

X-ray Free Electron Lasers

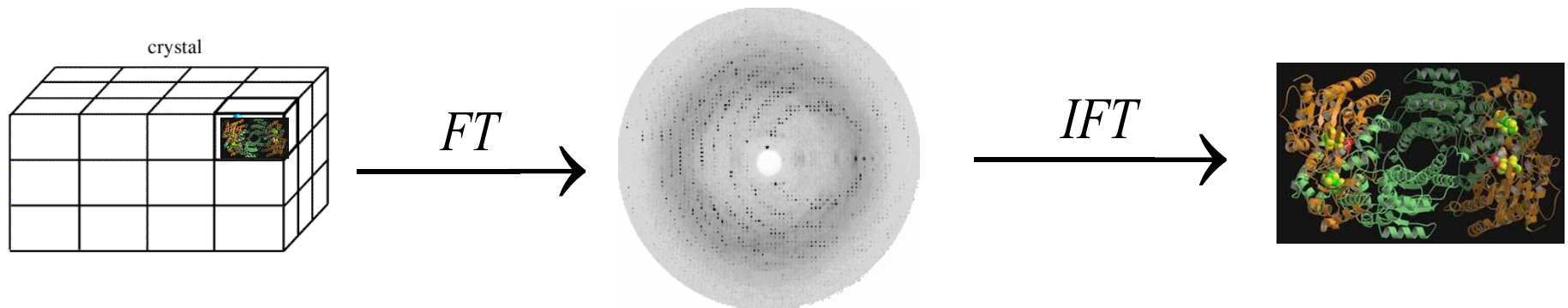
Daniel Ratner, June 27, 2013

Outline

1. Why you should care about FELs
2. How FELs work
3. How FELs *should* work

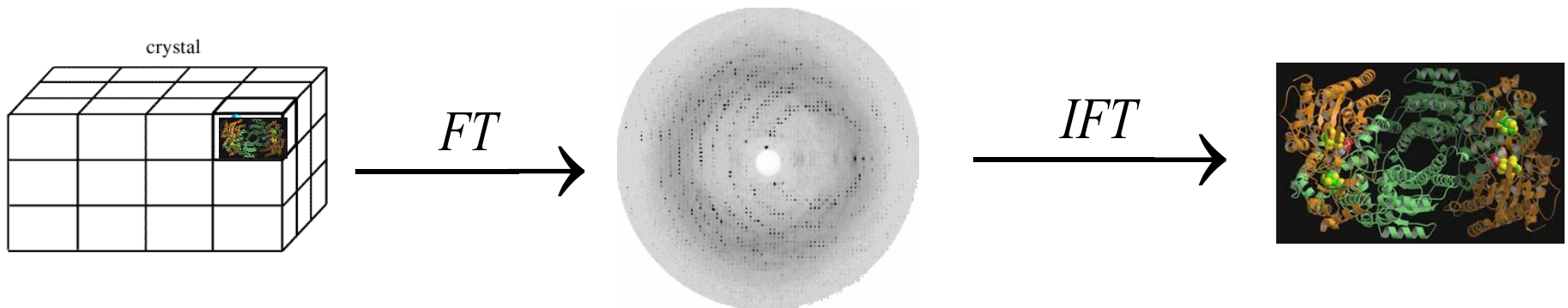
Structural biology in 4 steps:

- Isolate and make protein
- Crystallize protein
- Measure diffraction pattern from crystal
- Recover structure from diffraction data



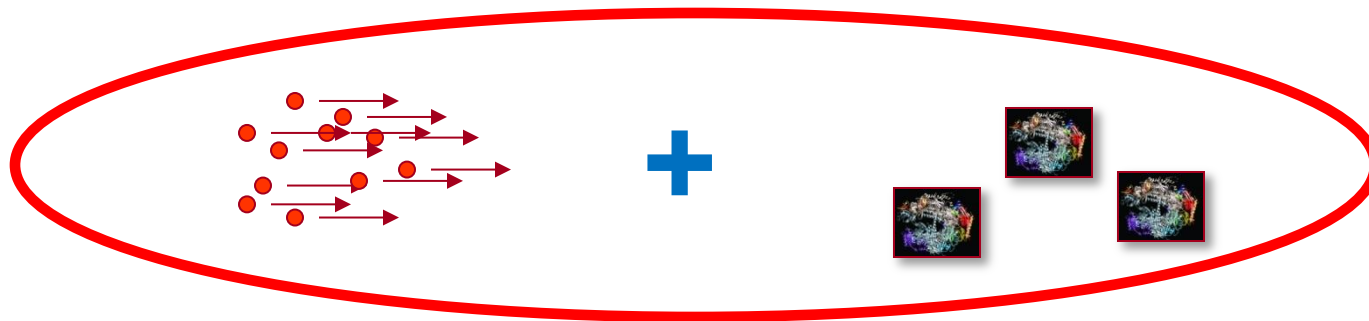
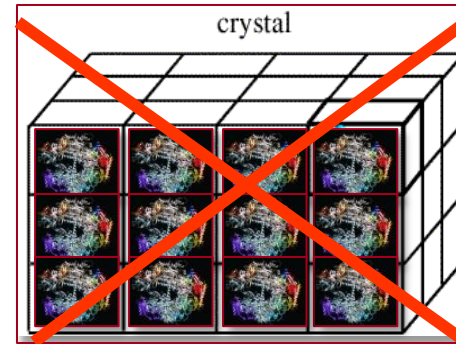
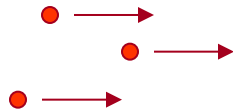
Structural biology in 4 steps:

- Isolate and make protein
- Crystallize protein – Can we avoid bottleneck?
- Measure diffraction pattern from crystal
- Recover structure from diffraction data



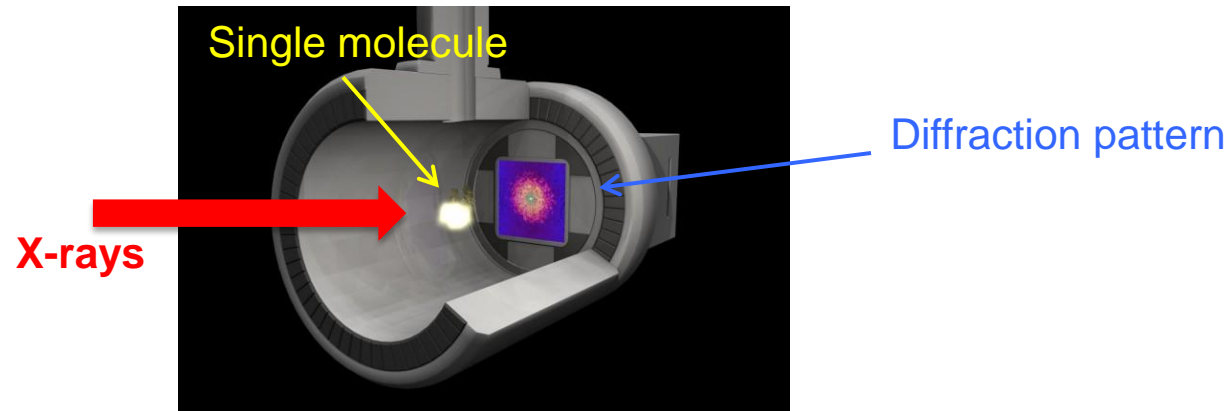
Two paths to molecular image:

Photons



Only possible with an X-ray laser!

Single molecule imaging!



... or at least really really small crystals: **nanocrystallography**

Simultaneous Femtosecond X-ray Spectroscopy and Diffraction of Photosystem II at Room Temperature

Jan Kern,^{1,2} Roberto Alonso-Mori,² Rosalie Tran,¹ Johan Hattne,¹ Richard J. Gildea,¹



Natively Inhibited Trypanosoma brucei Cathepsin B Structure Determined by Using an X-ray Laser

Lars Redecke *et al.*
Science **339**, 227 (2013);
DOI: 10.1126/science.1229663

LETTER

doi:10.1038/nature09750

Femtosecond X-ray protein nanocrystallography

Henry N. Chapman^{1,2}, Petra Fromme³, Anton Barty¹, Thomas A. White¹, Richard A. Kirian⁴, Andrew Aquila¹, Mark S. Hunter³,

LETTER

doi:10.1038/nature09748

Single mimivirus particles intercepted and imaged with an X-ray laser

M. Marvin Seibert^{1*}, Tomas Ekeberg^{1*}, Filipe R. N. C. Maia^{1*}, Martin Svenda¹, Jakob Andreasson¹, Olof Jönsson¹, Duško Odić¹,

Motivation

SLAC

And many many more fields...

Science



Real-Time Observation of Surface Bond Breaking with an X-ray Laser
M. Dell'Angela *et al.*
Science **339**, 1302 (2013);
DOI: 10.1126/science.1231711

LETTER

doi:10.1038/nature10721

Atomic inner-shell X-ray laser at 1.46 nanometres pumped by an X-ray free-electron laser

Nina Rohringer^{1†}, Duncan Ryan², Richard A. London¹, Michael Purvis², Felicie Albert¹, James Dunn¹, John D. Bozek³, Christoph Bostedt⁴, Alexander Graf¹, Randal Hill¹, Stefan P. Hau-Riege¹ & Jorge J. Rocca²

ARTICLES

PUBLISHED ONLINE: 11 NOVEMBER 2012 | DOI: 10.1038/NPHOTON.2012.261

nature
photonics

Ultra-efficient ionization of heavy atoms by intense X-ray free-electron laser pulses

Benedikt Rudek, Sang-Kil Son, Daniel Rolles *et al.**

Scienceexpress

Ultrafast Three-Dimensional Imaging of Lattice Dynamics in Individual Gold Nanocrystals

J. N. Clark,^{1*} L. Beitra,¹ G. Xiong,¹ A. Higginbotham,² D. M. Fritz,³ H. T. Lemke,³ D. Zhu,³ M. Chollet,³ G. J. Williams,³ M. Messerschmidt,³ B. Abbey,⁴ R. J. Harder,⁵ A. M. Korsunsky,^{6,7} J. S. Wark,² I. K. Robinson^{1,7}

LETTER

doi:10.1038/nature11627

An unexpectedly low oscillator strength as the origin of the Fe XVII emission problem

S. Bernitt¹, G. V. Brown², J. K. Rudolph^{1,3}, R. Steinbrügge¹, A. Graf², M. Leutenegger^{4,5}, S. W. Epp^{1,6}, S. Eberle¹, K. Kubiček^{1†}, V. Mäckel^{1†}, M. C. Simon⁷, E. Träbert², E. W. Magese², C. Beilmann¹, N. Hell^{2,8}, S. Schippers³, A. Müller³, S. M. Kahn⁹, A. Surzhykov^{10,11}, Z. Harman^{1,12}, C. H. Keitel¹, J. Clementson², F. S. Porter⁴, W. Schlott¹³, J. J. Turner¹³, J. Ullrich^{1†}, P. Beiersdorfer² & J. R. Crespo López-Urrutia¹

PRL 109, 245003 (2012)

PHYSICAL REVIEW LETTERS

week ending
14 DECEMBER 2012

Resonant $K\alpha$ Spectroscopy of Solid-Density Aluminum Plasmas

B. I. Cho,^{1,*} K. Engelhorn,¹ S. M. Vinko,² H.-K. Chung,³ O. Ciricosta,² D. S. Rackstraw,² R. W. Falcone,^{1,4} C. R. D. Brown,⁵ T. Burian,⁶ J. Chalupský,⁶ C. Graves,⁷ V. Hájková,⁶ A. Higginbotham,² L. Juha,⁶ J. Krzywinski,⁷ H. J. Lee,⁷ M. Messerschmidt,⁷ C. Murphy,⁷ Y. Ping,⁸ N. Rohringer,⁹ A. Scherz,⁷ W. Schlott⁷, S. Toleikis,¹⁰ J. J. Turner,⁷ L. Vysin,⁶ T. Wang,⁷ B. Wu,⁷ U. Zastra¹¹, D. Zhu,⁷ R. W. Lee,⁷ B. Nagler,⁷ J. S. Wark,² and P. A. Heimann⁷

PRL 108, 217402 (2012)

PHYSICAL REVIEW LETTERS

week ending
25 MAY 2012

Ultrafast Transitions from Solid to Liquid and Plasma States of Graphite Induced by X-Ray Free-Electron Laser Pulses

S. P. Hau-Riege,^{1,*} A. Graf,¹ T. Döppner,¹ R. A. London,¹ J. Krzywinski,² C. Fortmann,¹ S. H. Glenzer,¹ M. Frank,¹ K. Sokolowski-Tinten,³ M. Messerschmidt,² C. Bostedt,² S. Schorb,² J. A. Bradley,¹ A. Lutman,² D. Rolles,^{4,5} A. Rudenko,^{4,6} and B. Rudek^{4,6}

PRL 108, 253006 (2012)

PHYSICAL REVIEW LETTERS

week ending
22 JUNE 2012

Transient X-Ray Fragmentation: Probing a Prototypical Photoinduced Ring Opening

Vladimir S. Petrović,^{1,2,*} Marco Siano,³ James L. White,^{2,4} Nora Berrah,⁵ Christoph Bostedt,⁶ John D. Bozek,⁶ Douglas Broege,^{2,4} Max Chalfin,^{1,2} Ryan N. Coffee,⁶ James Cryan,^{1,2} Li Fang,⁵ Joseph P. Farrell,^{1,2} Leszek J. Frasinski,³ James M. Glowina,^{2,4} Markus Gühr,² Matthias Hoener,⁵ David M. P. Holland,⁷ Jaehee Kim,^{1,2} Jonathan P. Marangos,³ Todd Martinez,^{2,8} Brian K. McFarland,^{2,4} Russell S. Minns,⁹ Shungo Miyabe,^{2,8} Sebastian Schorb,⁶ Roseanne J. Senson,¹⁰ Limor S. Spector,^{1,2} Richard Squibb,³ Hongli Tao,^{2,8} Jonathan G. Underwood,⁹ and Philip H. Bucksbaum^{1,2,4}

The Free Electron Laser

John Madey, 1971

JOURNAL OF APPLIED PHYSICS

VOLUME 42, NUMBER 5

APRIL 1971

Stimulated Emission of Bremsstrahlung in a Periodic Magnetic Field

JOHN M. J. MADEY

Physics Department, Stanford University, Stanford, California 94305

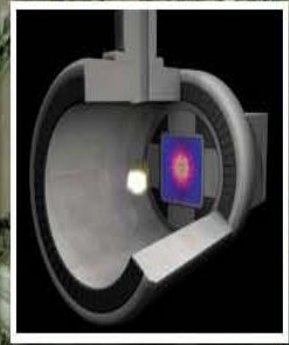
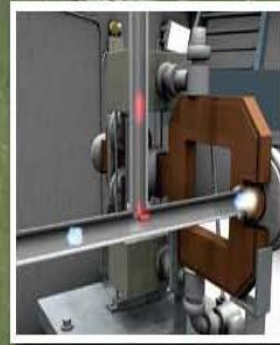
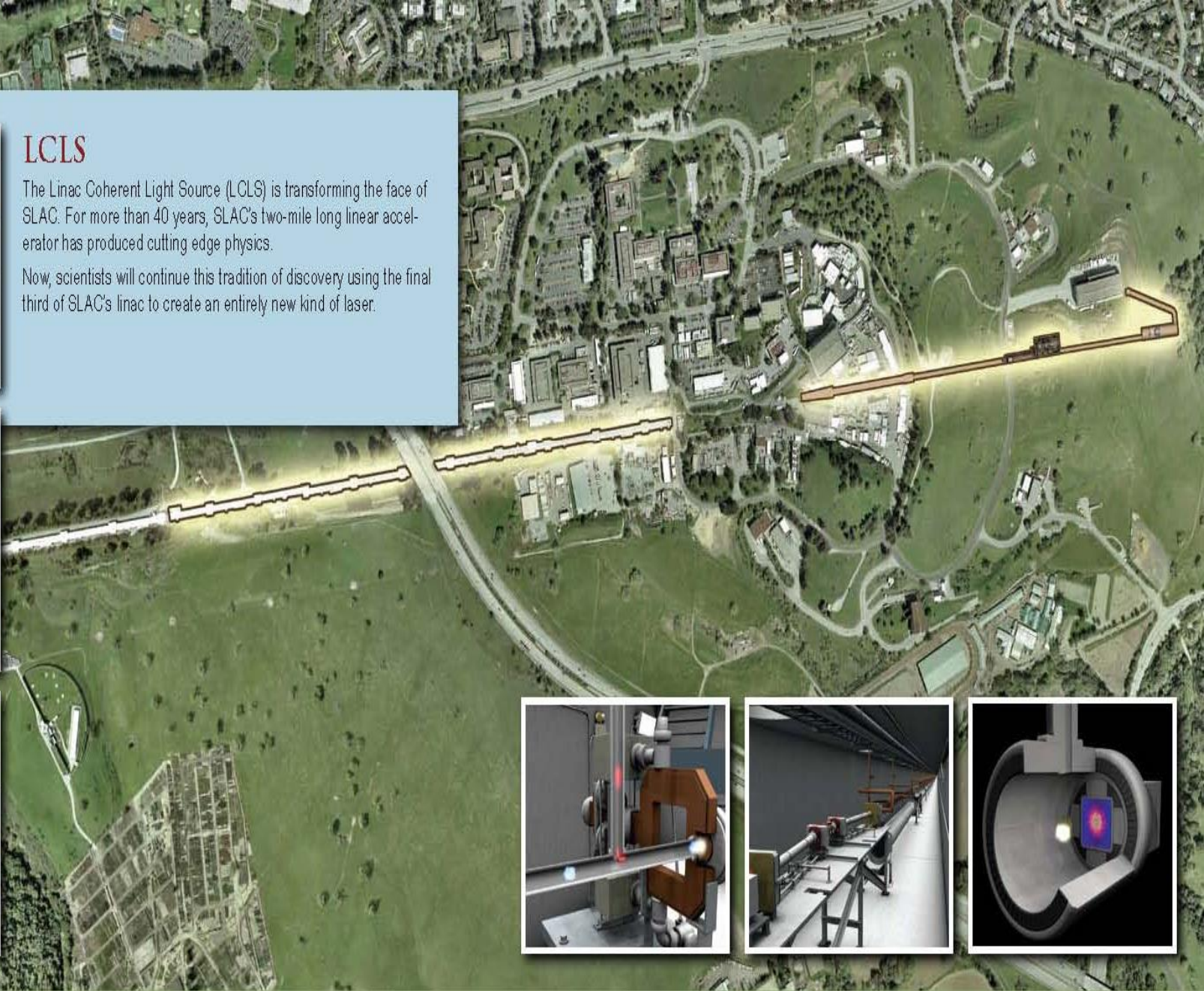
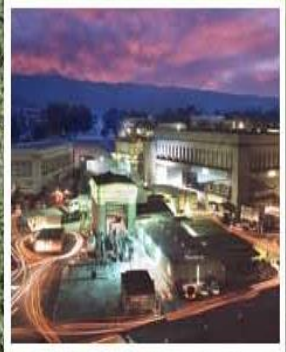
(Received 20 February 1970; in final form 21 August 1970)

The Weizsäcker-Williams method is used to calculate the gain due to the induced emission of radiation into a single electromagnetic mode parallel to the motion of a relativistic electron through a periodic transverse dc magnetic field. Finite gain is available from the far-infrared through the visible region raising the possibility of continuously tunable amplifiers and oscillators at these frequencies with the further possibility of partially coherent radiation sources in the ultraviolet and x-ray regions to beyond 10 keV. Several numerical examples are considered.

LCLS

The Linac Coherent Light Source (LCLS) is transforming the face of SLAC. For more than 40 years, SLAC's two-mile long linear accelerator has produced cutting edge physics.

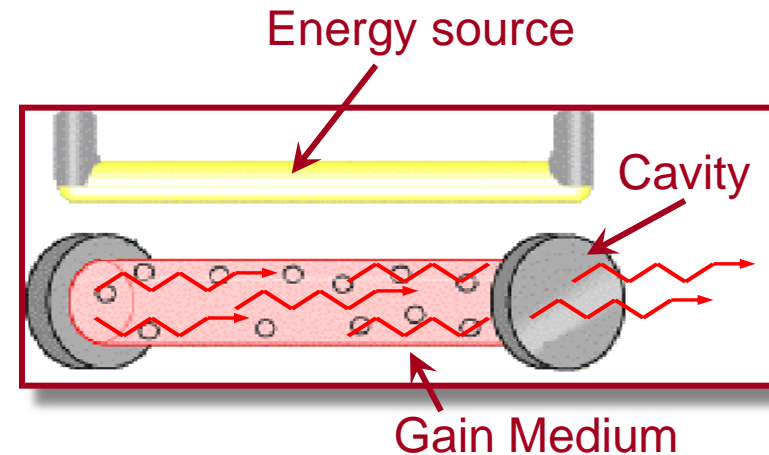
Now, scientists will continue this tradition of discovery using the final third of SLAC's linac to create an entirely new kind of laser.



The World's First Hard X-ray Free-Electron Laser

Laser Components

1. Energy Source (e.g. flashlamp)
2. Radiation Source (electronic transition)
3. Wavelength Selection (gain medium):
4. Gain (oscillator cavity)



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Stimulated Emission of Bremsstrahlung in a Periodic Magnetic Field

JOHN M. J. MADEY

Physics Department, Stanford University, Stanford, California 94305

(Received 20 February 1970; in final form 21 August 1970)

The Weizsäcker-Williams method is used to calculate the gain due to the induced emission of radiation into a single electromagnetic mode parallel to the motion of a relativistic electron through a periodic transverse dc magnetic field. Finite gain is available from the far-infrared through the visible region raising the possibility of continuously tunable amplifiers and oscillators at these frequencies with the further possibility of partially coherent radiation sources in the ultraviolet and x-ray regions to beyond 10 keV. Several numerical examples are considered.

Free Electron Laser Basics: FEL Components

Energy source: SLAC Linac

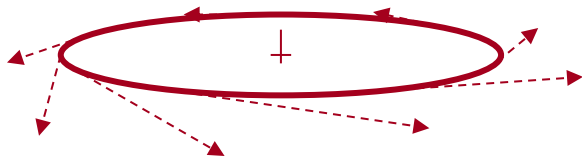
1 km can produce ~ 15 GeV beam \sim TW peak power

XFEL extracts less than 0.1% as radiation



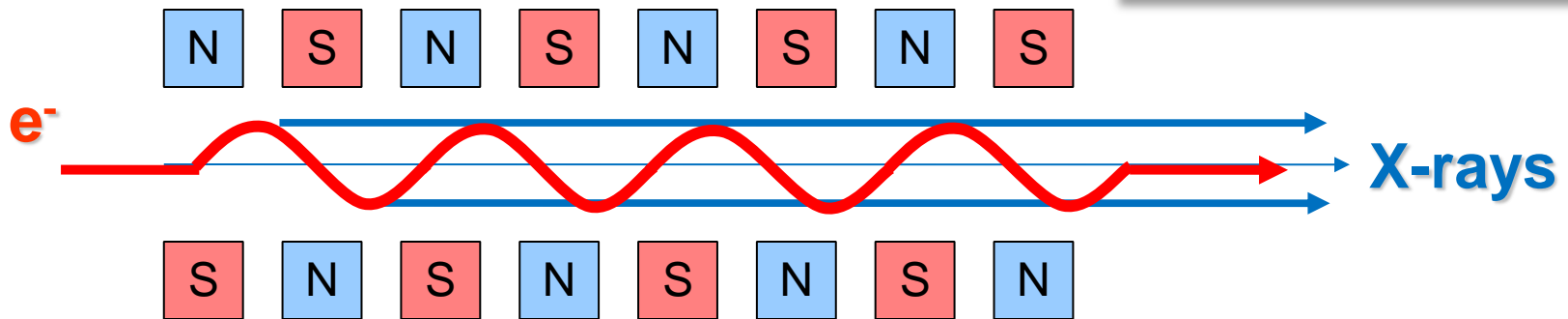
Free Electron Laser Basics: Radiation Source

Bending high energy electrons → X-rays



Synchrotron Radiation

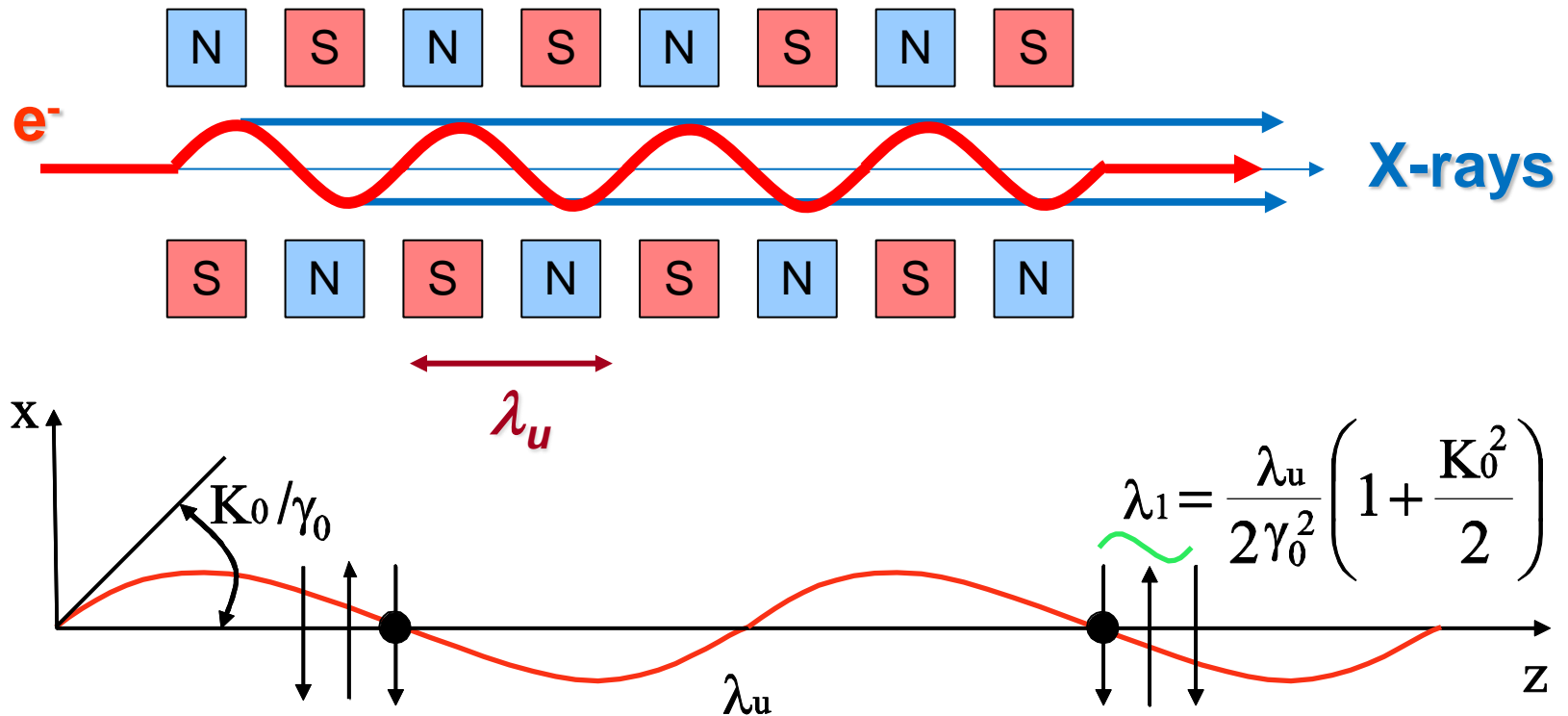
Modern light sources use Undulators:



Free Electron Laser Basics: Resonant Condition

Electrons travel farther than photons

- Match slippage to exactly one radiation wavelength
- Only resonant wavelength is amplified

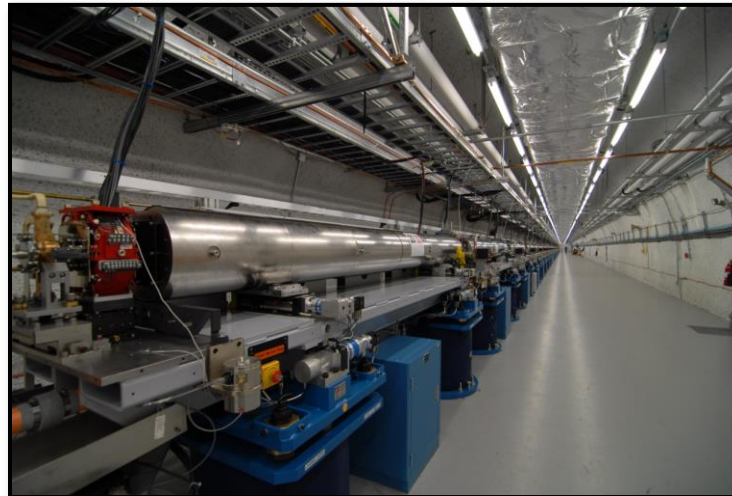
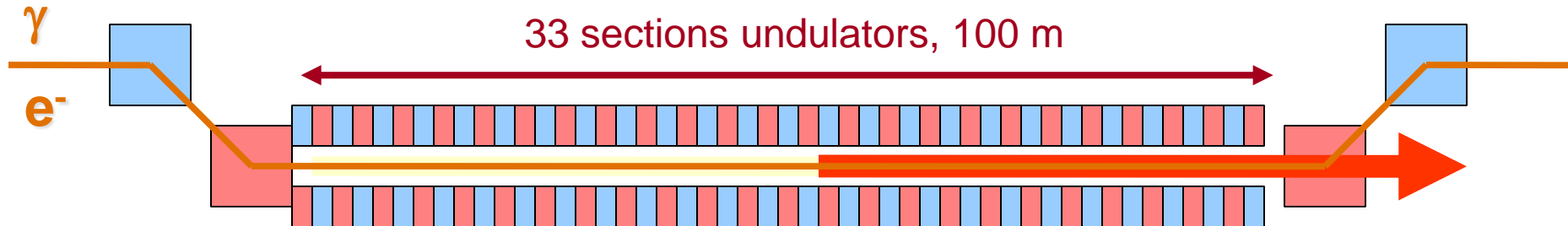


Free Electron Laser Basics: Gain

High Gain FEL: single pass for electrons

No mirrors, no cavity

LCLS uses ~3000 periods



1D FEL Theory

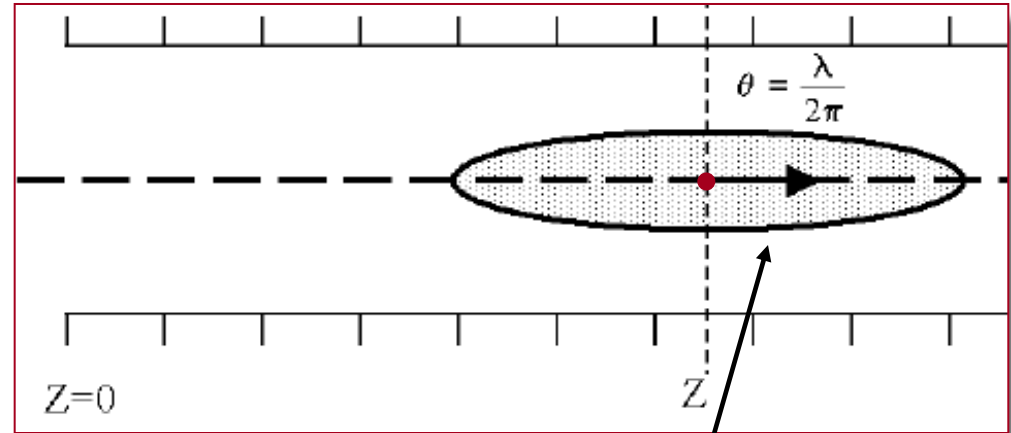
Define new variables

energy $\eta = (\gamma - \gamma_0) / \gamma_0$

phase $\theta = (k_r + k_u)z - \omega_r t$

radiation wavenumber undulator wavenumber

arrival time at undulator distance



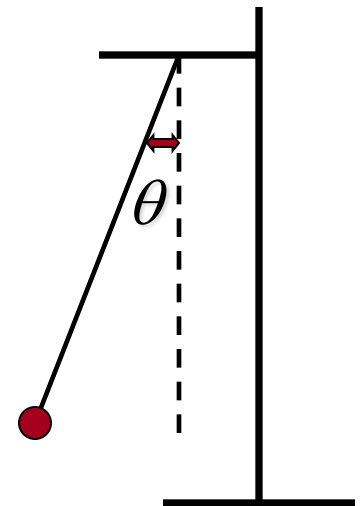
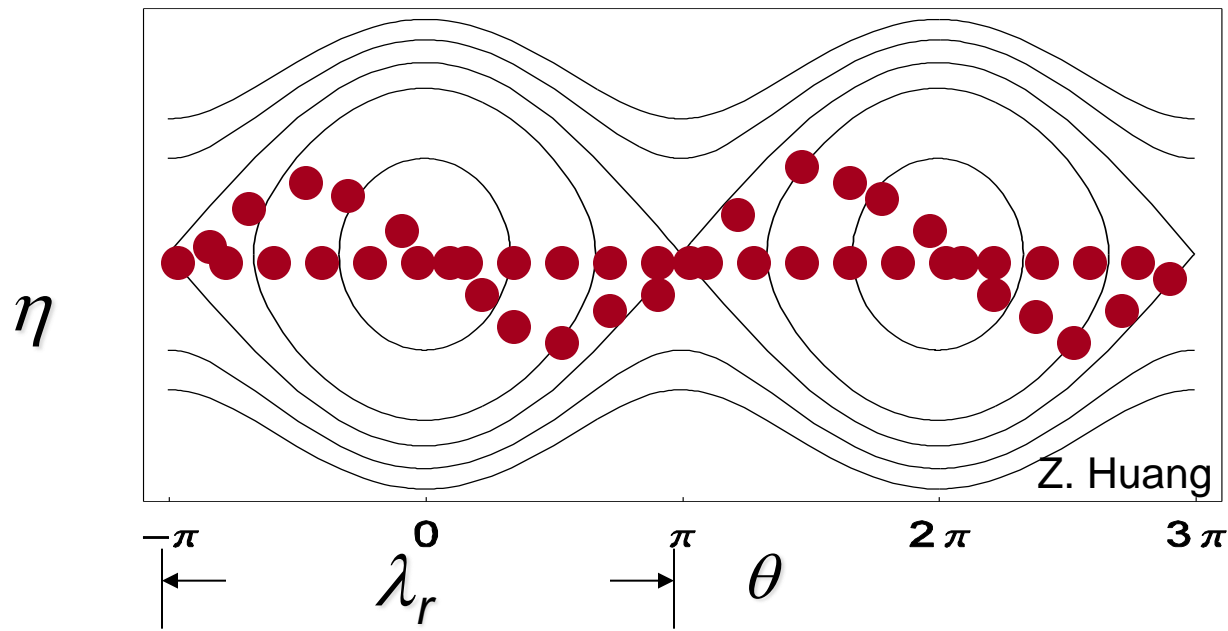
Electron phase, θ , is longitudinal position relative to radiation phase

$$\frac{dq}{dz} = 2hk_u, \quad \frac{dh}{dz} = c_1 \left(\tilde{E}e^{iq} + \tilde{E}^*e^{-iq} \right)$$

field amplitude

$$\chi_1 = \frac{eK[\text{JJ}]}{(2\gamma_0^2 mc^2)}, \quad [\text{JJ}] = J_0 \left(\frac{K^2}{4 + 2K^2} \right) - J_1 \left(\frac{K^2}{4 + 2K^2} \right) \quad (\text{planar undulator})$$

$$K = eB_0/(mck_u) = 0.94B_0[\text{Tesla}]\lambda_u[\text{cm}]$$



Intro to FEL Theory

Radiation scales as e⁻ bunching:



$$\frac{d\tilde{E}}{dz} \propto \mu \langle e^{-iq_j} \rangle_{\text{Slice}} \propto b$$

e⁻ bunching

Combining 3 coupled equations

$$\frac{dq}{dz} = 2hk_u, \quad \frac{dh}{dz} = c_1 \left(\tilde{E}e^{iq} + \tilde{E}^*e^{-iq} \right), \quad \frac{d\tilde{E}}{dz} \propto \mu \langle e^{-iq_j} \rangle_{\text{Slice}}$$

$$\rightarrow \frac{d^3 \tilde{a}}{d\bar{z}^3} \propto i \tilde{a}$$

$$\bar{z} = 2k_u r z$$

$$\tilde{a} = \frac{c_1}{2k_u r^2} \tilde{E}$$

$$r_0 \propto \frac{I}{8\rho I_A} \frac{K[JJ]}{1 + K^2/2} \frac{\sigma}{S_A} \frac{g l_1^2}{\theta} \frac{\dot{u}}{u}^{1/3}$$

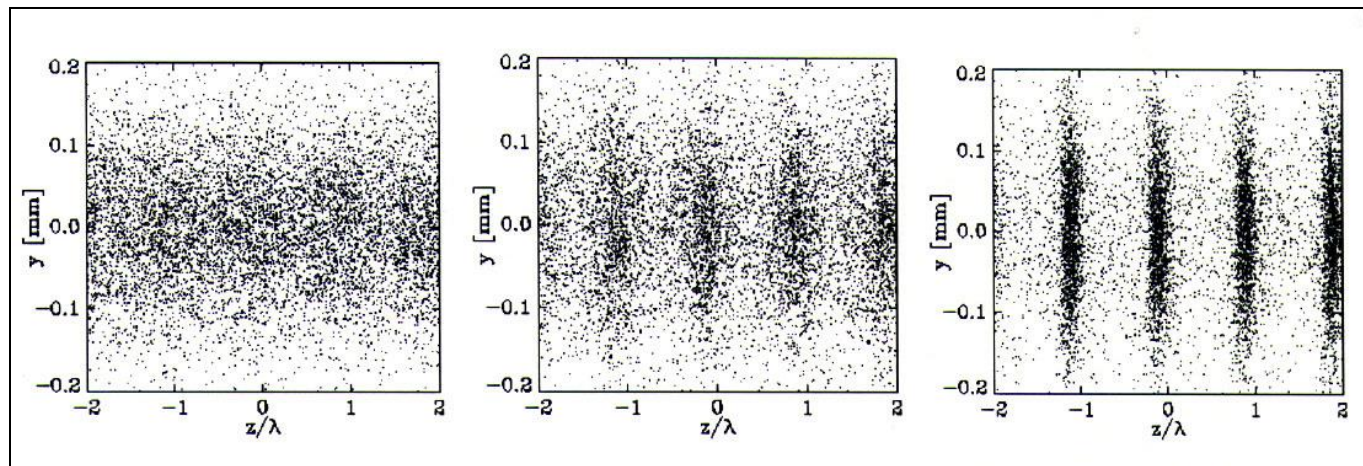
↑
Alfven current
↑
beam cross section

And finally exponential radiation growth

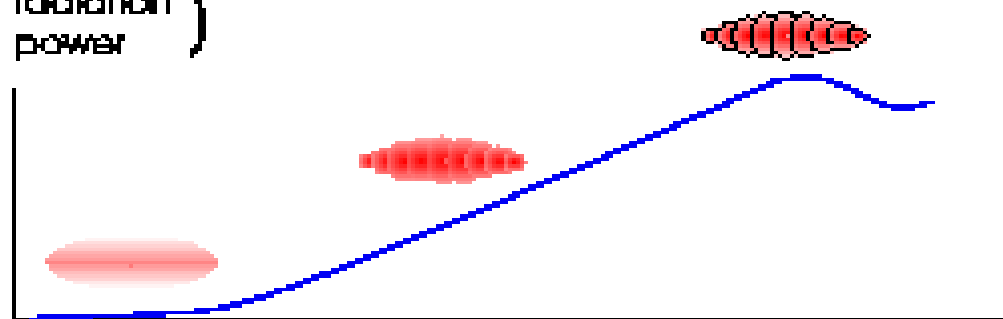
$$\tilde{A}(\bar{z}) \approx \frac{1}{3} \left(\tilde{A}(0) - i \frac{b(0)}{\mu_3} - iP(0)\mu_3 \right) e^{-i\mu_3 \bar{z}}, \quad \mu_3 \equiv \frac{-1 + \sqrt{3}i}{2}$$

↑
Radiation
↑
Bunching
↑
Momentum

X-ray FELs start from shot noise



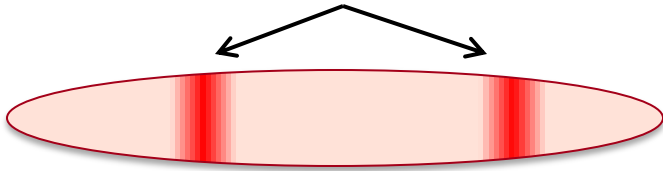
$\log(\text{radiation power})$



distance

Implications of shot noise:

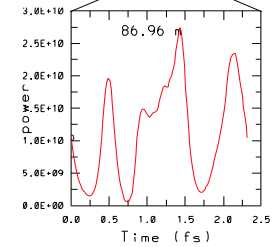
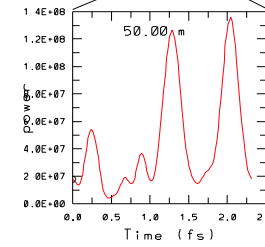
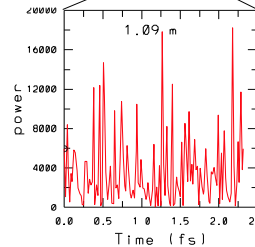
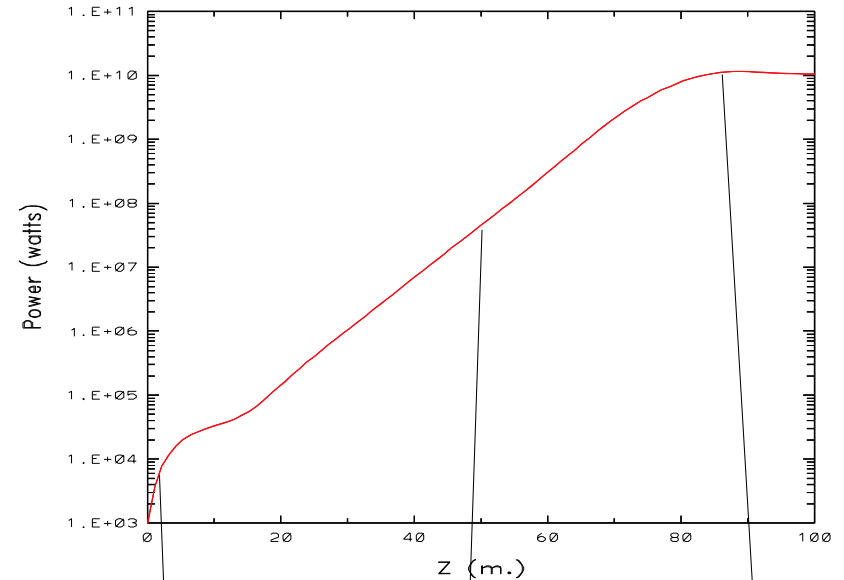
Different slices don't communicate



Each slice lases independently!

Upshot: SASE FELs have complicated temporal structure

Avg. Field Power vs. Z



1 % of X-Ray Pulse Length

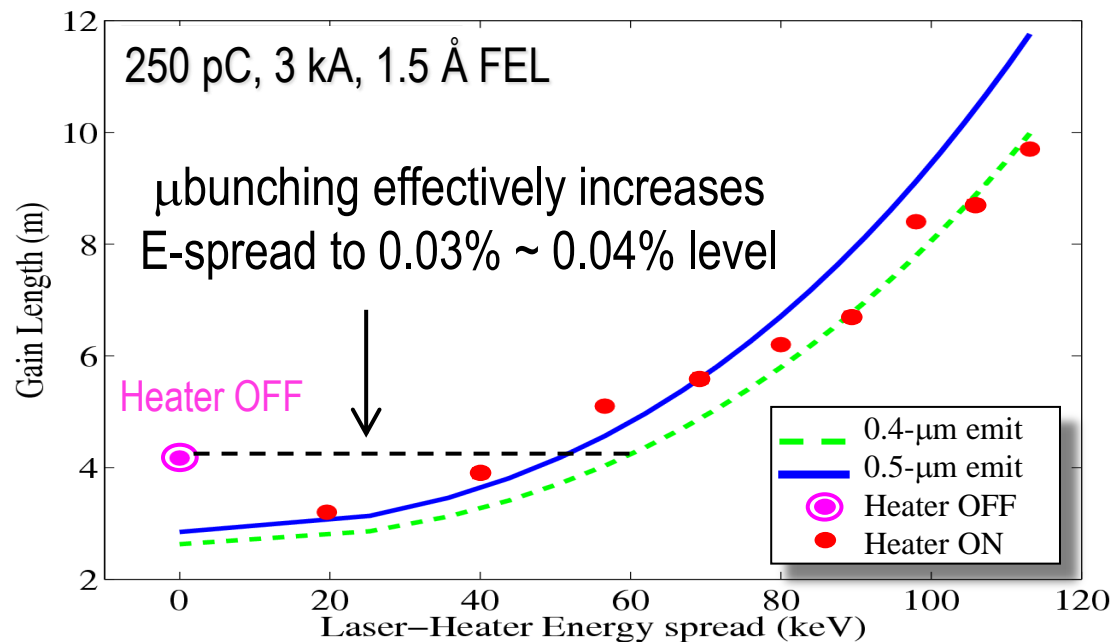
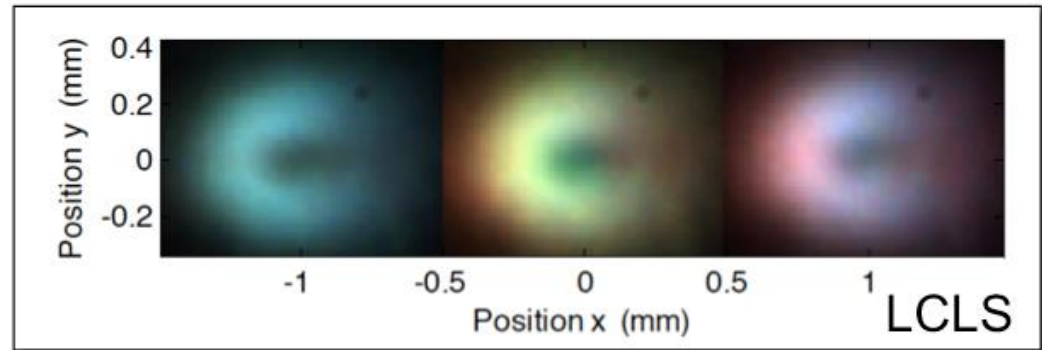
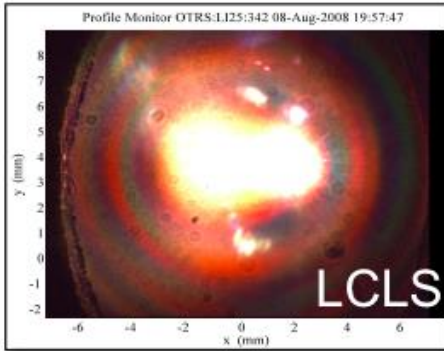
LCLS accelerator parameters:

Parameter	Value
Electron energy range	2.5-15.8 GeV
Electron charge	20-250 pC
Slice emittance (normalized)	0.2-0.4 μm
Electron pulse length	\sim 5-500 fs
Peak current	1-3 kA
Initial slice energy spread	1-2 MeV
Electron energy jitter	0.04-0.07 %
Undulator period	3 cm
Number of undulator periods	3000
Gain length	1.5-3 m

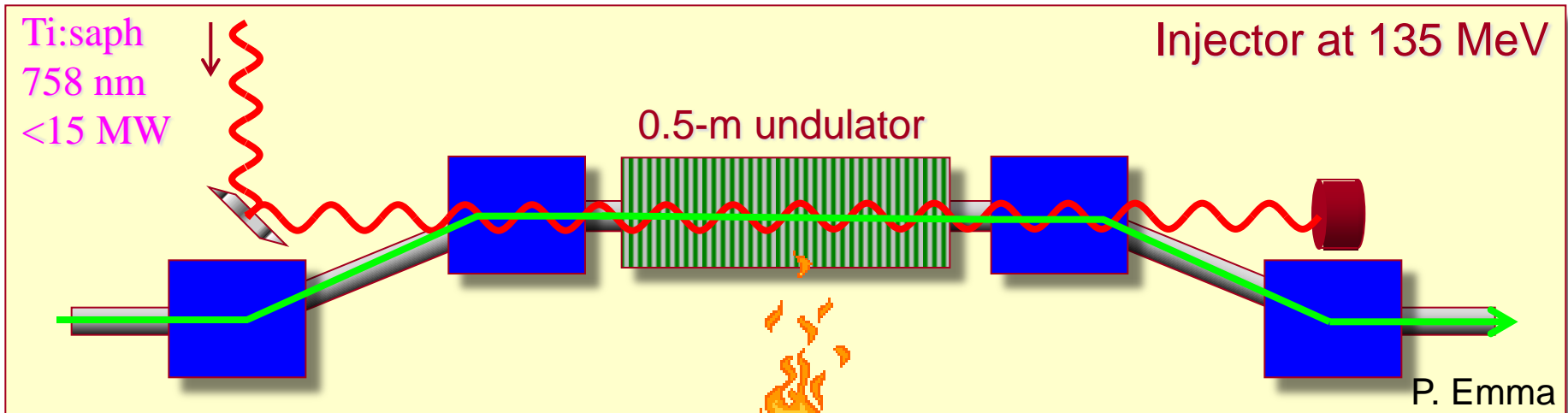
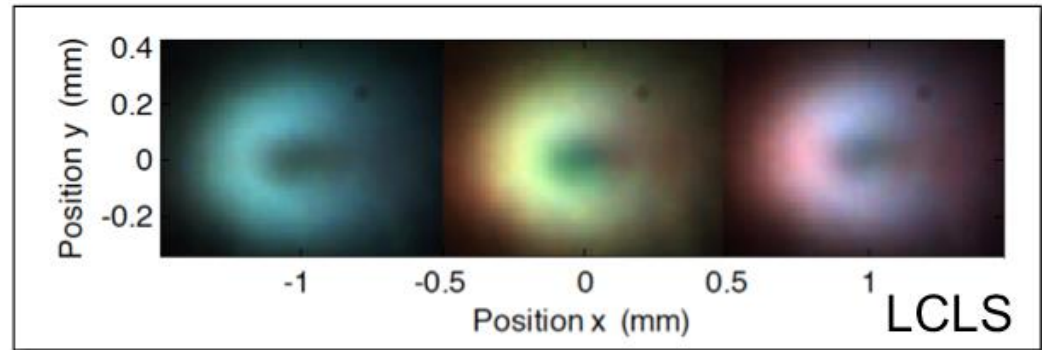
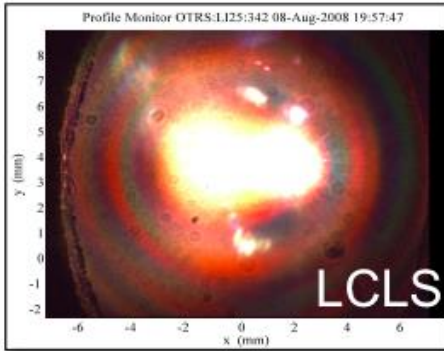
LCLS X-ray performance:

Parameter	Value
Photon energy range (fundamental)	0.3-11.2 keV
Photon wavelength range	0.11-4 nm
Typical pulse energy	2 mJ
Typical number of photons	$10^{12} - 10^{13}$
Bandwidth (non-seeded)	0.1-0.5 %
Pulse length	<10-400 fs

Microbunching Instability



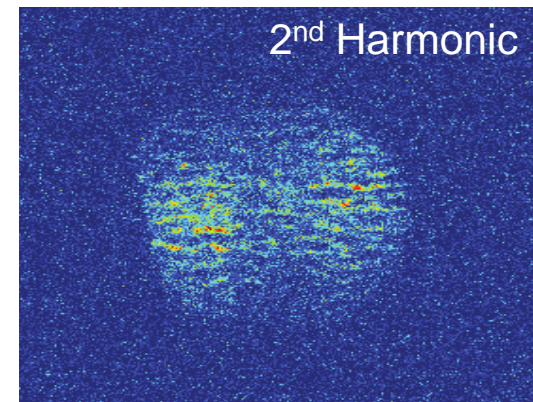
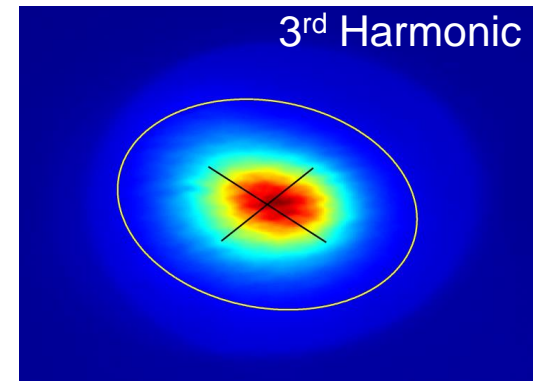
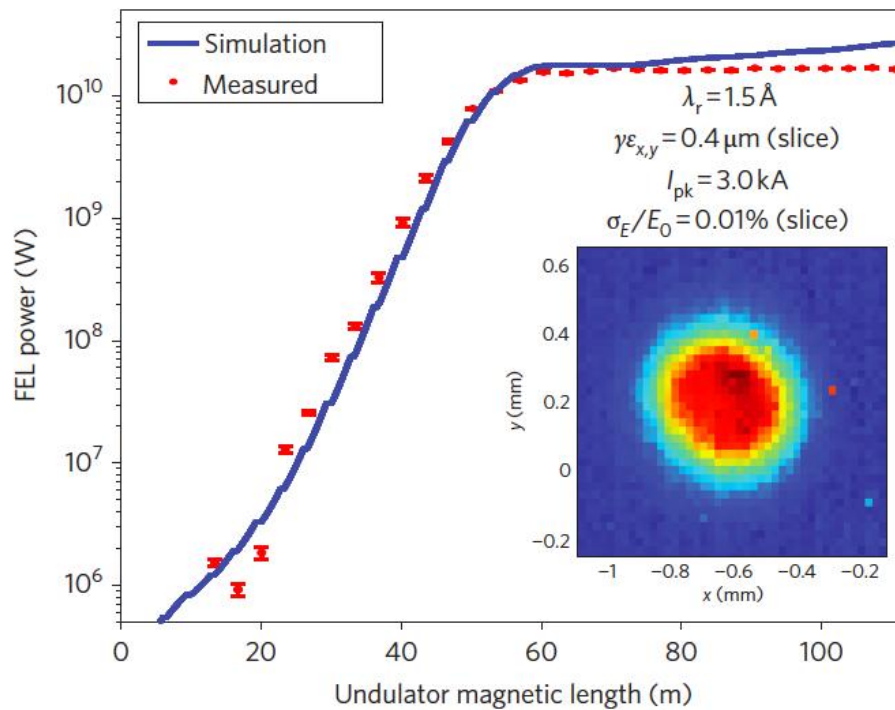
Microbunching Instability



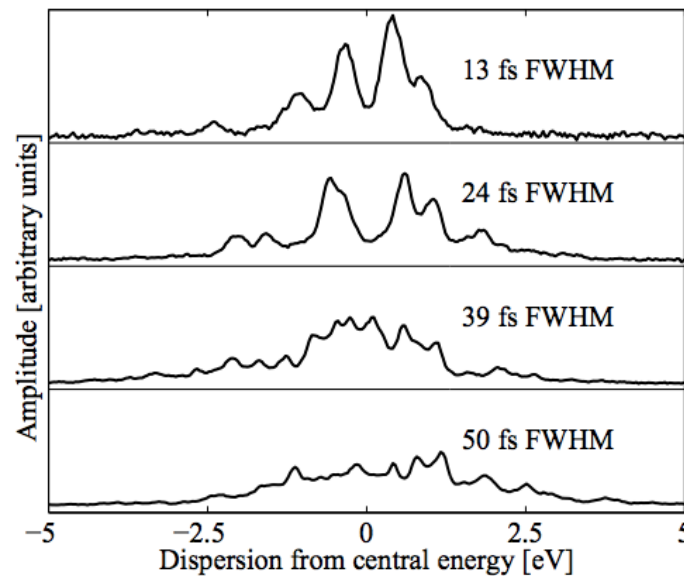
'Laser heater' suggested by Saldin et al., NIMA, 2004;²³
independently by J. Galayda

LCLS design study: Z. Huang et al., PRST 2004
(chicane suggested by T. Smith)

LCLS data: Transverse structure



LCLS data: Longitudinal structure

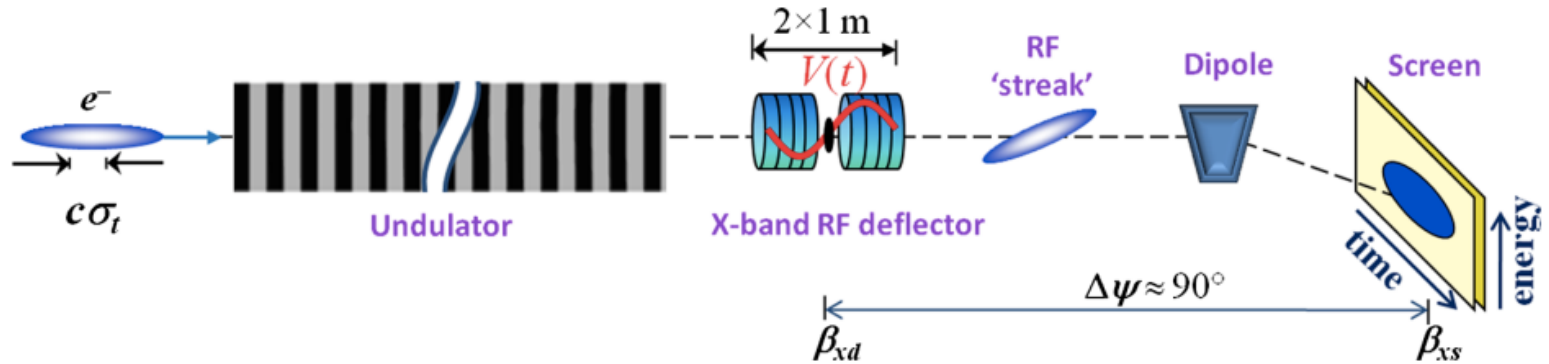


PHYSICAL REVIEW SPECIAL TOPICS - ACCELERATORS AND BEAMS **15**, 030705 (2012)

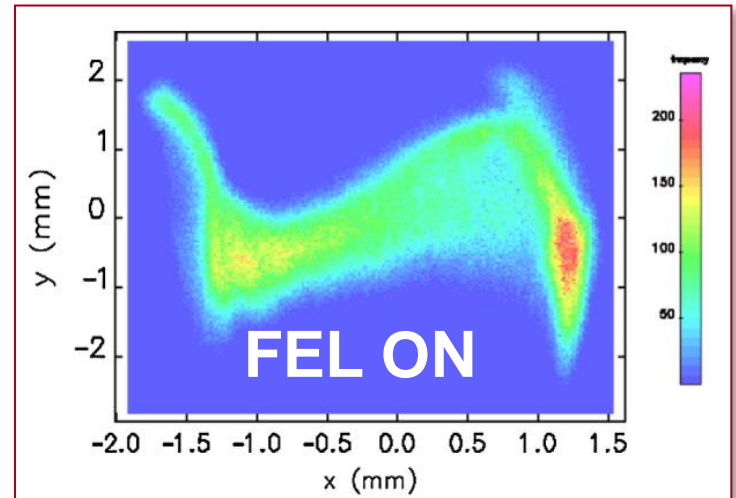
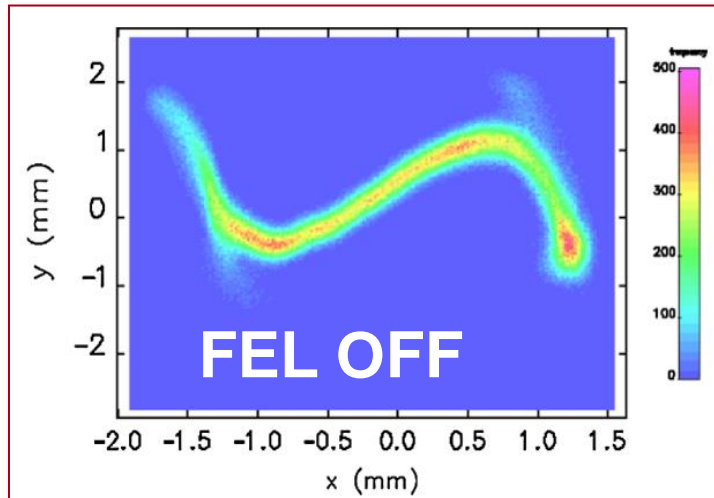
Femtosecond x-ray free electron laser pulse duration measurement from spectral correlation function

A. A. Lutman,^{*} Y. Ding, Y. Feng, Z. Huang, M. Messerschmidt, J. Wu, and J. Krzywinski

X-Band Transverse Cavity



Energy ↑



Time →

Moving Beyond the Vanilla FEL

Baseline modern X-ray FEL:

- High power (GW) in the X-ray regime
- Good transverse coherence, poor longitudinal coherence
- Need ~1km and ~\$1 billion to build

Looking towards the future:

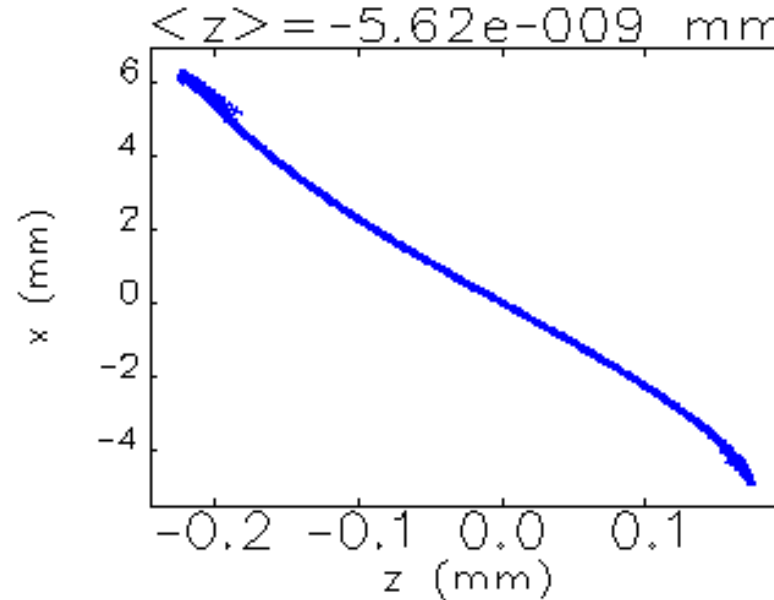
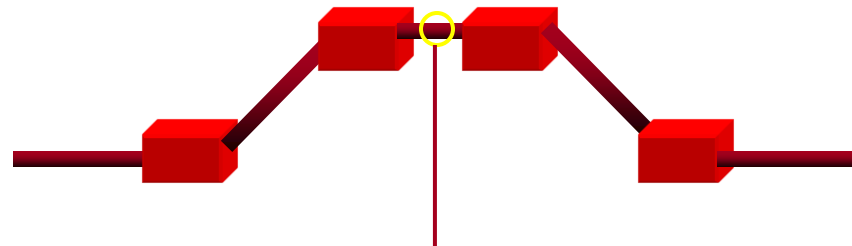
- Shorter pulses/higher power
- More energy per pulse
- Coherent control
- Smaller and cheaper!

Slotted-spoiler

Large x-z correlation inside a bunch compressor chicane

LCLS BC2

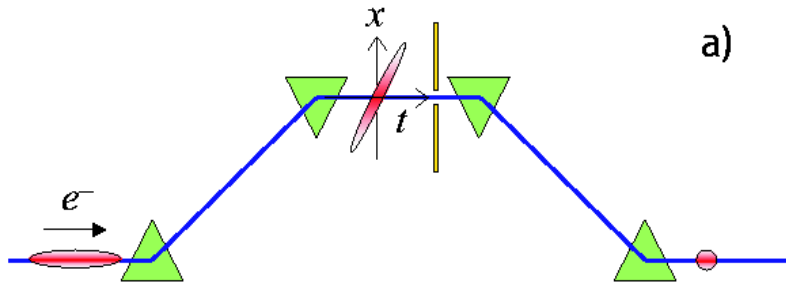
2.6 mm rms



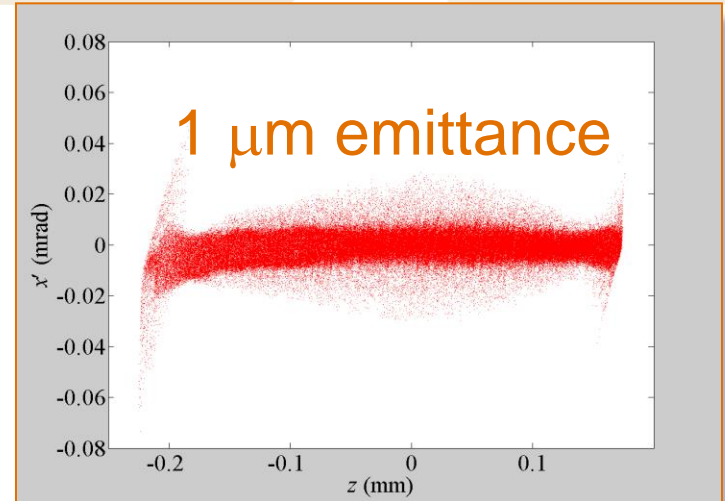
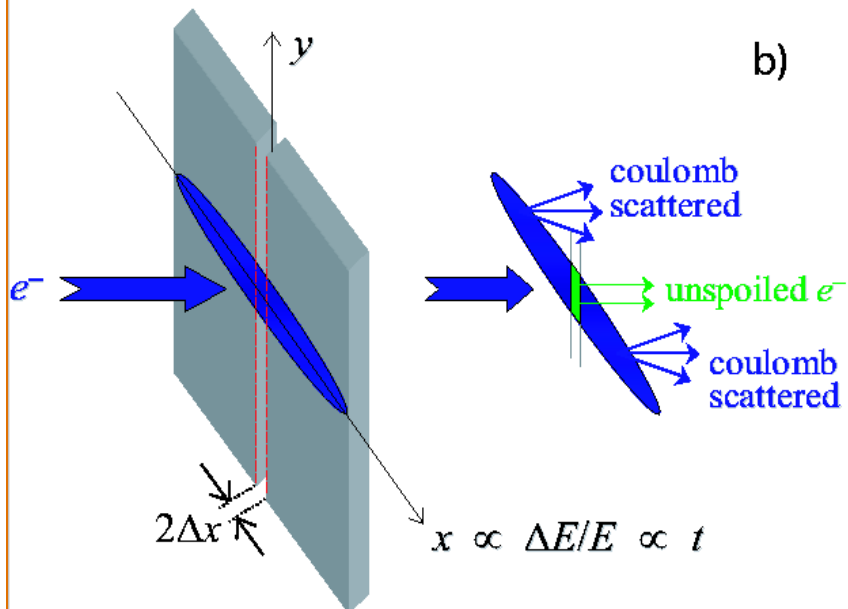
← Easy access to *time* coordinate along bunch

0.1₂₈ mm rms

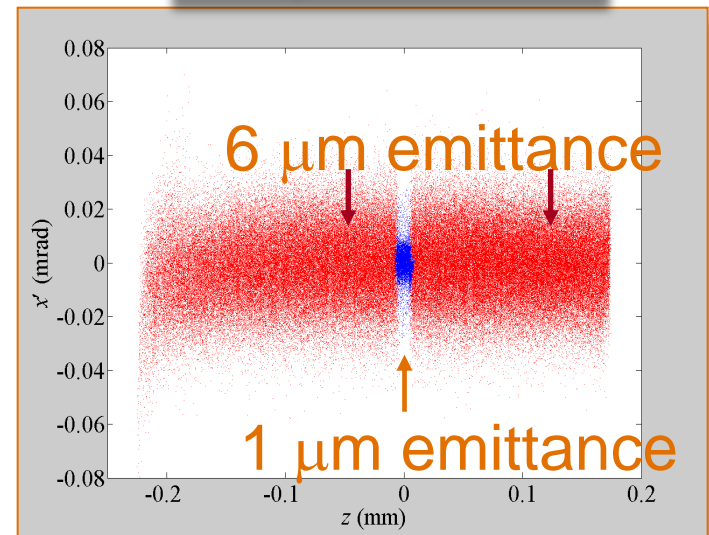
Slotted-spoiler



P. Emma et al. PRL92, 074801 (2004)



15- μm Be foil



Low charge mode

→ Short pulse, low emittance



nominal: 150-250 pC



low charge mode: 10-40 pC

PRL 102, 254801 (2009)

PHYSICAL REVIEW LETTERS

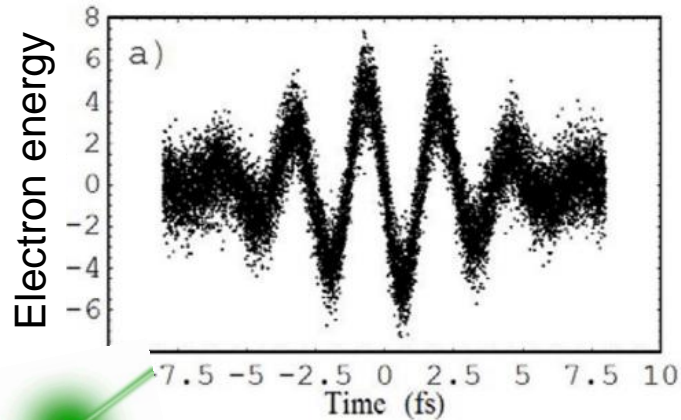
week ending
26 JUNE 2009

Measurements and Simulations of Ultralow Emittance and Ultrashort Electron Beams in the Linac Coherent Light Source

Y. Ding, A. Brachmann, F.-J. Decker, D. Dowell, P. Emma, J. Frisch, S. Gilevich, G. Hays, Ph. Hering, Z. Huang,
R. Iverson, H. Loos, A. Miahnahri, H.-D. Nuhn, D. Ratner, J. Turner, J. Welch, W. White, and J. Wu

enhanced-SASE (eSASE)

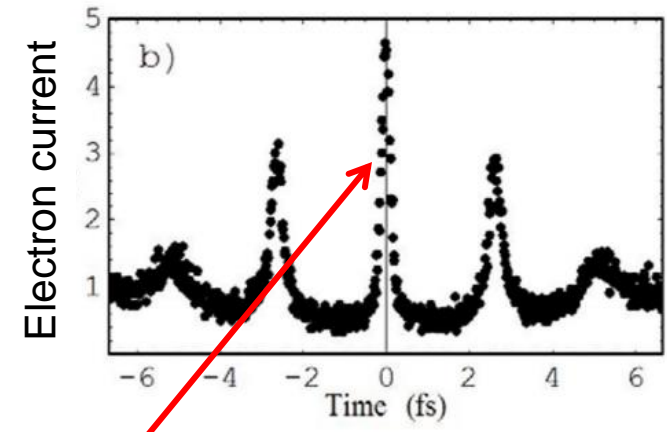
Energy modulation
from laser



Dispersion



Density modulation



Only current spike makes X-rays

PHYSICAL REVIEW SPECIAL TOPICS - ACCELERATORS AND BEAMS 8, 040701 (2005)

Method of an enhanced self-amplified spontaneous emission for x-ray free electron lasers

Alexander A. Zholents

Coherent Control

Two Color:

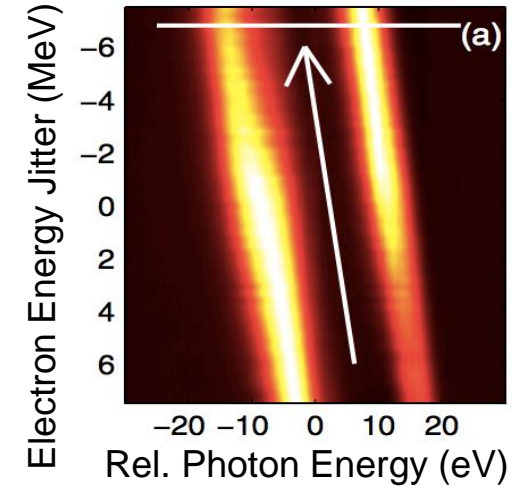
PRL 110, 134801 (2013)

PHYSICAL REVIEW LETTERS

week ending
29 MARCH 2013

Experimental Demonstration of Femtosecond Two-Color X-Ray Free-Electron Lasers

A. A. Lutman, R. Coffee, Y. Ding,* Z. Huang, J. Krzywinski, T. Maxwell, M. Messerschmidt, and H.-D. Nuhn



Polarization Control:

Nuclear Instruments and Methods in Physics Research A 347 (1994) 83–86

Analyses for a planar variably-polarizing undulator

Shigemi Sasaki

APPLE-II, BESSY



Modelocking:

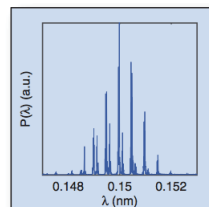
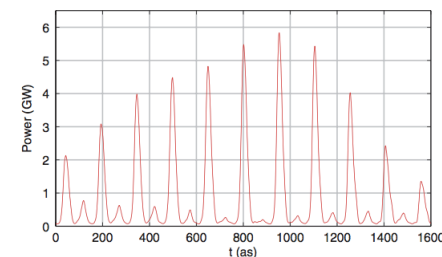
PRL 100, 203901 (2008)

PHYSICAL REVIEW LETTERS

week ending
23 MAY 2008

Mode Locking in a Free-Electron Laser Amplifier

N. R. Thompson^{1,2,*} and B. W. J. McNeil^{1,†}



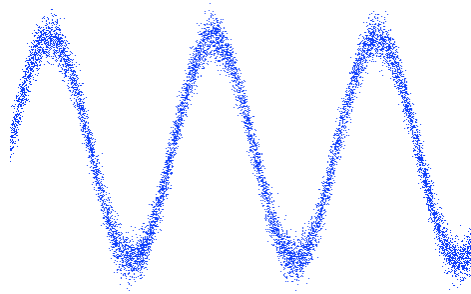
SASE FEL: Start from shot noise

Seeded FEL: Start from radiation

$$\tilde{a}(\bar{z}) \gg \frac{1}{3} \underbrace{e^{i\bar{z}} \tilde{a}(0)}_{\text{Radiation}} \underbrace{- i \frac{b(0)}{m_3}}_{\text{Bunching}} - iP(0) \underbrace{m_3}_{\text{Momentum}} e^{-im_3\bar{z}}$$

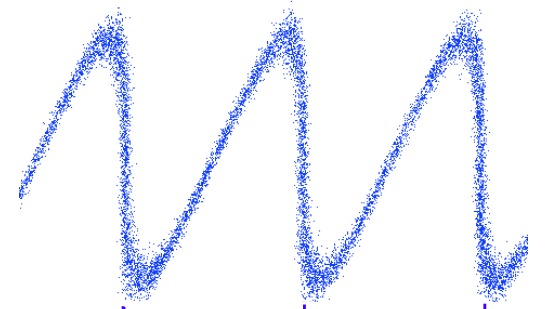


Energy

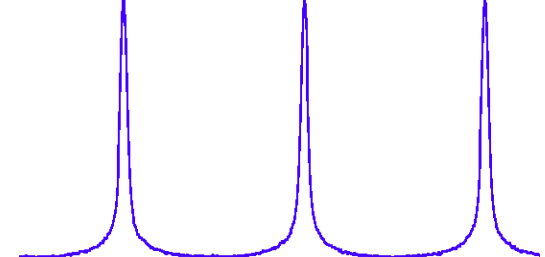


Position

Dispersion

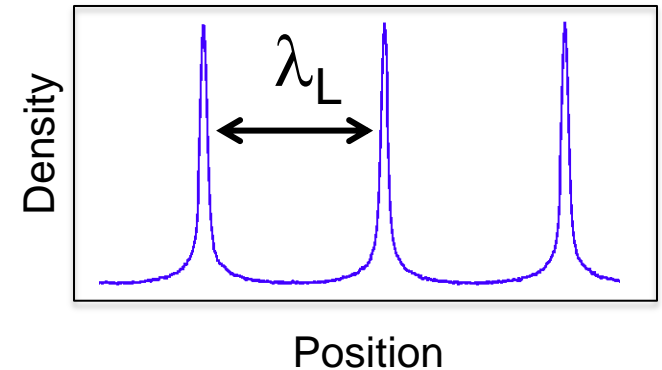


Density



Seeded FEL: Start from radiation

$$\tilde{a}(\bar{z}) \gg \frac{1}{3} \tilde{a}(0) - i \frac{b(0)}{m_3} - i P(0) m_3 \ddot{\theta} e^{-im_3 \bar{z}}$$



Short-wavelength seeding:

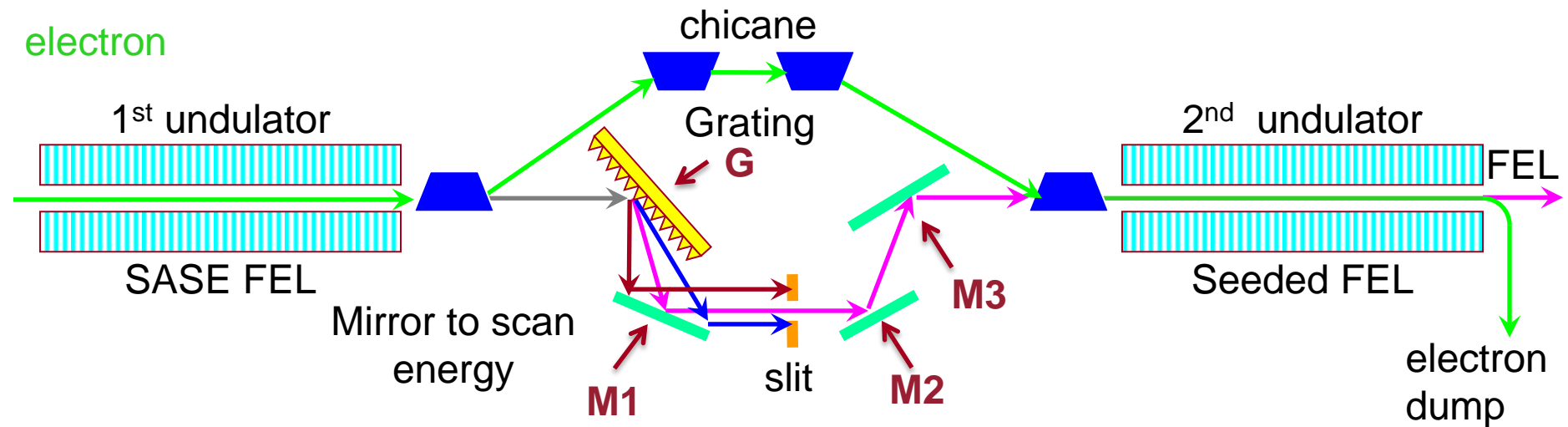
1. High Harmonic Generation (HHG): **small λ_L**
2. Harmonic seeding: **$\lambda_L \rightarrow \lambda_L/H$**
 High Gain Harmonic Generation (HG)
 - Echo-enabled Harmonic Generation (EEHG)
3. Self-seeding: **use λ_{FEL}**

Self-Seeding: First half of FEL seeds second half

Two components:

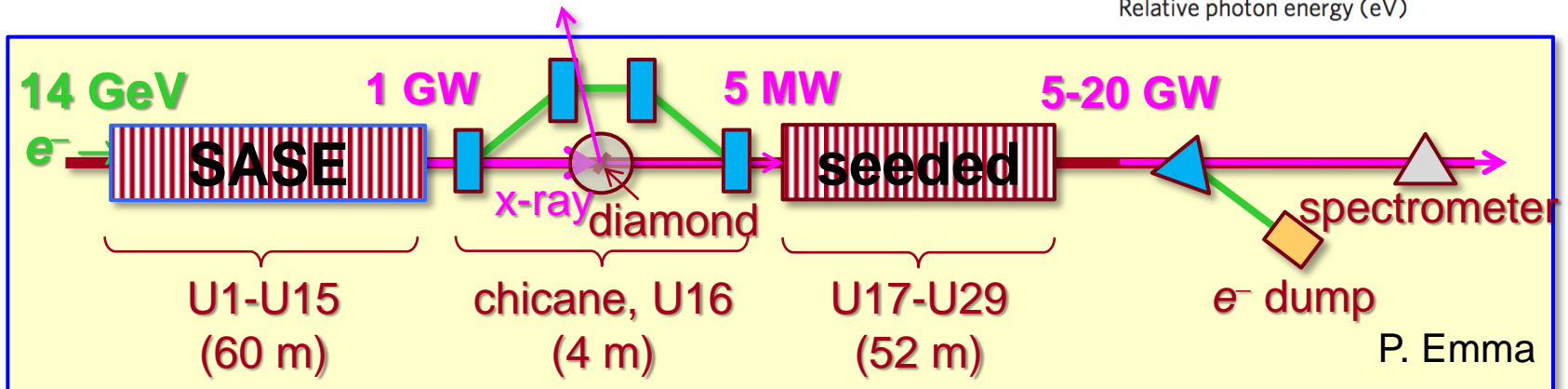
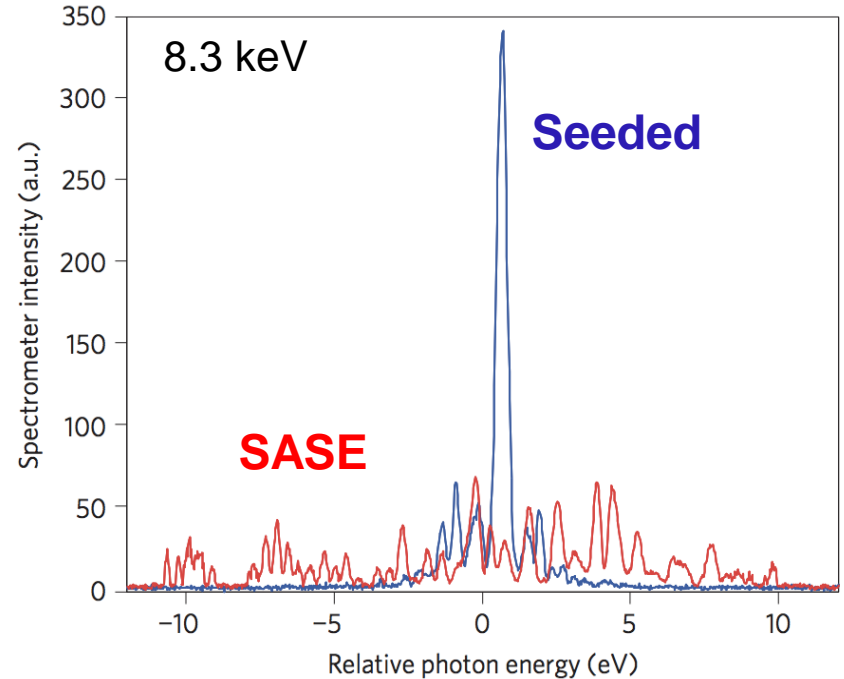
- a) Monochromator makes narrow-bandwidth seed
- b) Chicane resets electron bunch

Soft X-ray Self-Seeding Design

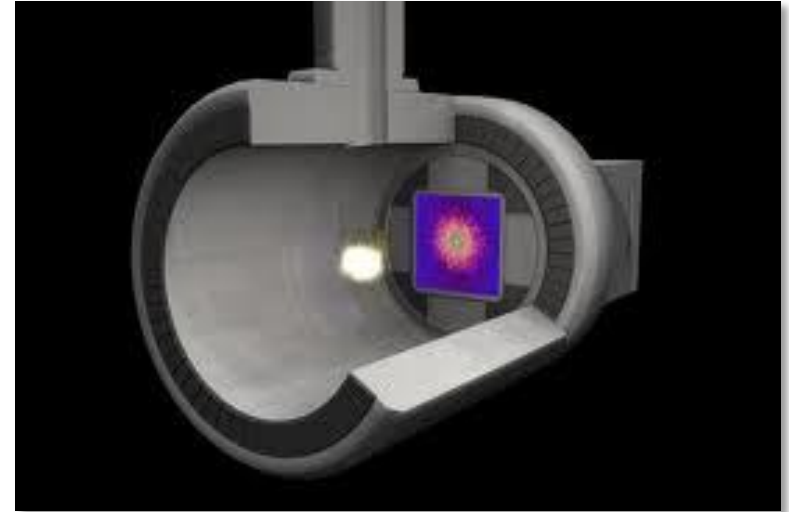


Self-Seeding: Hard X-rays

Diamond Bragg reflection produces monochromatic wake



**XFEL dream:
Single molecule imaging
...but need TW FEL!!**



LCLS currently saturates around 10 GW

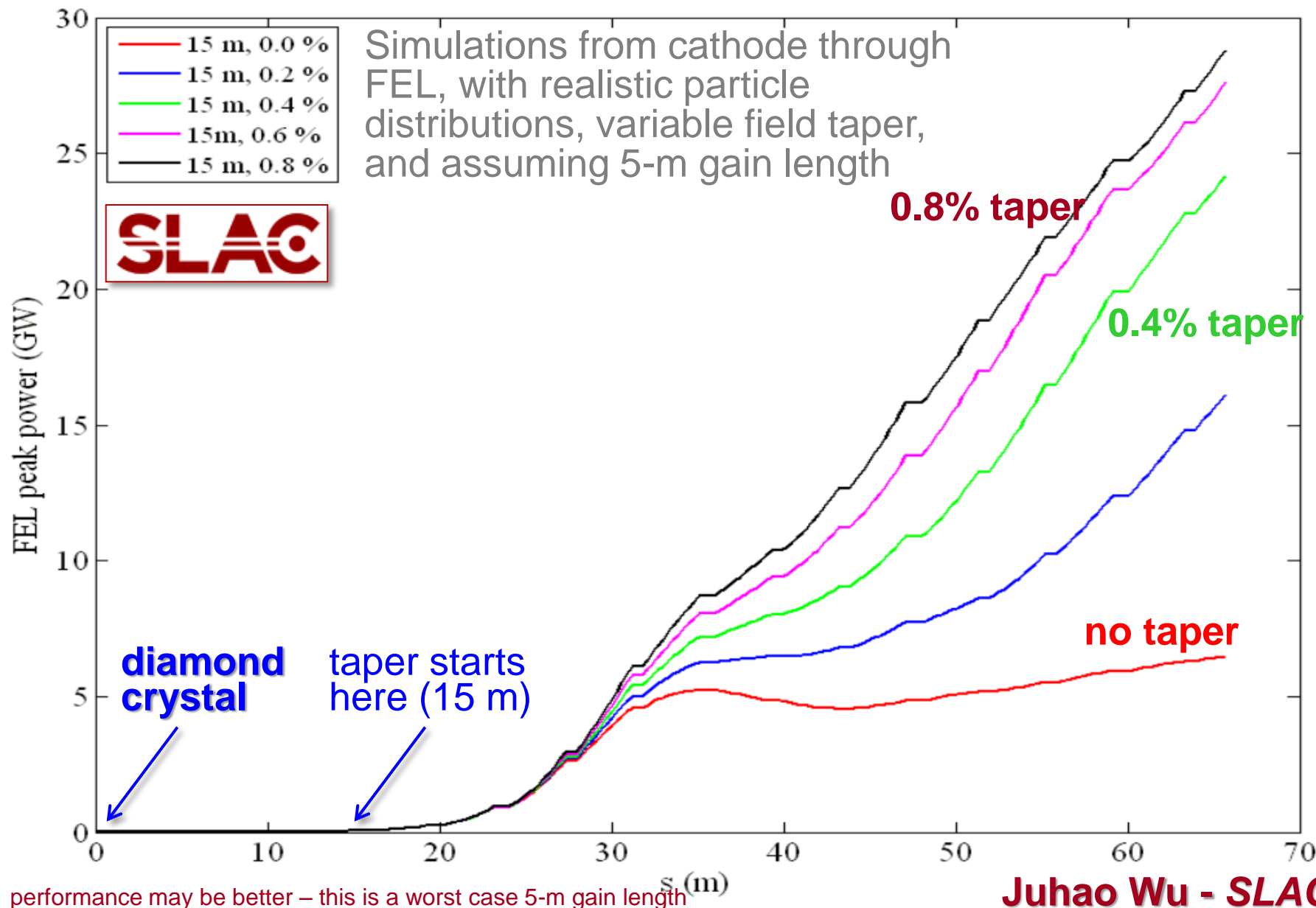
1. Bunching maximal
 → exponential growth ends
2. e- energy drops
 → Resonant frequency changes

Offset with drop in K

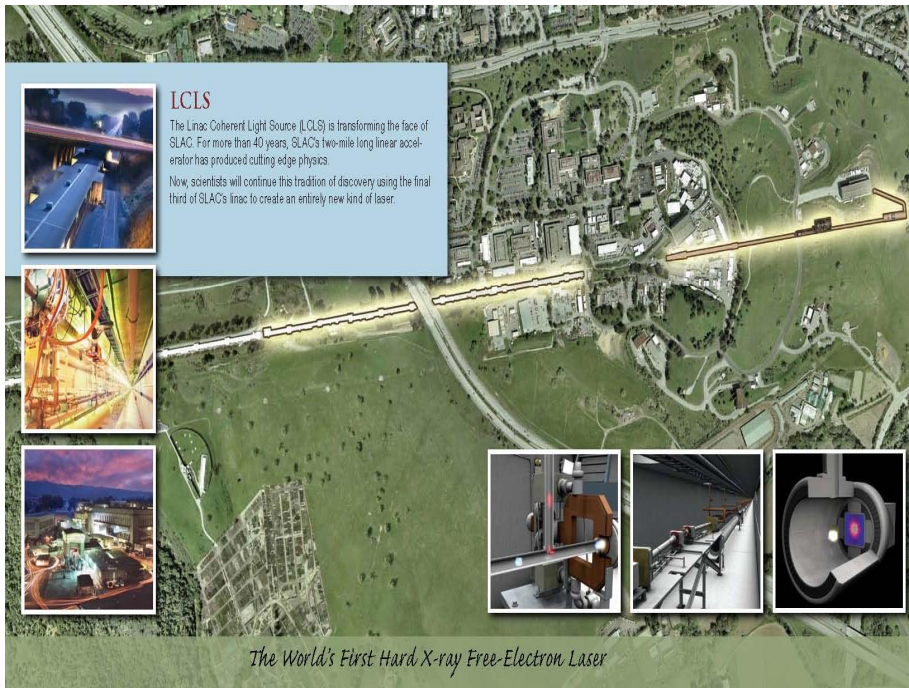
$$I_{sat} = I_u \frac{[1 + K^2 / 2]}{2(g_0 - Dg)^2} > I_1$$

Energy drops

Start-to-End HXRSS Simulations (U17-U33)



Grand challenge in FELs: Miniaturize the X-ray laser!

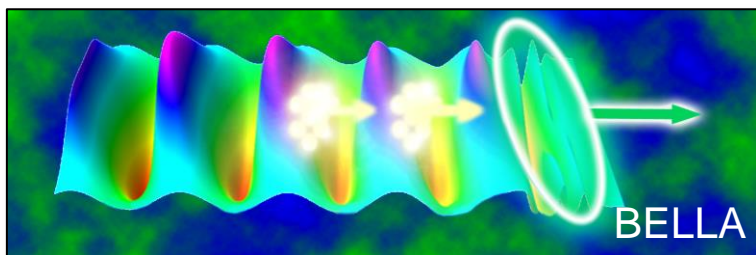


Path to a Miniature X-ray FEL: Miniaturize the Accelerator

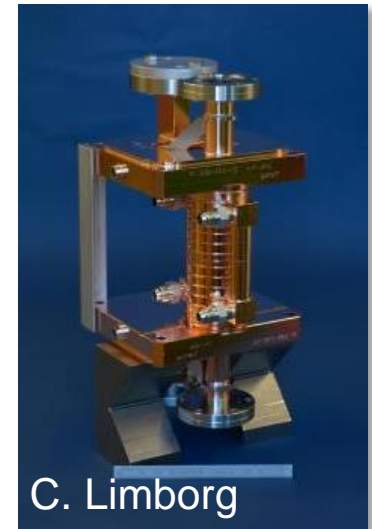
**Small step:
X-band guns, accelerators**

**Big step:
Novel acceleration methods**

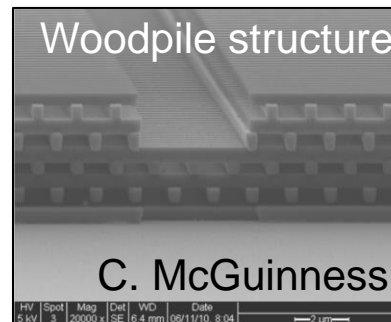
e.g. Laser wakefield
and dielectrics:



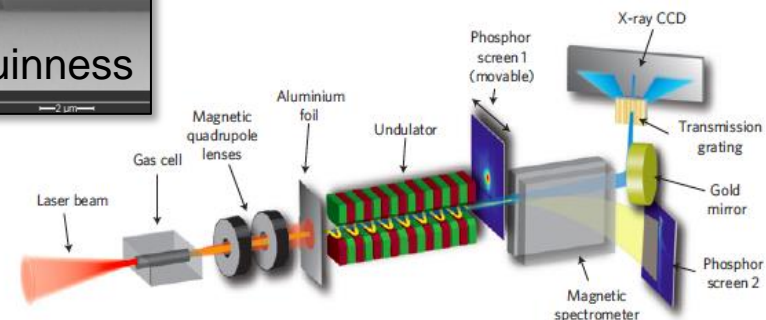
C. Limborg



C. Limborg



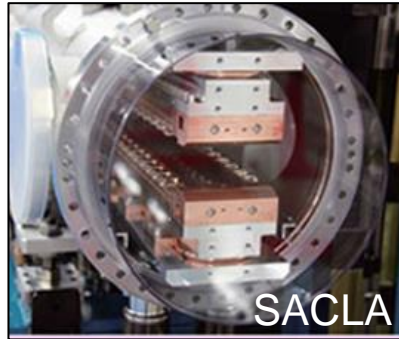
C. McGuinness



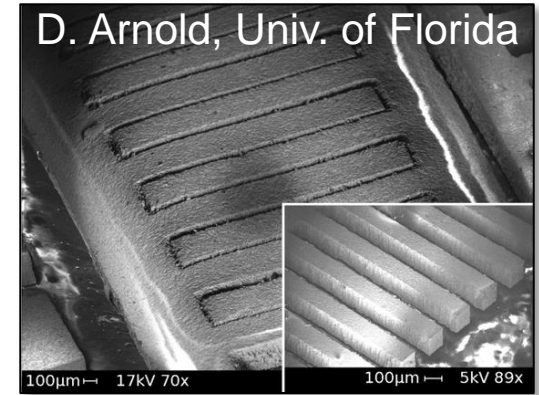
M. Fuchs et al., Nature 2009

Path to a Miniature X-ray FEL: Miniaturize the **Undulator**

Smaller periods:

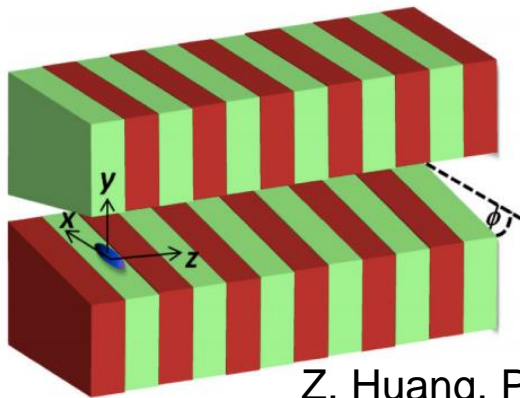


In vacuum



Micromachining

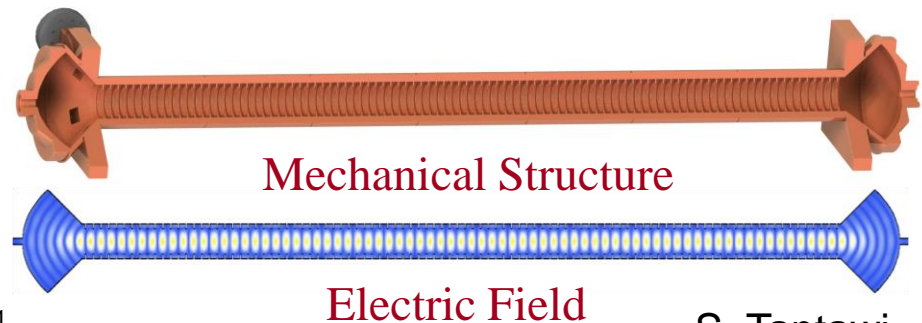
Undulators for compact accelerators:



Z. Huang, PRL 2012

Transverse Gradient Undulator

Electromagnetic undulators



Path to a Miniature X-ray FEL: Miniaturize the **Accelerator**
Miniaturize the **Undulator**

It's up to you to put them together!

FEL References

References:

K.-J. Kim and Z. Huang, FEL lecture note, available electronically upon request (zrh@slac.stanford.edu)

Saldin, Schneidmiller, Yurkov, The Physics of Free Electron Lasers (Springer, 1999), more SASE but much more technical

Thanks for help with figures from Y. Ding, B. Fawley, Z. Huang, C. Limborg, S. Reiche, J. Wu