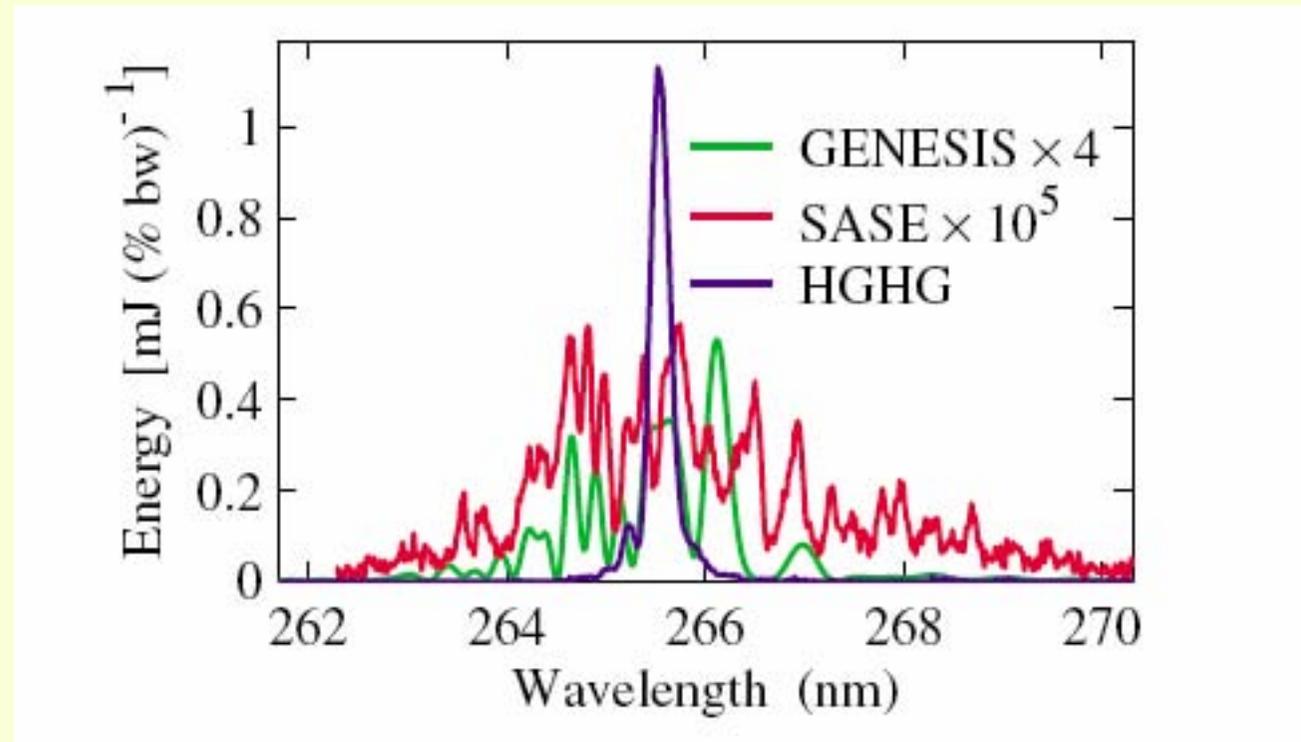


Very good transverse coherence!

High Gain Harmonic Generation experiments



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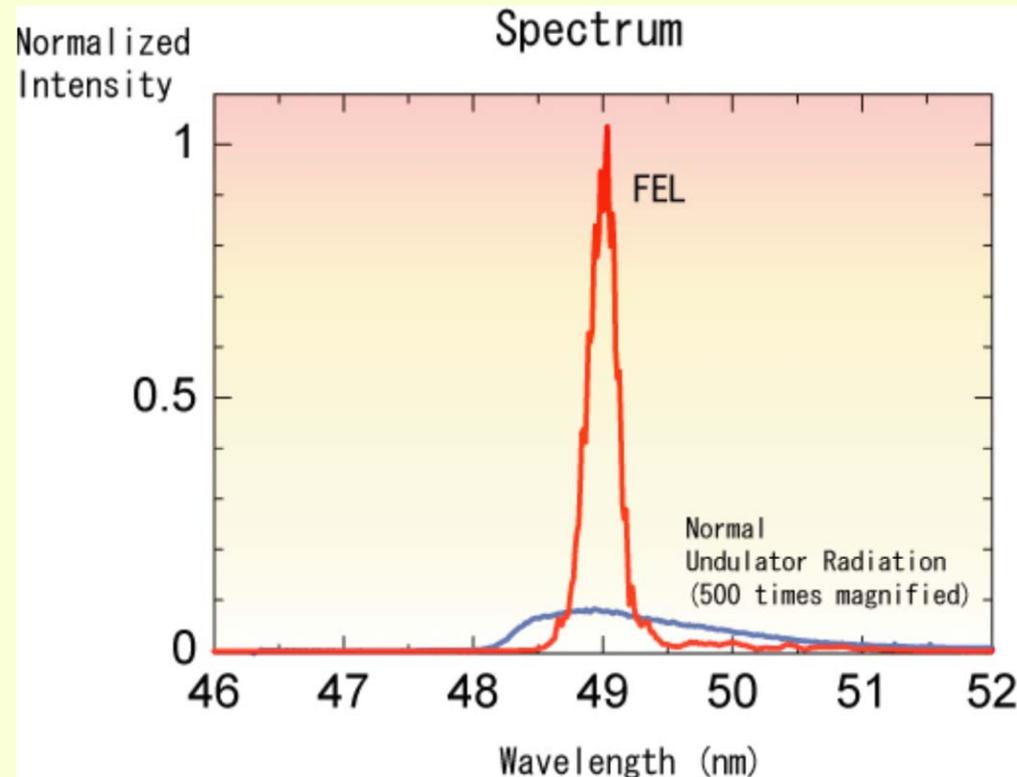


Measured HGHG for the third harmonic, and the SASE spectra at the BNL-DUV FEL. Seed laser $\lambda=800$ nm. A. Doyuran et al., PRST, 7, 050701 (2004)

New result from the SCSS prototype at this conference



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First lasing at 49 nm in SCSS prototype accelerator (250 MeV, SASE-FEL, with 500 kV thermoionic gun).

Summary of theoretical and experimental work



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The theory works quite well! The agreement between experimental results and theoretical/simulation work is remarkable.

But to fit the data we have to use the real beam properties - longitudinal and transverse phase-space distributions, including coupling between different degrees of freedom- which in most cases are quite complex.

To understand the FEL radiation we need to have very good and complete beam diagnostics and do complete start-to-end simulations from the electron source to the undulator entrance.

Directions of development and challenges



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Some areas of possible FEL improvements are:

Greater stability of electron beam energy. Electron beam energy shot to shot fluctuations of about 0.1% produce a wavelength fluctuation of $\sim 0.2\%$, 5 times larger than the line-width, giving large intensity fluctuations when using a monochromator or in seeded systems.

Longitudinal coherence is limited. Seeding with external lasers and self-seeding schemes have been proposed, but are sensitive to wakefields and the energy distribution along a bunch.

Reduced beam emittance and short period undulators would allow the design of lower beam energy, less expensive systems.

Progress in producing lower emittance, reliable, high repetition rate electron sources is very important.

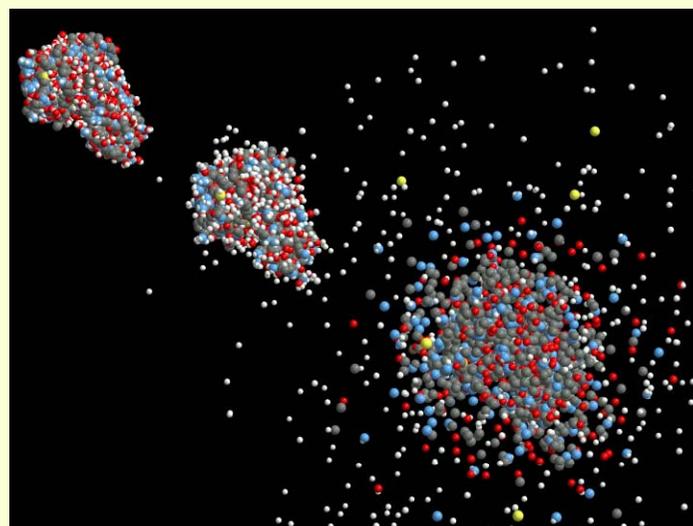
Directions of development and challenges



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The main directions of development, beyond the present status of FLASH, for the soft X-ray region, and the initial expected performance of LCLS for the Ångstrom region, are:

1. Short, few to 10 femtosecond, pulses
2. Smaller line-width, nearly transform limited
3. Higher intensity, getting near to the N_e^2 limit.



Experiments like single shot imaging of a protein structure require more than 10^{12} photons in about 10 fs. This is an important challenge.

Coulomb Explosion of Lysozyme (50 fs). J. Haidu

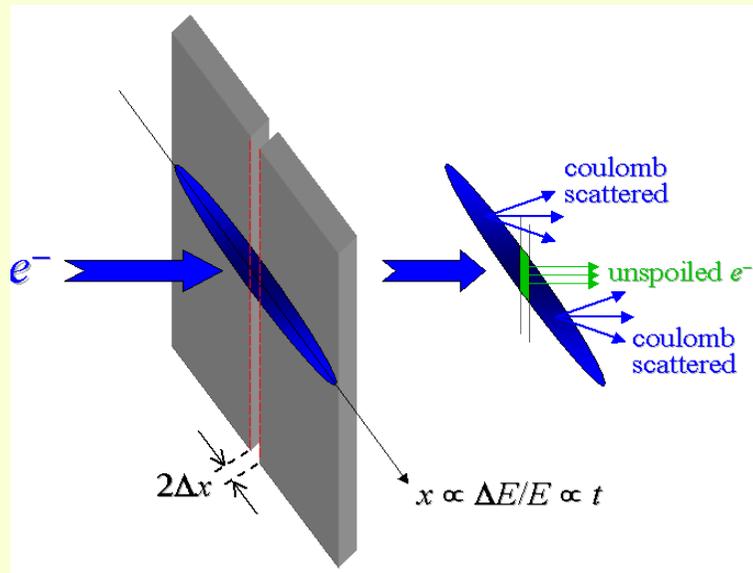
C Pellegrini, EPAC 2006

Reducing the LCLS Pulse Length



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Many ideas have been proposed to reduce the X-ray pulse length: using the dependence of the pulse length on the electron bunch length, as in the TTF-VUV results; or chirping the electron beam energy and the radiation pulse wavelength in a two undulator system; or producing a local increase of the electron bunch emittance and/or energy spread.

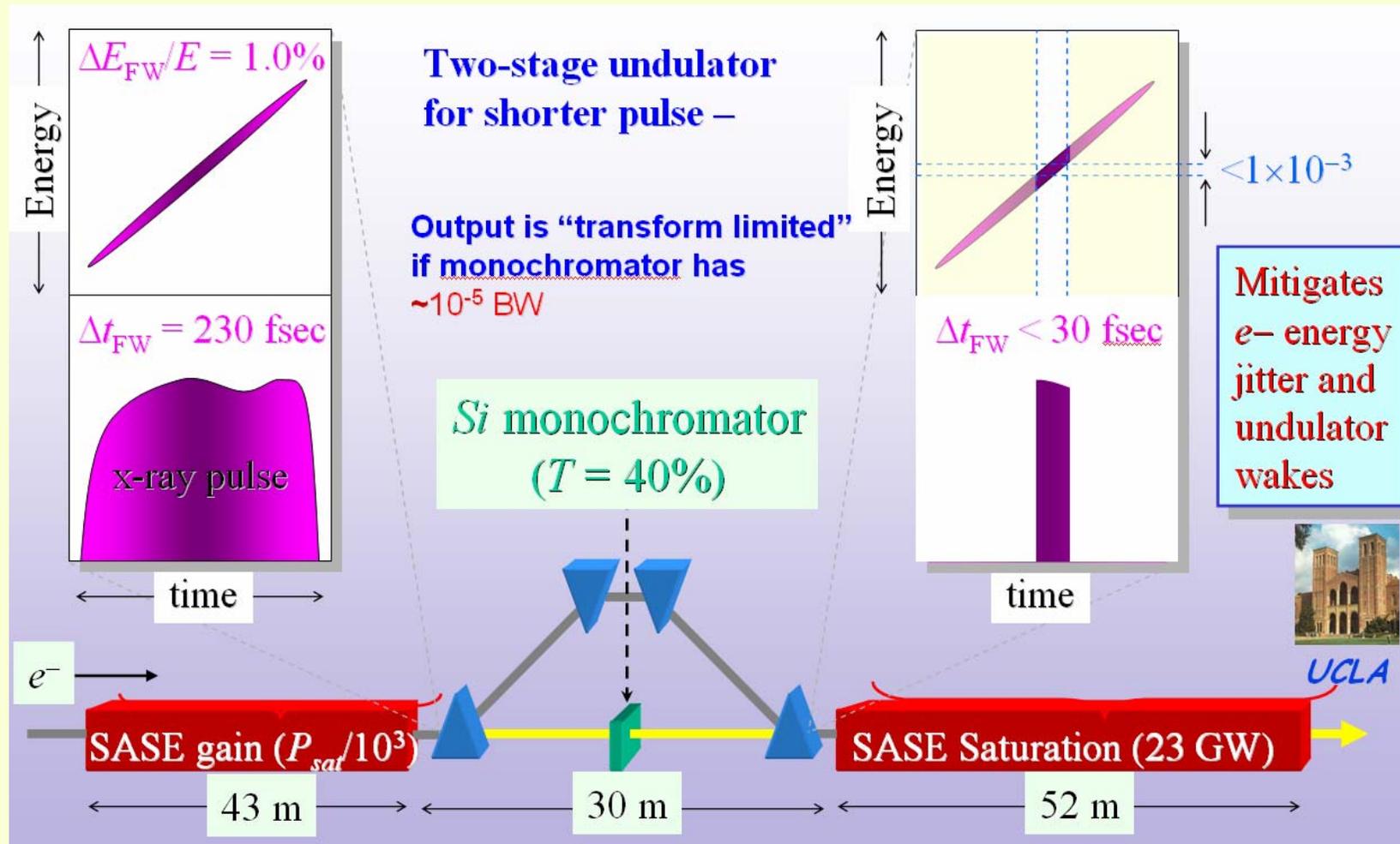


The emittance spoiler method can produce few fs long pulses.
P. Emma, Z. Huang, et al., Ph. Rev. Lett. 2004.

Two-Stage Chirped-Pulse Self-Seeding in LCLS



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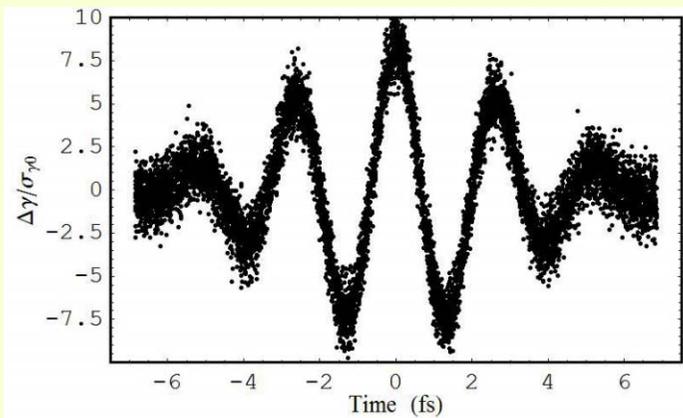
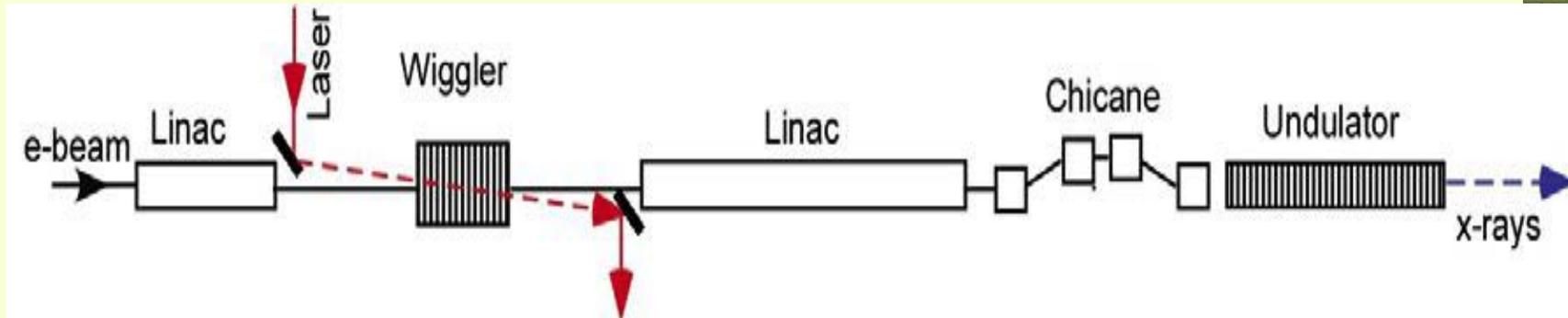
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C. Schroeder et al., JOSA B 19, 1782-1789, (2002).

Enhanced SASE. A. Zholents et al, Phys. Rev. Lett.



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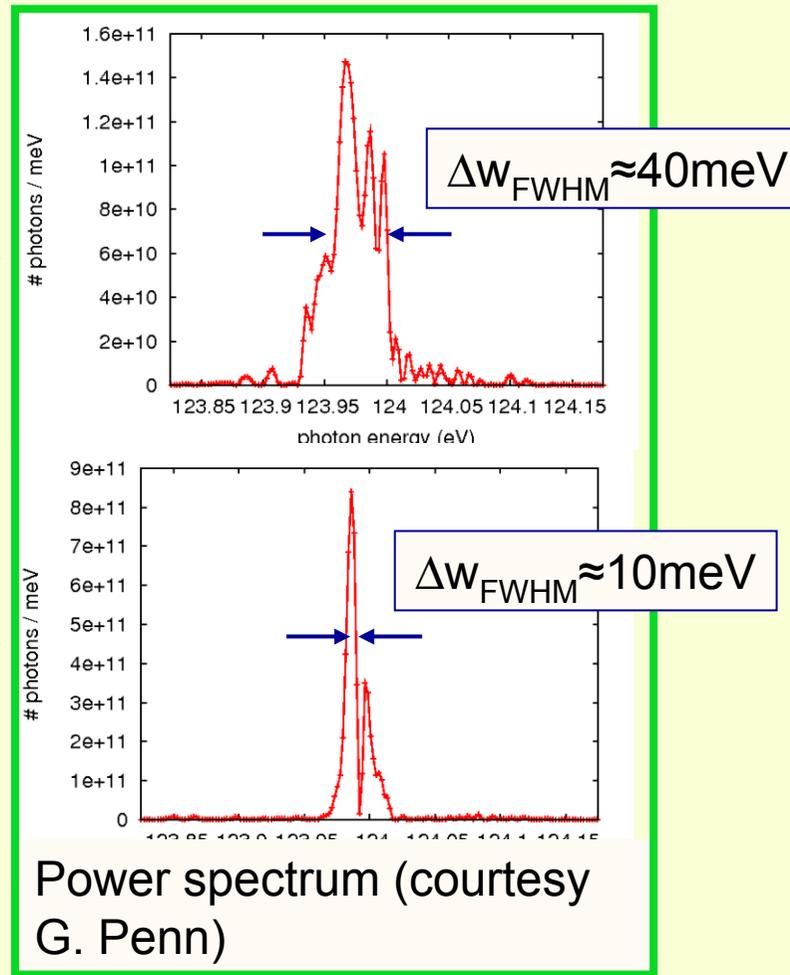
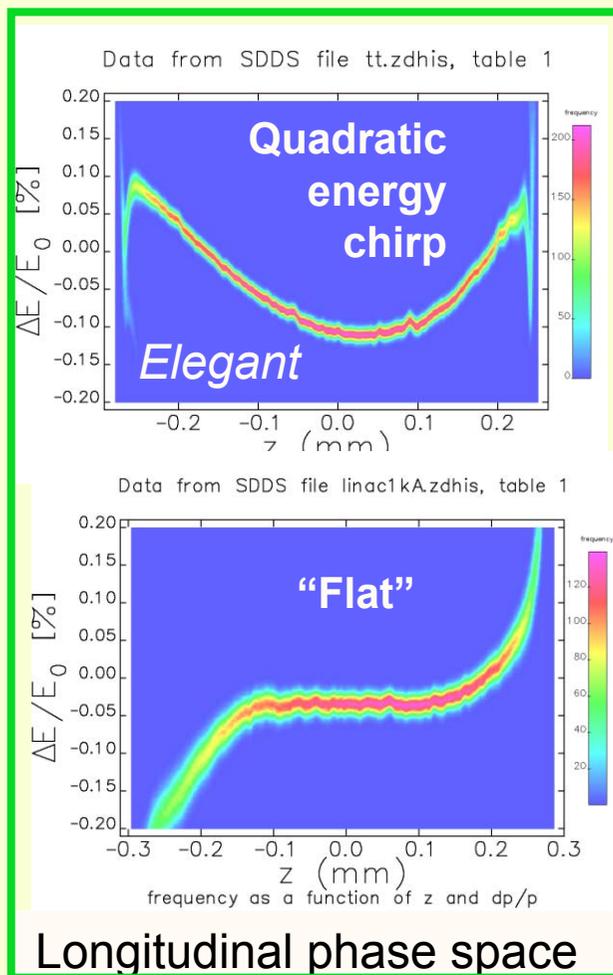
Modulating Laser: 6 GW, $l = 2.2$ mm

X-ray output: 230 GW peak, pulse length 0.2 fs.

Small line-width sensitivity to bunch energy profile



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Two examples using two different electron beams. How to go from the bad to the good is in M. Cornacchia et al. THOPA01

Conclusions



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The great progress in the physics and technology of high brightness electron beams, and the exploitation of the FEL collective interaction, has made possible to design and build powerful X-ray FELs in the 1 Å spectral region, opening the way to new opportunities to explore the properties of matter at the atomic level.

R&D work should be continued in many areas like high brightness electron sources, beam stability, diagnostics, undulators, X-ray optics, synchronization of the X-ray probe pulse with a pump pulse, short fs pulses, higher peak power, to increase even more the potential of X-ray FELs.