X-Ray Free-Electron Lasers: An Introduction

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2022 National School on Neutron & X-ray Scattering
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U.S. DEPARTMENT OF ENERGY
Stanford University
SLAC NATIONAL ACCELERATOR LABORATORY

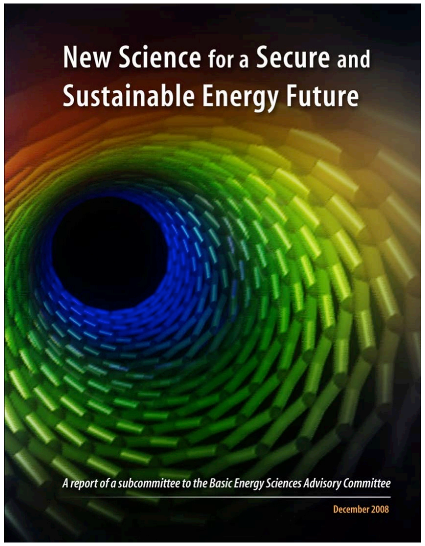
Fundamental Questions in Materials Science

What materials are present?

Where are the materials located?

When do crucial transformations and processes occur?

Why does a material have its structure and properties?



Advanced x-ray techniques provide unique information by looking into and through complex materials and devices.

Coupled with theory and advanced computing capabilities, this information enables a detailed understanding of material processing technologies and device physics.

Transformational Control and X-Rays

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The ability to make new materials and to shape them into useful objects is the heart of materials science and technology.

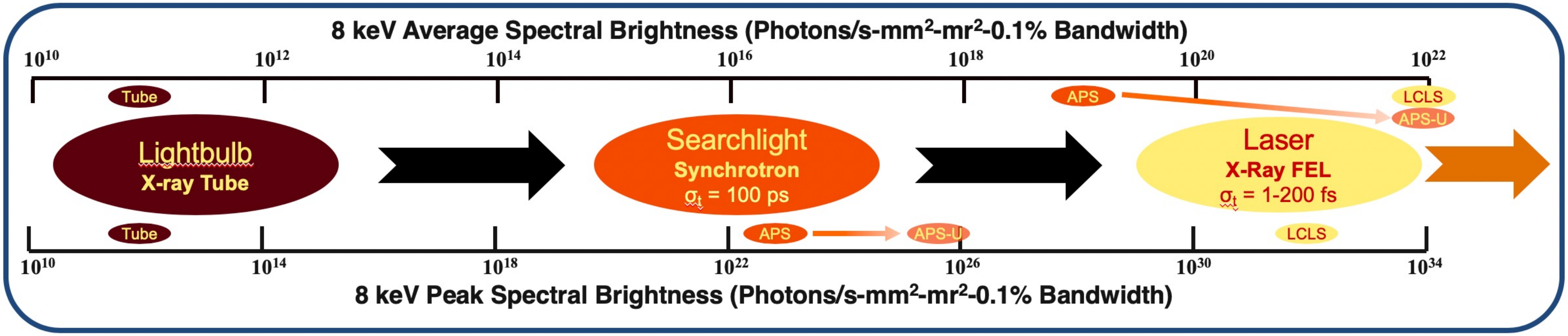
In order to meet current challenges, the cycle of material design, creation and optimization needs to be fast.

- Steel took thousands of years.
- Silicon technology took 50 years.

X-ray synchrotron radiation provides a unique window into the transformation of:

- raw materials into complex materials.
- complex materials into useful implements.

Extraordinary X-Ray Sources



Typical XFEL Performance – LCLS

- 3 mJ/pulse (2×10^{12} 10 keV photons)
- <100 femtosecond long pulses
- 120 pulses/second
- Full transverse coherence (it is a laser)
- Stochastic energy spectrum with 0.1% width

Light source advances enable:

- X-ray measurements of ultrafast behavior
- Coherent scattering studies of atomic structure and dynamics

These allow development of new analysis techniques and deeper insight into materials processes.

Evolution of Accelerator X-Ray Sources

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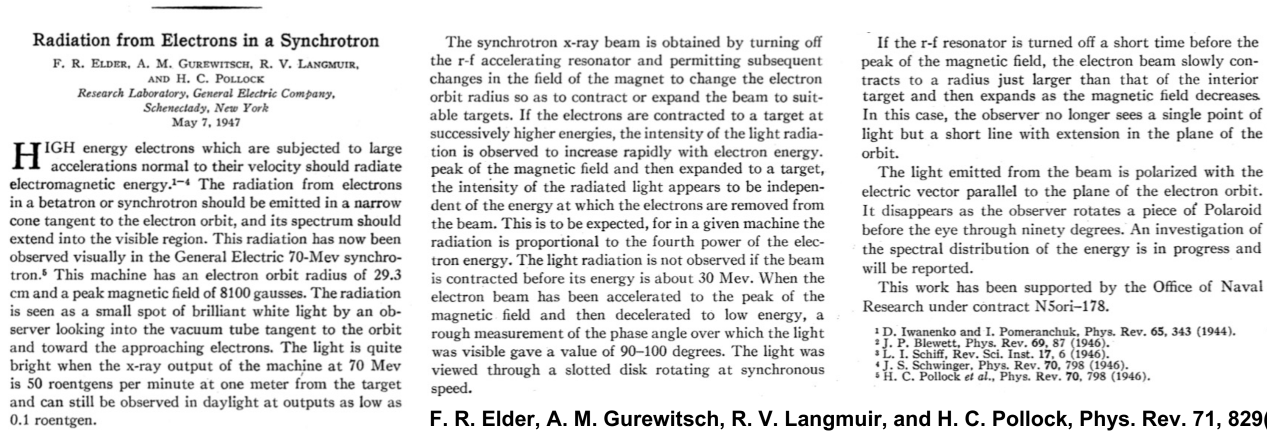
- 1944 - Blewett infers SR at GE 100 MeV Betatron
- **1947 - Pollack observes SR at GE 70 MeV Synchrotron**
- 1947 - Vitaly Ginzburg invents undulator
- 1949 - Schwinger simplifies undulator calculations
- 1952 - Motz, et al demonstrate IR undulator*
- 1956 - First use of SR for atomic spectroscopy at Cornell synchrotron
- 1961 - NBS synchrotron source available
- 1964 - Parasitic use of DESY, Hamburg
- 1968 - Tantalus-I storage ring, Univ. of Wisconsin
- 1971 - Parasitic use of NINA cyclic synchrotron
- 1971 - Parasitic use of ACO storage ring, Orsay
- 1971 - Parasitic use of CEA, Harvard



Radiation from Electrons in a Synchrotron

F. R. Elder, A. M. Gurewitsch, R. V. Langmuir, and H. C. Pollock
Research Laboratory, General Electric Company, Schenectady, New York
May 7, 1947

HIGH energy electrons which are subjected to large accelerations normal to their velocity should radiate electromagnetic energy.[1-4] The radiation from electrons in a betatron or synchrotron should be emitted in a narrow cone tangent to the electron orbit, and its spectrum should extend into the visible region. This radiation has now been observed visually in the General Electric 70-Mev synchrotron.[5] This machine has an electron orbit radius of 29.3 cm and a peak magnetic field of 8100 gausses. The radiation is seen as a small spot of brilliant white light by an observer looking into the vacuum tube tangent to the orbit and toward the approaching electrons. The light is quite bright when the x-ray output of the machine at 70 Mev is 50 roentgens per minute at one meter from the target and can still be observed in daylight at outputs as low as 0.1 roentgen.

The synchrotron x-ray beam is obtained by turning off the r-f accelerating resonator and permitting subsequent changes in the field of the magnet to change the electron orbit radius so as to contract or expand the beam to suitable targets. If the electrons are contracted to a target at successively higher energies, the intensity of the light radiation is observed to increase rapidly with electron energy. peak of the magnetic field and then expanded to a target, the intensity of the radiated light appears to be independent of the energy at which the electrons are removed from the beam. This is to be expected, for in a given machine the radiation is proportional to the fourth power of the electron energy. The light radiation is not observed if the beam is contracted before its energy is about 30 Mev. When the electron beam has been accelerated to the peak of the magnetic field and then decelerated to low energy, a rough measurement of the phase angle over which the light was visible gave a value of 90–100 degrees. The light was viewed through a slotted disk rotating at synchronous speed.

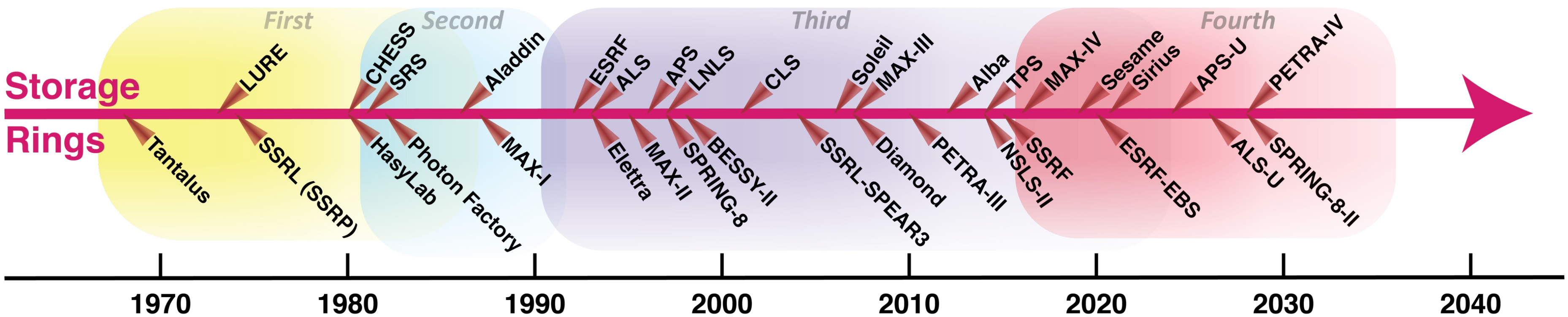
If the r-f resonator is turned off a short time before the peak of the magnetic field, the electron beam slowly contracts to a radius just larger than that of the interior target and then expands as the magnetic field decreases. In this case, the observer no longer sees a single point of light but a short line with extension in the plane of the orbit.

The light emitted from the beam is polarized with the electric vector parallel to the plane of the electron orbit. It disappears as the observer rotates a piece of Polaroid before the eye through ninety degrees. An investigation of the spectral distribution of the energy is in progress and will be reported.

This work has been supported by the Office of Naval Research under contract N5ori–178.

1 D. Iwanenko and I. Pomeranchuk, Phys. Rev. **65**, 343 (1944).
2 J. P. Blewett, Phys. Rev. **69**, 87 (1946).
3 L. I. Schiff, Rev. Sci. Inst. **17**, 6 (1946).
4 J. S. Schwinger, Phys. Rev. **70**, 798 (1946).
5 H. C. Pollock *et al.*, Phys. Rev. **70**, 798 (1946).

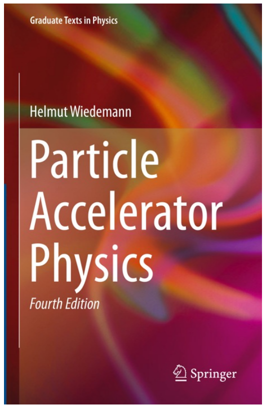
F. R. Elder, A. M. Gurewitsch, R. V. Langmuir, and H. C. Pollock, Phys. Rev. 71, 829(1947)



Most table data from Williams and Winick, Synchrotron Radiation News, **28**, 2(2015)

*H. Motz, W. Thon, and R. N. Whitehurst, J. Appl. Phys **24**, 826(1953)

Two Key Accelerator Concepts



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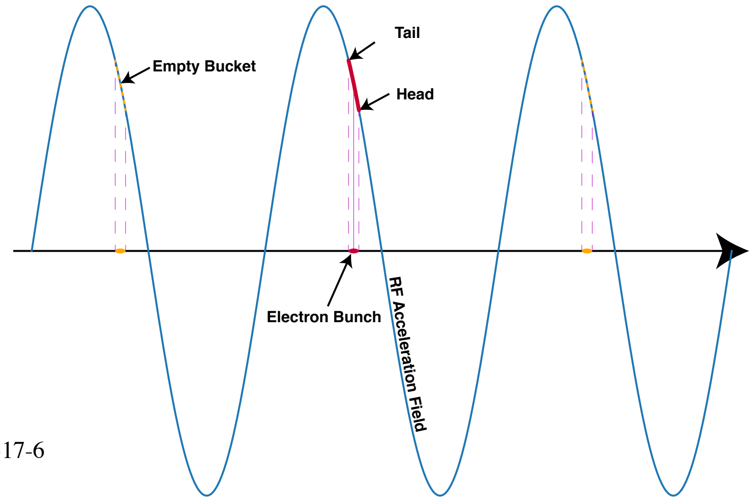
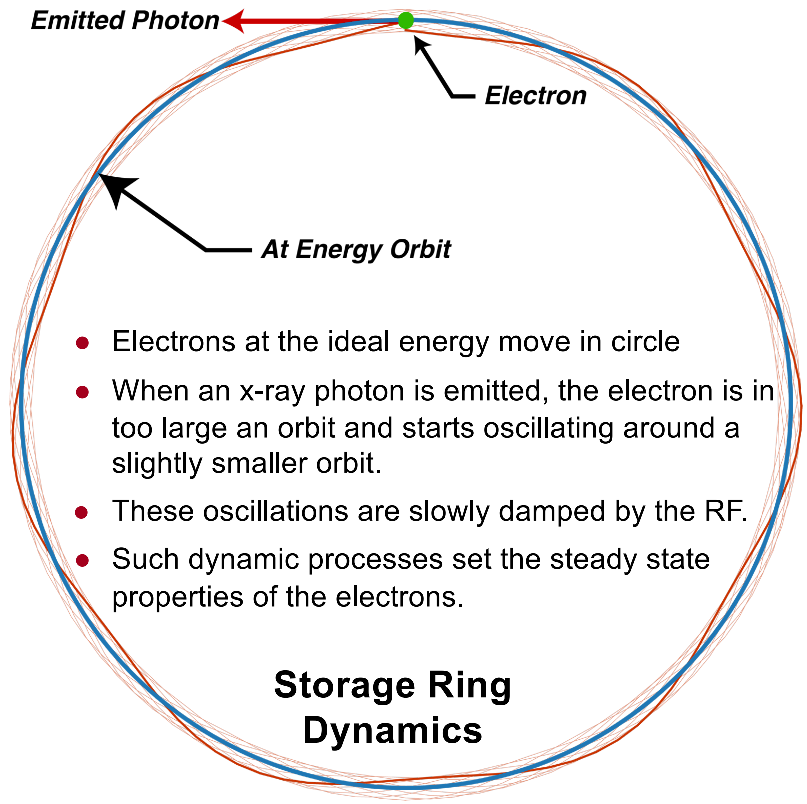


- The electrons can be thought of as surfing on the RF accelerating field.
- The tail of the pulse sees a bigger acceleration than the head.
- Each stable point on the RF field is referred to as a “RF Bucket”.



- Electrons at the ideal energy move in circle
- When an x-ray photon is emitted, the electron is in too large an orbit and starts oscillating around a slightly smaller orbit.
- These oscillations are slowly damped by the RF.
- Such dynamic processes set the steady state properties of the electrons.

Storage Ring Dynamics

Key Properties of Photon Beams

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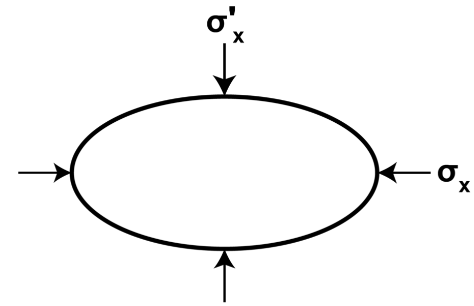
Flux	Typically expressed as the number of photons per second. But at FEL facilities it is usually expressed as by mJ/pulse.
Spectral Brightness	$B = \frac{N_{photons}}{4\pi^2 \Sigma_x \Sigma'_x \Sigma_y \Sigma'_y \frac{dE}{E}}$ Photons/(sec-mm^2-mrad^2-0.1%BW) is typically cited.
Peak Brightness	Critical for ultrafast measurements. FELs can generate pulses of attosecond duration with significant intensity.
Pulse Bandwidth	Critical for spectroscopy and, to a lesser extent, scattering. FEL's can create transform limited pulses. In that case, there is a strict relationship between pulse length and bandwidth. $\hbar = 0.658\ meV{-}ps$
Polarization	Storage rings and FELs typically have a horizontal polarization vector which generally requires scattering in the vertical plane. The LCLS-II hard x-ray undulator has a vertical polarization vector. Circular polarization is possible and important for magnetic measurements.
Number of Modes	The number of modes is important for coherent scattering measurements. Storage rings typically have large numbers, FEL's a few. The goal with lasers is often to have all the photons in a single mode.
Pulses per Second	Storage rings can produce well over a million pulses/second. Room temperature FELs typically are 60-120 pulses/second. Superconducting FELs can produce up to a million pulses/second.

Phase Space Ellipse

(One for each dimension)



$$\Sigma = \sqrt{\sigma^2_{electrons} + \sigma^2_{x-rays}}$$

$$\Sigma' = \sqrt{\sigma'^2_{electrons} + \sigma'^2_{x-rays}}$$

The Goal: Extend the Diffraction Limit to Hard X-Rays

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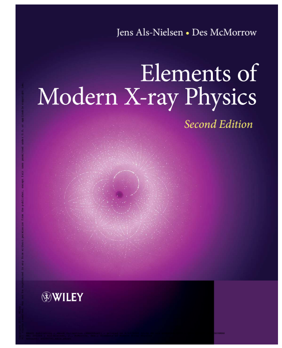
Why: At the diffraction limit, the x-rays are almost completely transversely coherent.
Coherent x-ray scattering techniques can yield unique structural information.

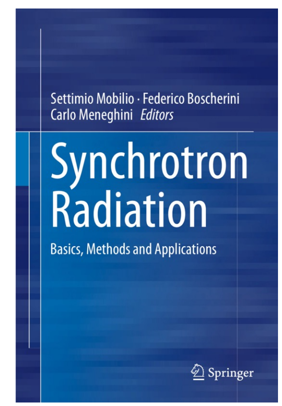


Look at the ESRF-EBS

- Horizontal emittance of 110 pm-rad yields a diffraction limited wavelength of ≈13.8Å.
- Vertical emittance of 5 pm-rad yields a diffraction limited wavelength of ≈0.6Å.

Even the best of the current generation of storage ring sources don't reach the full diffraction limit for typical hard x-ray experiments.

$$
\begin{aligned}
\epsilon &= 2\pi\sigma_x\sigma_x{}' \\
&= \frac{\lambda}{4\pi} \\
&= \frac{0.1\ nm}{4\pi} = 8\ pm\text{-}rad
\end{aligned}
$$



https://www.esrf.eu/home/UsersAndScience/Accelerators/ebs---extremely-brilliant-source/ebs-parameters.html

Scaling of Electron Emittance

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The emittance is an equilibrium property in a storage ring driven by quantum fluctuations (the emission of x-ray photons). For a storage ring, the emittance scales like:

$$\mathcal{E}_x \propto E^2 \theta^3$$

Where:

E = Electron Energy

θ = Angular deviation per period

This suggests three ways to reduce the emittance and raise brightness.

- Use many optical elements to make the angle θ small (expensive but can give order of magnitude improvement)
- Run the storage ring at low electron energy (possibly unstable and reduces undulator performance)
- Use extremely large ring such as PETRA-IV or build a machine in Fermilab's Tevatron tunnel (high capital cost)

Linear Accelerators Emerge

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Nuclear Instruments and Methods in Physics Research A264 (1988) 497–501 497
North-Holland, Amsterdam

HIGH ENERGY ELECTRON ACCELERATOR BASED SYNCHROTRON RADIATION SOURCES

P.H. FUOSS

AT&T Bell Laboratories, Crawfords Corner Road, Holmdel, NJ 07733, USA

Received 5 May 1986 and in revised form 28 July 1987

This paper discusses the possibility of using electron linear accelerators as picosecond synchrotron radiation sources. Calculations presented show that the Stanford Linear Collider could exceed the spectral brilliance of existing storage rings (although at a much lower total flux) while producing 3 ps long pulses at a repetition rate of 180 pulses per second. Higher performance sources might be feasible but would require major modifications of existing linear accelerators or the development of new facilities.

Status in 1987	Emittance	Electrons per pulse	Pulse Length	Electrons per picosecond
Advanced Light Source	17 nm-rad	5×10^{9}	20 ps	2.5×10^{8}
ESRF	11 nm-rad	7×10^{9}	27 ps	2.6×10^{8}
SLAC Linear Collider	0.3 nm-rad	5×10^{10}	3 ps	1.7×10^{10}

This paper suggested a spontaneous source – like a storage ring – but without the reuse of the electrons.

A similar concept (with bunch compressors for much shorter pulses) was implemented at the SPPS facility at SLAC in the early 2000s.

The FemtoMax facility at MAX-IV is implementing a spontaneous source.*

But there is a much better use of a high performance accelerator
The Free Electron Laser

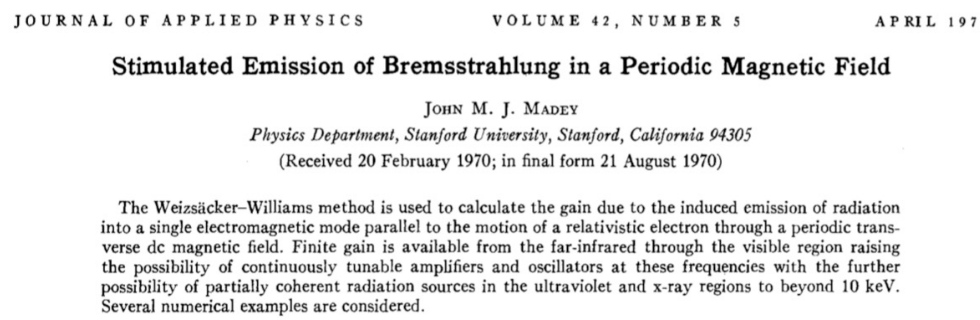
*https://www.maxiv.lu.se/accelerators-beamlines/beamlines/femtomax/

A Brief History: Invention of the Free Electron Laser

John Madey at Stanford University first proposed a free-electron laser (FEL) 50 years ago in the Journal of Applied Physics

Early FEL development focused on producing infrared and visible light.

Advances in theory and accelerator technology led to proposals in the early 90’s for x-ray FEL’s.



JOURNAL OF APPLIED PHYSICS VOLUME 42, NUMBER 5 APRIL 1971

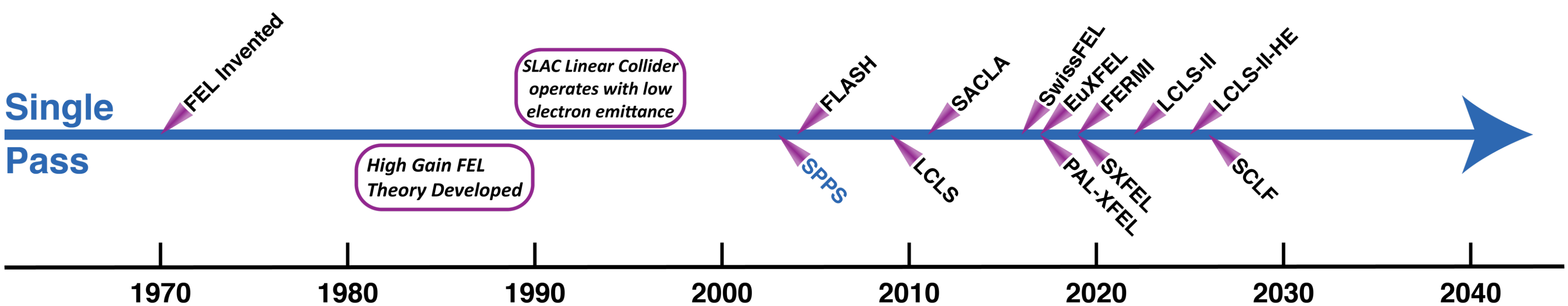
Stimulated Emission of Bremsstrahlung in a Periodic Magnetic Field

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.



A Brief History: Invention of the Free Electron Laser

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Volume 50, number 6 OPTICS COMMUNICATIONS 15 July 1984

COLLECTIVE INSTABILITIES AND HIGH-GAIN REGIME IN A FREE ELECTRON LASER

R. BONIFACIO *, C. PELLEGRINI
National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY 11973, USA

and

L.M. NARDUCCI
Physics Department, Drexel University, Philadelphia, PA 19104, USA

Received 5 April 1984

We study the behavior of a free electron laser in the high gain regime, and the conditions for the emergence of a collective instability in the electron beam-undulator-field system. Our equations, in the appropriate limit, yield the traditional small gain formula. In the nonlinear regime, numerical solutions of the coupled equations of motion support the correctness of our proposed empirical estimator for the build-up time of the pulses, and indicate the existence of optimum parameters for the production of high peak-power radiation.

Eur. Phys. J. H
DOI: 10.1140/epjh/e2012-20064-5

THE EUROPEAN PHYSICAL JOURNAL H

The history of X-ray free-electron lasers

C. Pellegrini[1,2,a]

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[2] SLAC National Accelerator Laboratory, Menlo Park, 94025 California, USA

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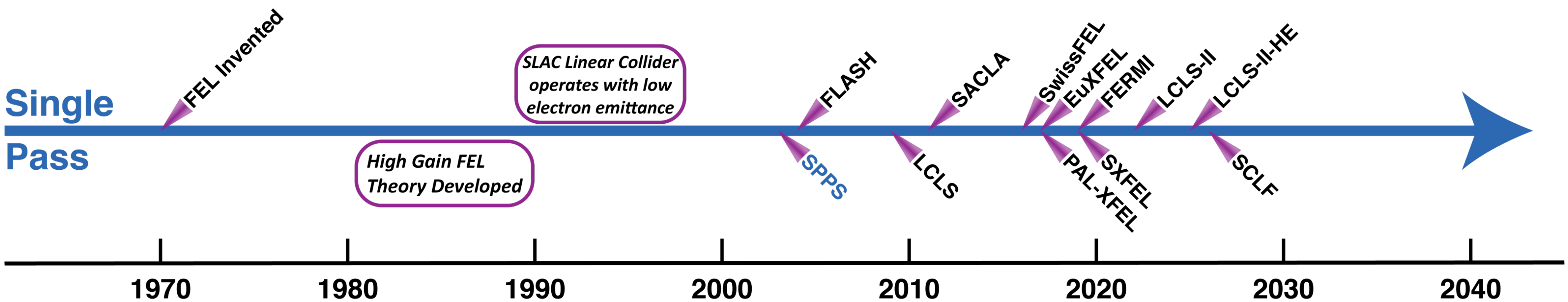

Electron Paths in an Undulator

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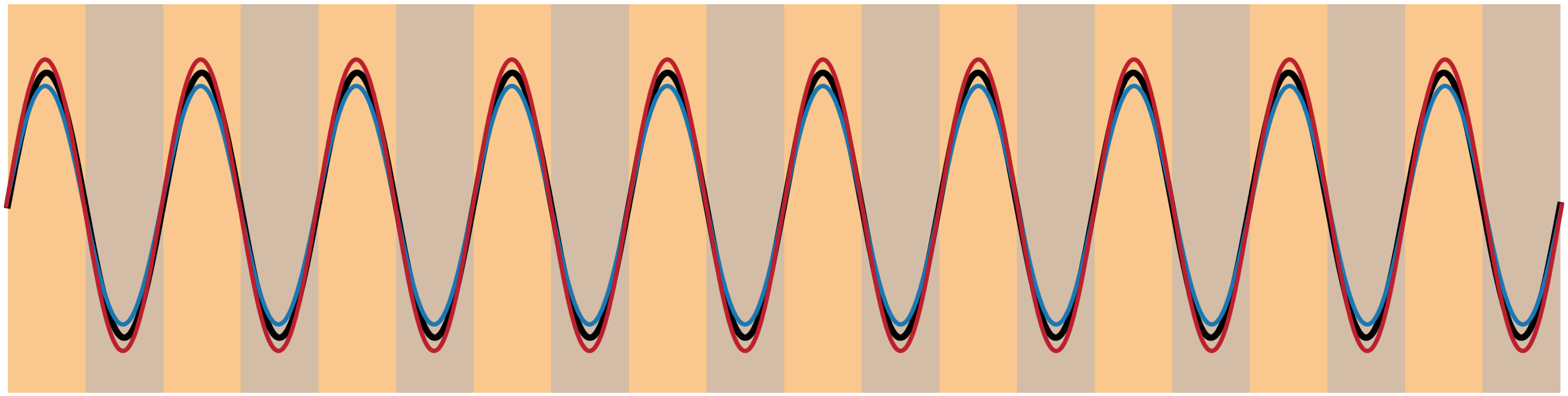


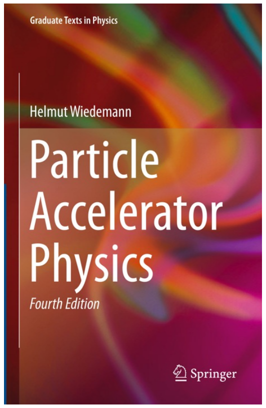
Ideally, electrons take a sinusoidal path through an undulator

Electrons with a slightly lower energy will take a longer path

Electrons with a slightly higher energy will take a shorter path

If there is an energy chirp placed on the electron pulse, the beam can be bunched.

A Non-Rigorous View of the FEL



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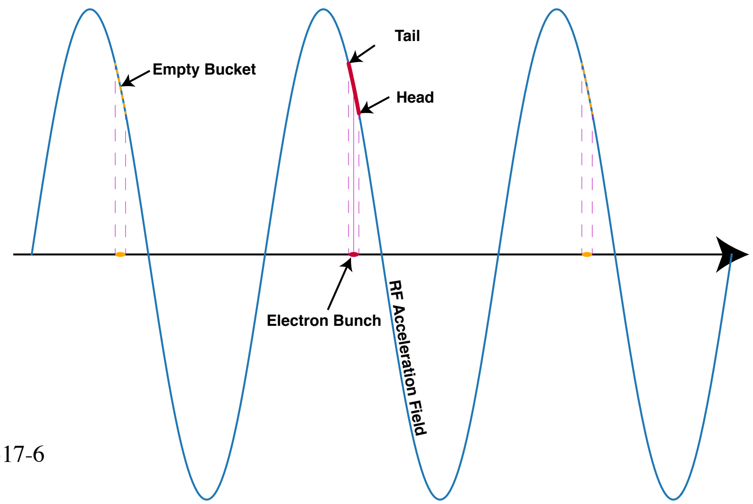
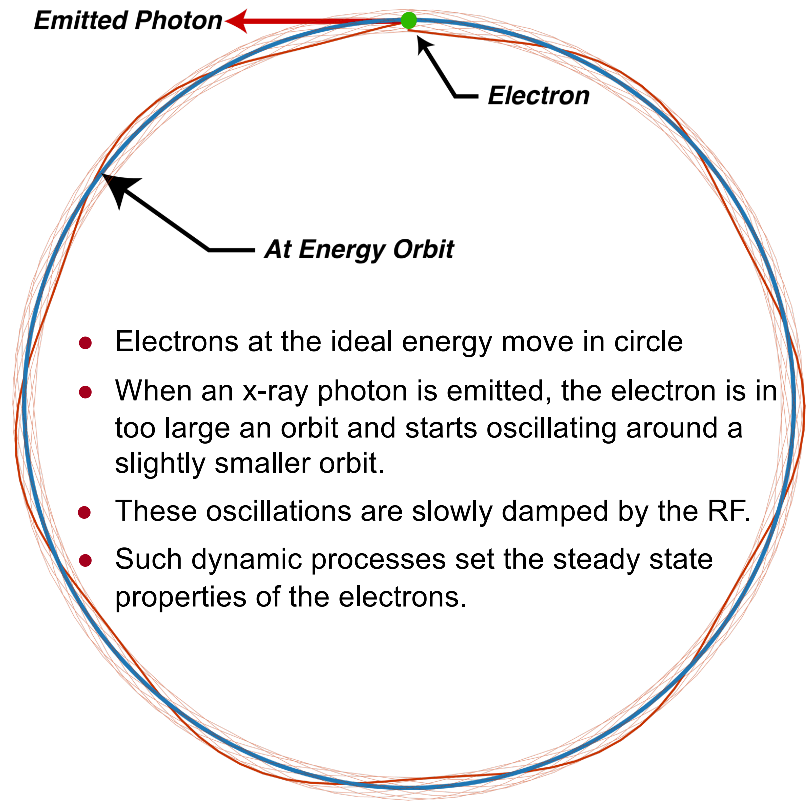


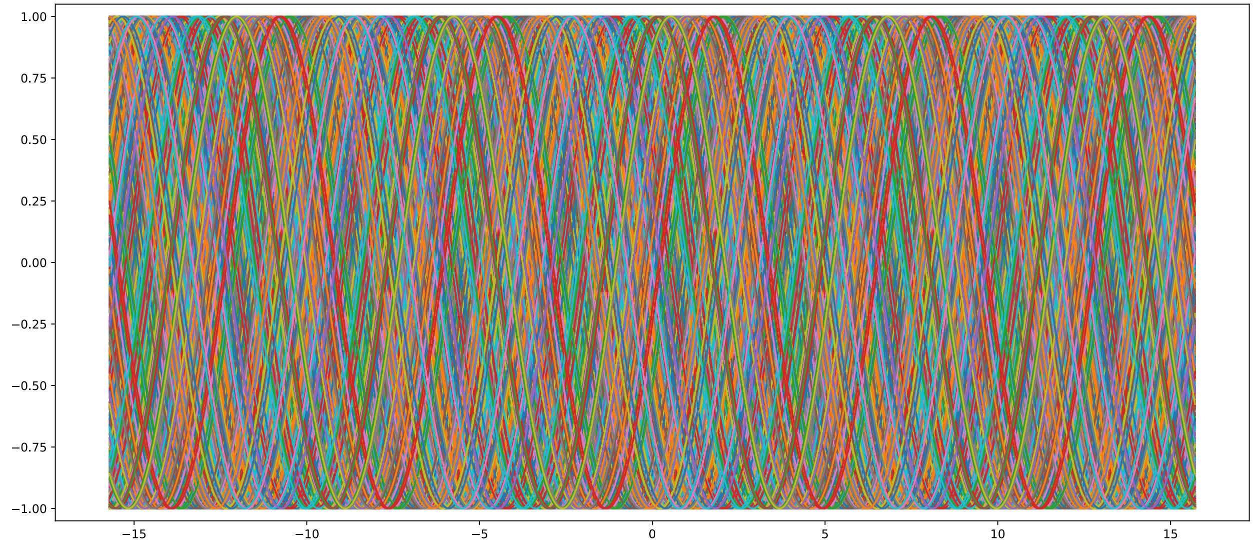
- The electrons can be thought of as surfing on the RF accelerating field.
- The tail of the pulse sees a bigger acceleration than the head.
- Each stable point on the RF field is referred to as a "RF Bucket".



- Electrons at the ideal energy move in circle
- When an x-ray photon is emitted, the electron is in too large an orbit and starts oscillating around a slightly smaller orbit.
- These oscillations are slowly damped by the RF.
- Such dynamic processes set the steady state properties of the electrons.

The X-Rays Make the Field

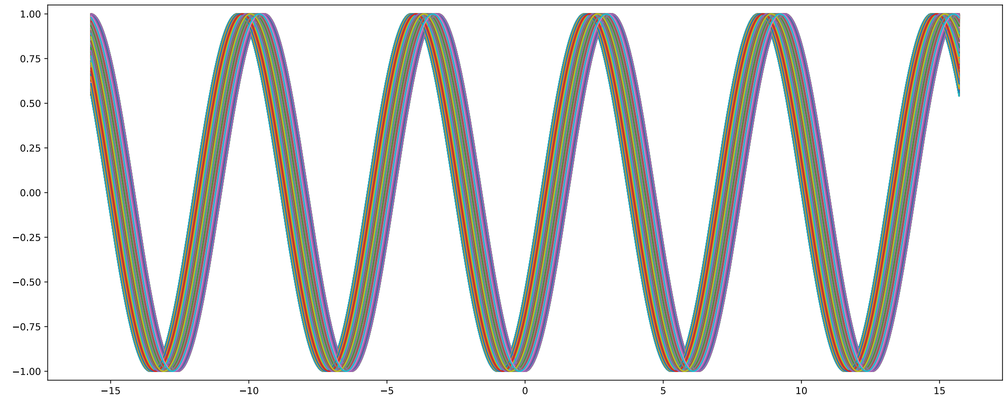
NO THEY CAN'T – They radiate with random phase

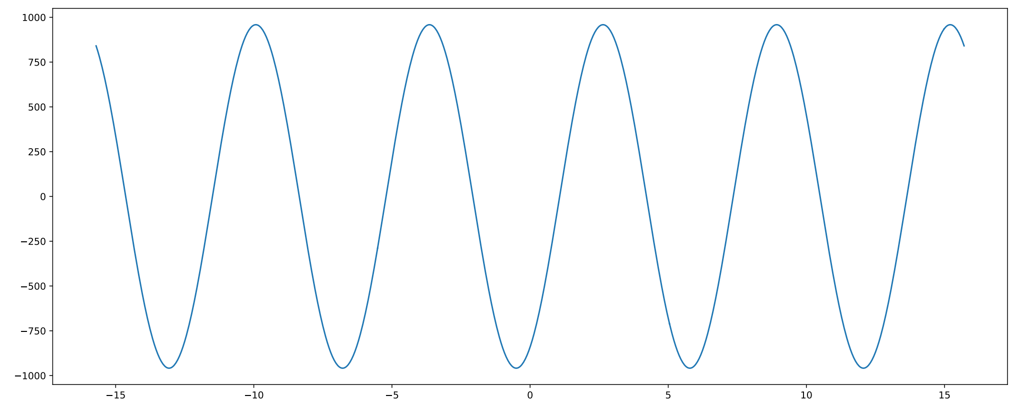


The X-Rays Make the Field

YES THEY CAN

- **Fluctuations or imperfections will cause brief, localized coherence.**
- **That coherence can start to bunch the electrons.**
- **The bunching improves the coherence is a self-reinforcing process.**





A Non-Rigorous View of the FEL

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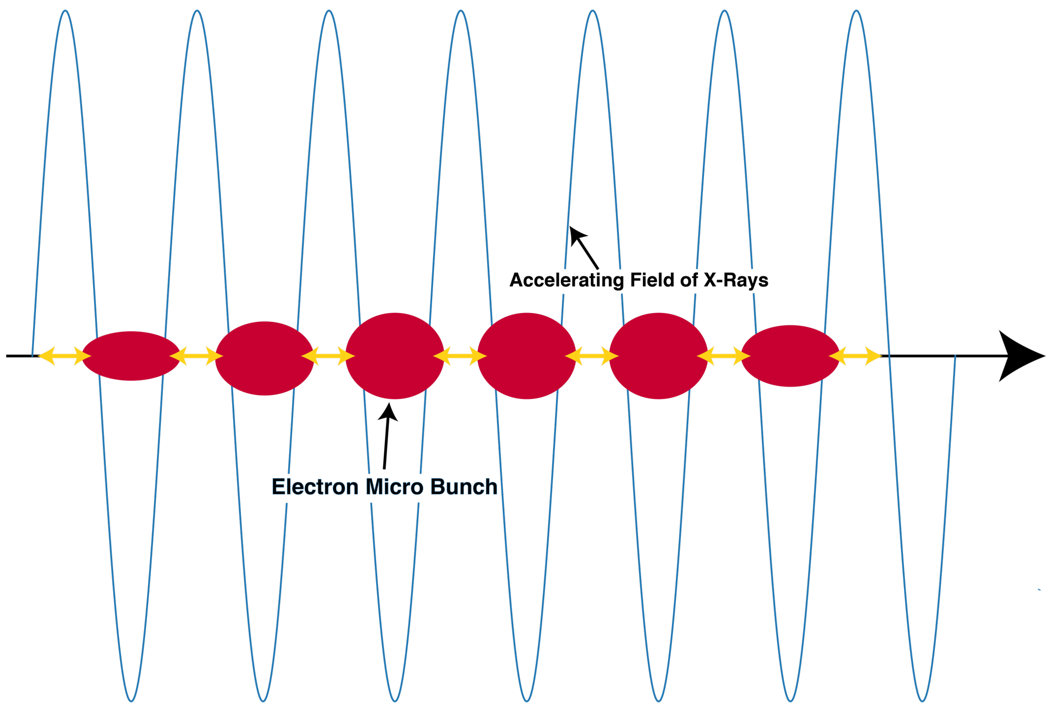
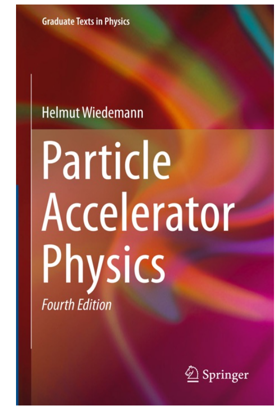
Self-Amplified Spontaneous Emission → SASE

- The x-rays create a weak accelerating field but with much shorter period than RF.
- The x-ray field pushes electrons into non-uniform bunch in the undulator.
- This non-uniform bunch creates a larger field because the electrons start radiation more coherently. This drives the process faster.
- The bunches become more well defined and the radiation goes like N_{bunch}^2





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Challenge: SASE is a weak process

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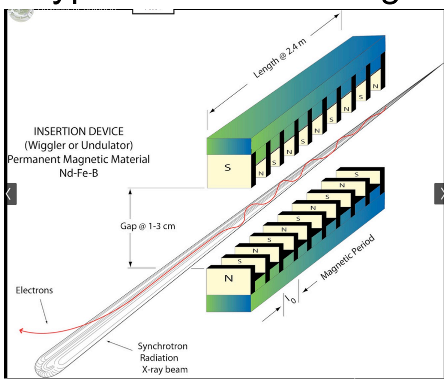
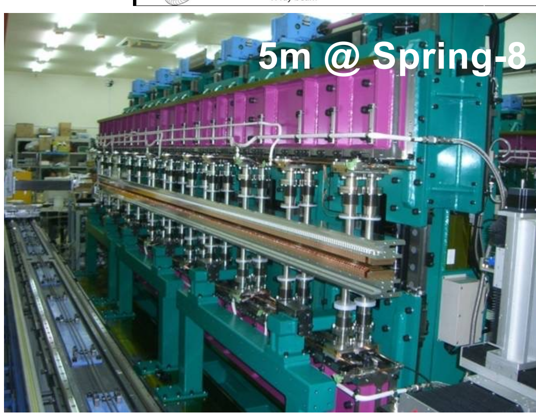
Synchrotrons

Typ. 1 to 5 meter long

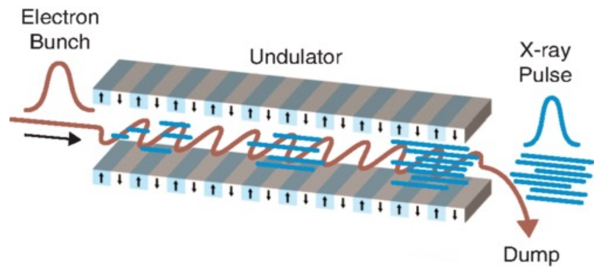


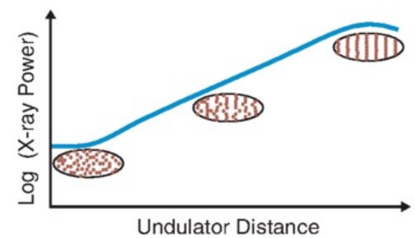


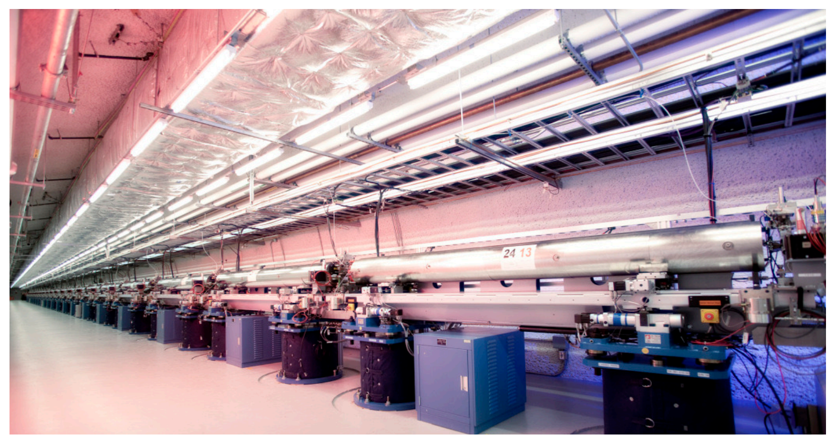
Free Electron Lasers

VERY long : typ. >100 meters

Small e-beam emittance







(Some) Technical Challenges for an FEL

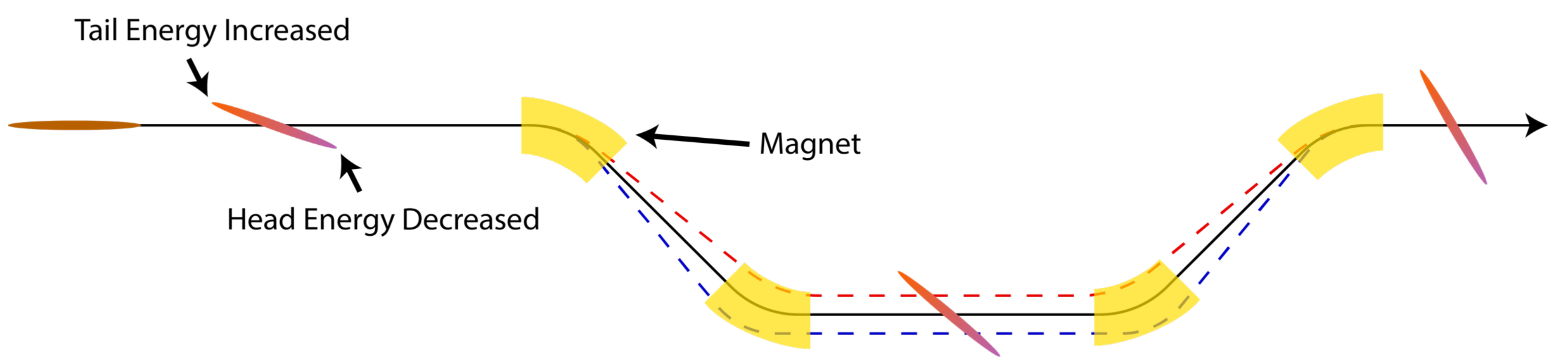
- A very high electron density is required to drive the SASE process.
  - This requires an electron gun with a very low electron emittance.
  - Periodic bunch compression is required to produce the extremely short electron pulses are needed.
- High electron density pulses have many instabilities that need to be controlled. Laser heaters can be used to destroy correlations.
- In the undulator, the photons go straight. The magnetic properties of the undulator have to be almost perfect to keep the photon and electron beams overlapped.
- Optics have to be able to handle high instantaneous photon power.
- The divergence of the photon beam is roughly a μrad. Precise control of the electron beam is required to keep the beam on the sample.
- The femtosecond long pulse is triggered two miles from the experiment. Precise timing synchronization is challenging.

Linacs are very flexible

A variety of optical elements can be put into the linac to aid in optimizing the electron parameters for individual experiments.

For example, a bunch compressor, show below, is critical for producing the high electron densities required for efficient SASE operation.

The flexibility of the linac is often a complication because setup time for different operating modes can be quite time consuming. Thus, facilities like LCLS have gravitated towards “standard configurations” to enhance operational efficiency and user productivity.



What Type Linear Accelerator?

While the conceptual physics is the same for all accelerators, the choice of cavities can have a big impact on the approach to experiments.

Warm Cu: Relatively low duty factor because heating of the RF cavity and power consumption. LCLS is a typical example.

Typically the cavities are filled with RF for a μsec about 60-120 times a second.

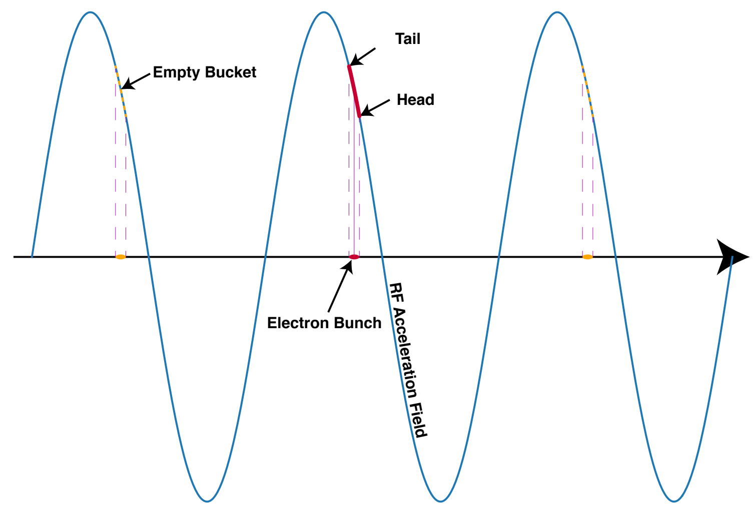
Also, multiple buckets can be filled within the μsec RF pulse.

Low Duty Superconducting: Many electron pulses within one train followed by a long recovery time between macro pulses. EuXFEL and FLASH are examples of this structure.

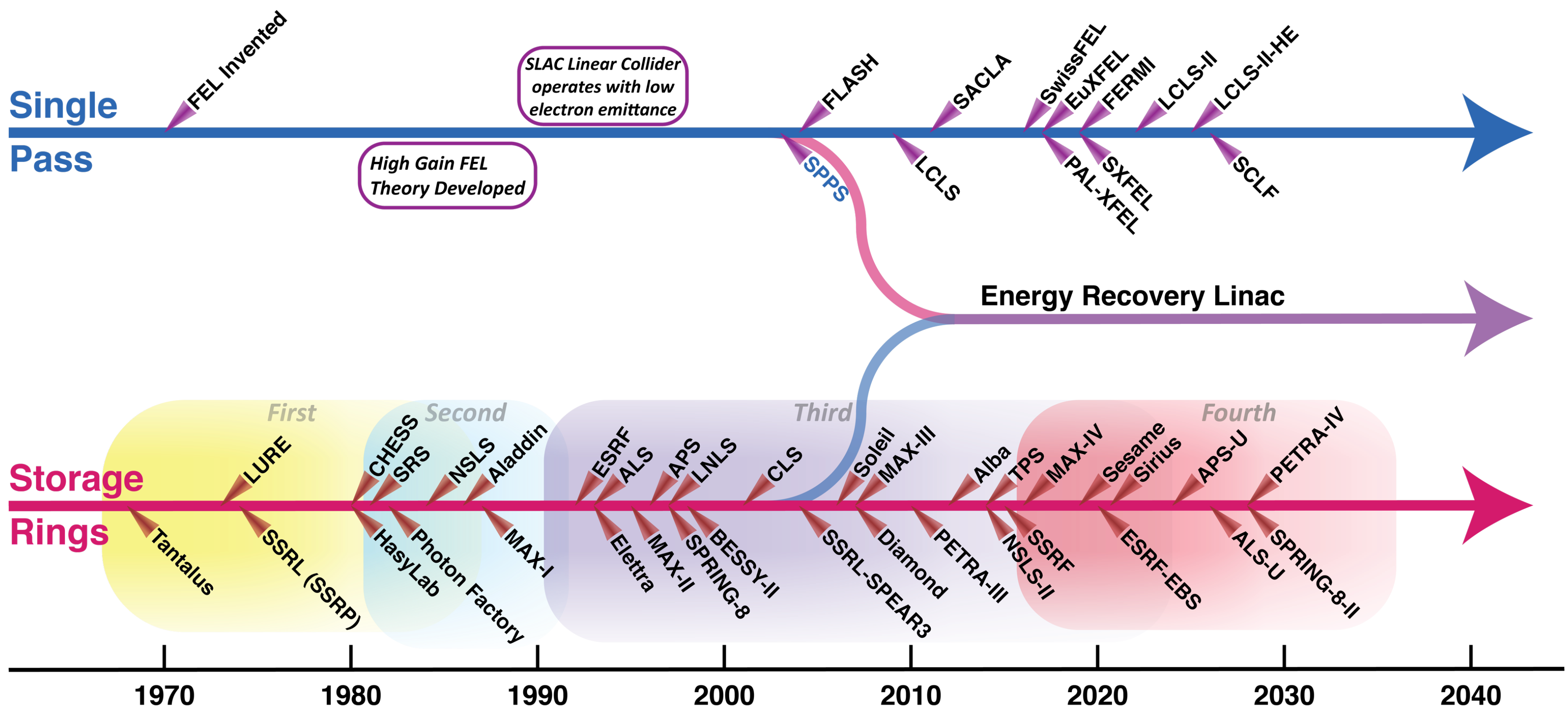
Pulses within a macro pulse can be directed to different instruments.

DC Superconducting: LCLS-II will have a continuous pulse train with the pulses separated by ≈1 μsec.

Individual pulses can be directed to different instruments.



Evolution of Hard X-Ray Sources



LCLS – Linac Coherent Light Source

At the beginning of 2019, almost 10 years after 1st light, LCLS shutdown to start a major upgrade, the LCLS-II project.

The first stage of that upgrade, the installation of new undulators, has been completed.

This talk will focus on where we're going, not where we've been.

However, there are great review articles summarizing the scientific and technical accomplishments of the last two decades. Here are two that appeared in the Reviews of Modern Physics after five years of LCLS operation.

REVIEWS OF MODERN PHYSICS, VOLUME 88, JANUARY–MARCH 2016

Linac Coherent Light Source: The first five years

Christoph Bostedt,[*] Sébastien Boutet, David M. Fritz, Zhirong Huang, Hae Ja Lee, Henrik T. Lemke,[†] Aymeric Robert, William F. Schlotter, Joshua J. Turner, and Garth J. Williams[‡]

SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA

(published 9 March 2016)

The physics of x-ray free-electron lasers

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(published 9 March 2016)

LCLS – Linac Coherent Light Source

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At the beginning of 2019, almost 10 years after 1st light, LCLS shutdown to start a major upgrade, the LCLS-II project.

The first stage of that upgrade, the installation of new undulators, has been completed.

I'll now focus on where we're going, not where we've been.

However, there are great review articles summarizing the scientific and technical accomplishments of the last two decades.

Phase 1: 2020

- **2 LCLS-II variable gap undulators**
- 0.25 to 25 keV (fundamental) at 120 Hz
- XLEAP pulse(s) at 200-400 attoseconds
- 4 pulses at 0.35 ns to >500 ns separation

Phase 2: 2022

- **LCLS-II 4 GeV CW SCRF accelerator**
- 0.25 to 5 keV at 1 MHz (CW, programmable)
- 5 new endstations

Phase 3: 2026/7

- **LCLS-II-HE 8 GeV CW SCRF accelerator**
- 0.25 to >15 keV at 1 MHz
- 5 new or upgraded endstations
- Reconfiguration to increase experimental capacity

Phase 4: 2026/7

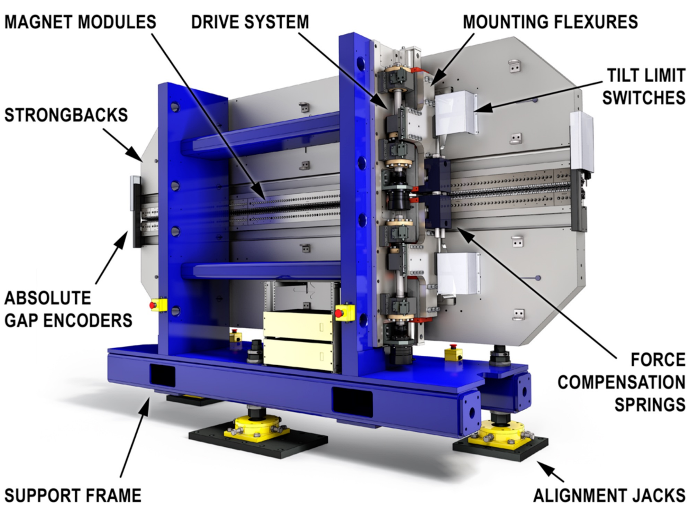
- **MEC Upgrade**
- 1 PW at 10 Hz, plus 1 kJ
- Dedicated experimental cavern

LCLS-II Undulators

Soft X-Ray Undulator

Horizontal Polarization

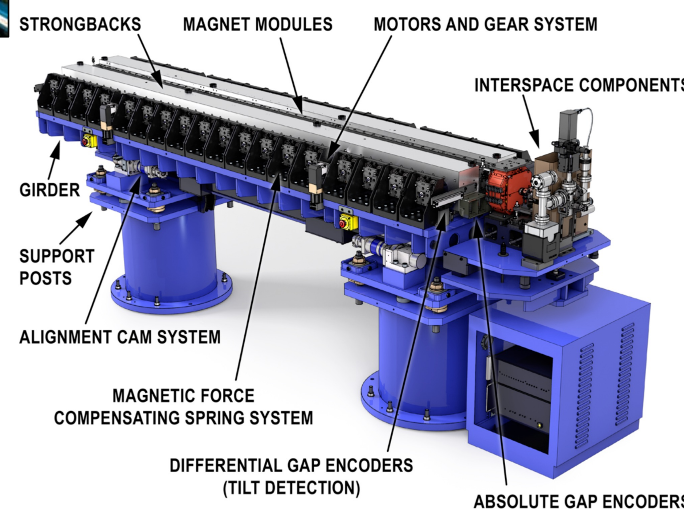
Undulator Period (mm):	39
Number of Modules:	21
Total Length (meters):	**71**



Hard X-Ray Undulator

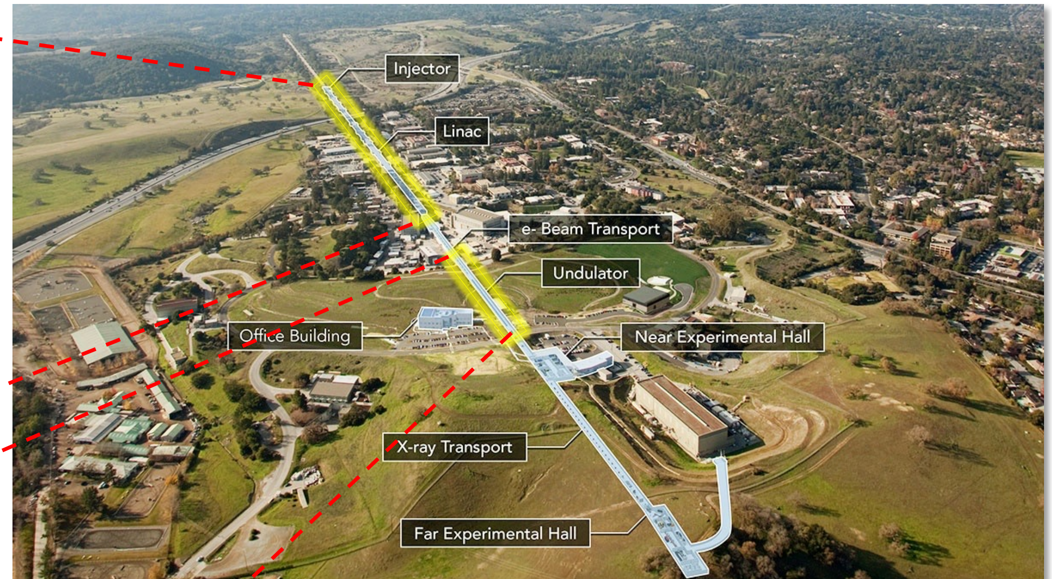
Vertical Polarization

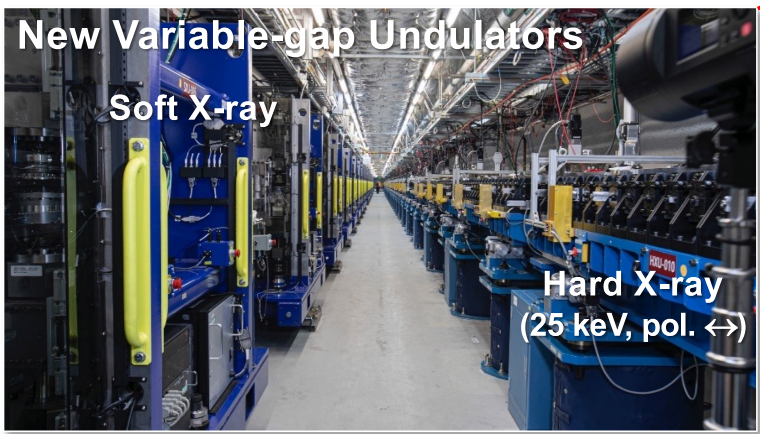
Undulator Period (mm):	26
Number of Modules:	32
Total Length (meters):	**109**

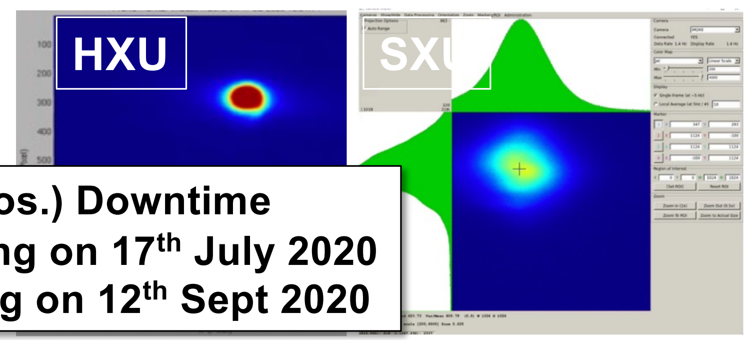


LCLS Today

SLAC



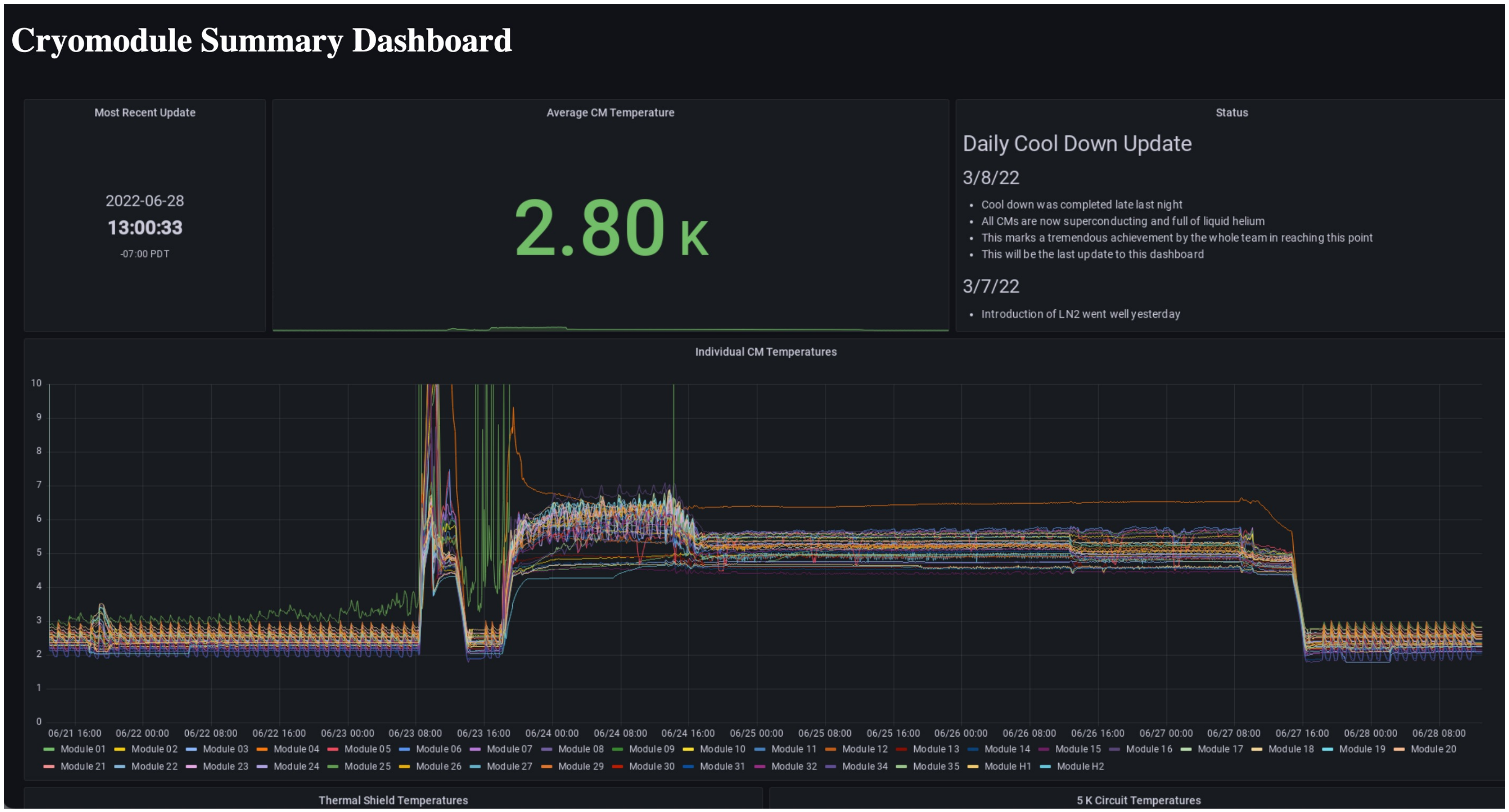




2019-2020 (18 mos.) Downtime

- **Hard X-ray lasing on 17th July 2020**
- **Soft X-ray lasing on 12th Sept 2020**

The Superconducting Accelerator is Cold!



https://pswww.slac.stanford.edu/swdoc/ecs_dashboards/cryomodule.html

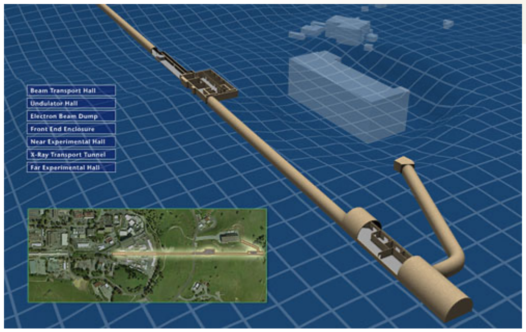
Synchrotron Sources



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

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

Free Electron Lasers



Measuring Ultra-Fast phenomena (< 100ps)

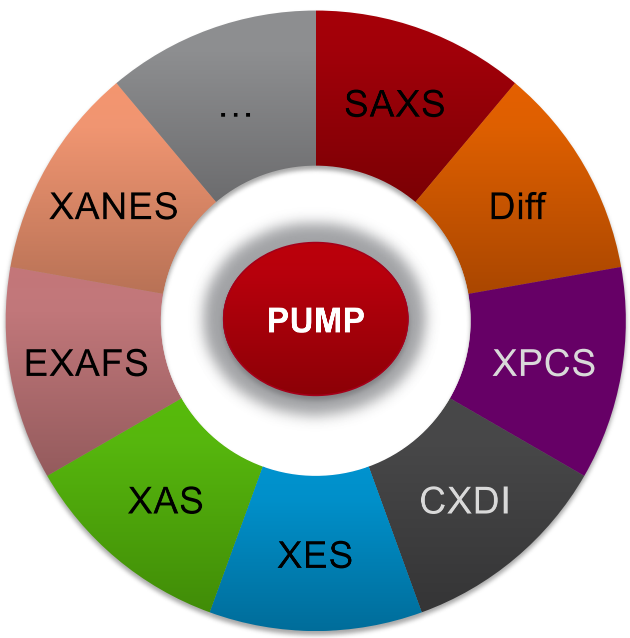
Parameter	Storage Ring	FEL
Time Structure	Continuous	**Pulsed**
Intensity	Stable	**Fluctuations**
Position/ pointing	Stable	**Fluctuations**
Energy spectrum	Stable	**Fluctuations**
Timing	Stable	**Fluctuations**
Coherence	Partial	**Full**

JITTER

Free Electron Lasers : using X-rays for Science

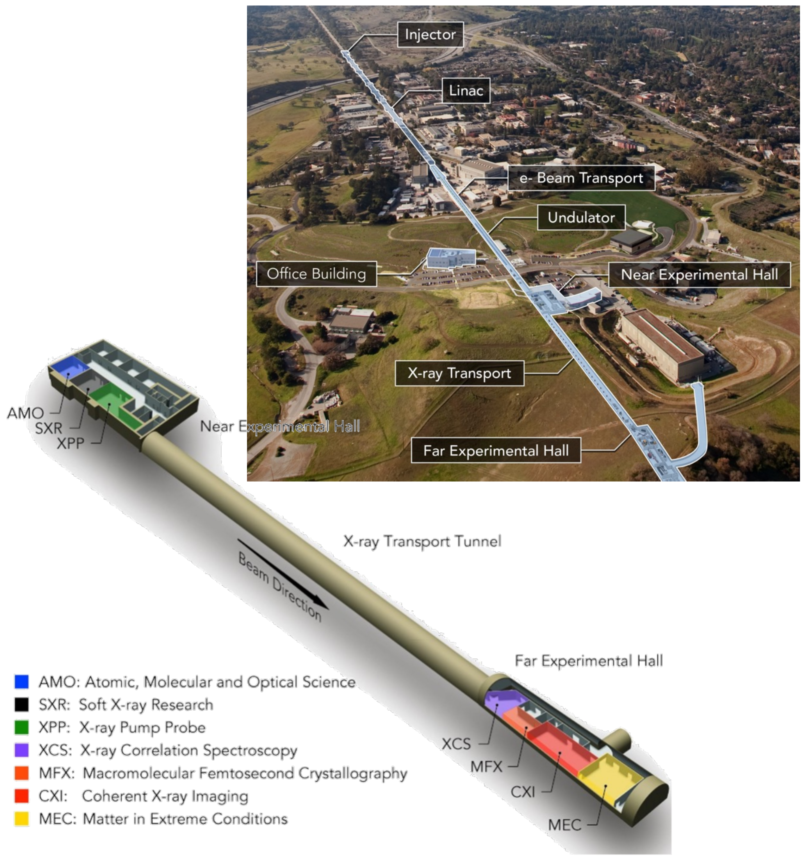
"Linac Coherent Light Source: the first five years", *Rev. Mod. Phys.* **88**, 015007 (2016)

Materials Science	Chemistry	Atomic & Molecular Dynamics	High Energy Density	Life Sciences



- **Relying on the long experience of synchrotron Storage Ring sources**
- Experiments use at least one of the FEL beam properties
- **Ideal for ultrafast dynamics, radiation sensitive samples, pump-probe (optical, THz, Field, etc.)**
- Some experiments use more than one technique simultaneously or sequentially

LCLS: Parameters Overview



White, Robert, Dunne, J. Synch. Rad. **22** (3), pp 472-476 (2015)

http://LCLS.slac.Stanford.edu

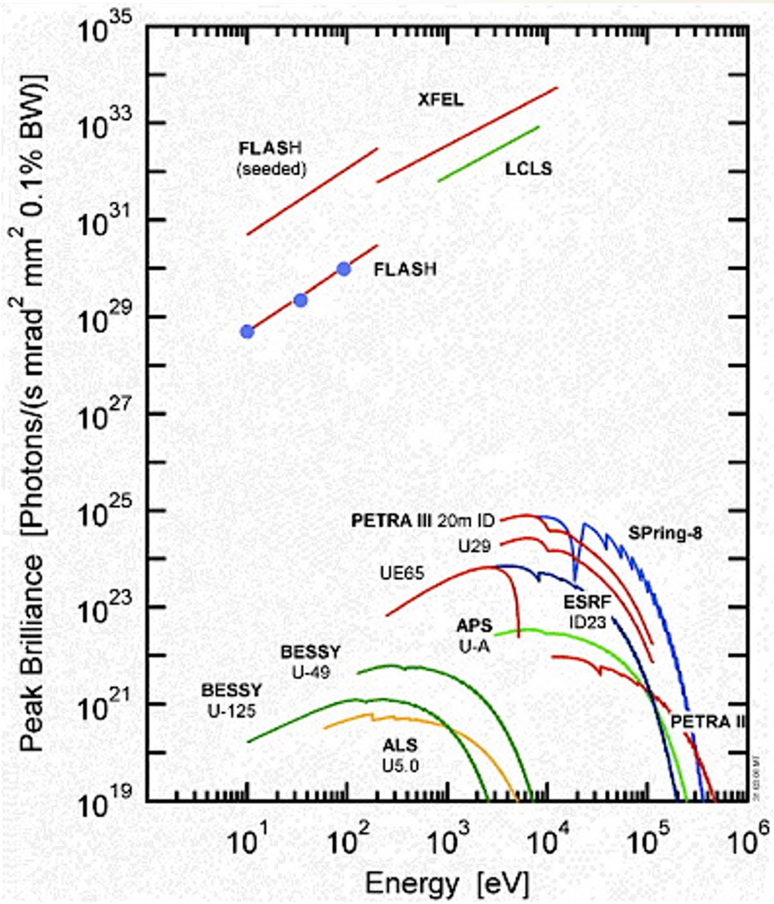
	LCLS PARAMETERS		Unit
Linac	e-beam energy	2.5-16.9	GeV
	Length	~1	km
	Slice emittance	0.5-1.2	μm
Undulator	Active Length	~112	m
	Period	30	mm
	K	3.5	--
	Peak Field	1.25	T
	Typical SASE Parameters		
X-ray Beam	Photon Energy (1st harm.)	0.28-12.8	keV
	Number Photons	$\sim 10^{12}$	ph/pulse
	Rep. Rate	Up to 120	Hz
	Pulse Duration	~1-200	fs
	Size (unfocused)	200-500	μm
	Divergence	1-2	μrad
	Trans. Coherence	Full	--
	Polarization	Horiz.	--
	Bandwidth $\Delta\lambda/\lambda$	0.1	%

SR vs FEL : Important Parameters

What are the important parameters ?

① Flux
② Collimated beam
③ Beam position
④ Intensity
⑤ Pulse durations
⑥ Temporal fluctuations
⑦ Energy spectrum
⑧ Coherence

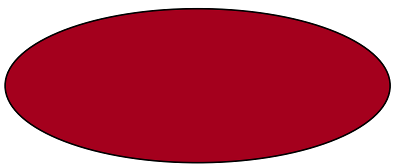
(1) FLUX



- FEL sources provide unprecedented peak brilliance
- This originates from the pulsed nature of these sources.
- One typically gets per shot what one gets per second on a SR

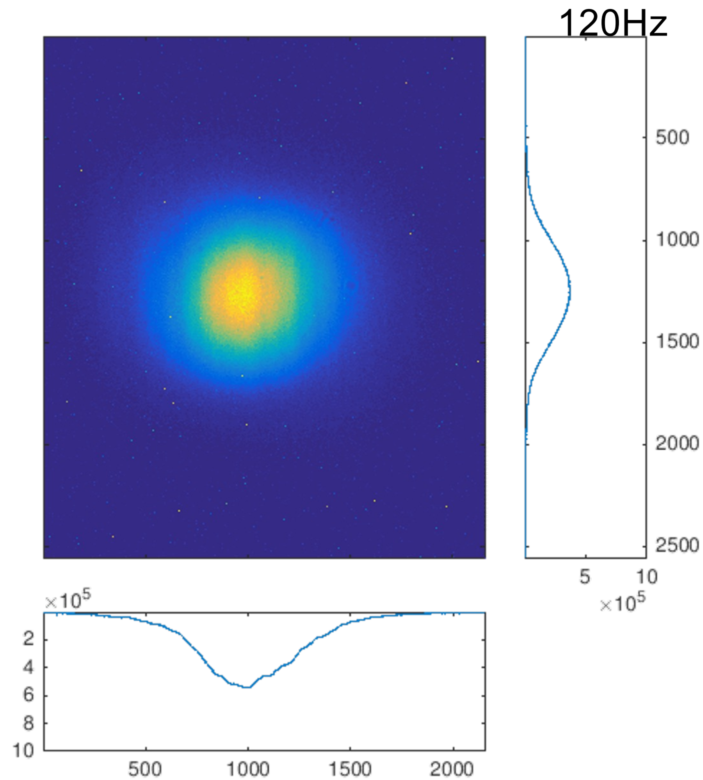
(3) POSITION

Storage Ring



Rock Stable !

Free Electron Laser



XPP Instrument

Beam fluctuates in position (>10% of its size)

(4) INTENSITY

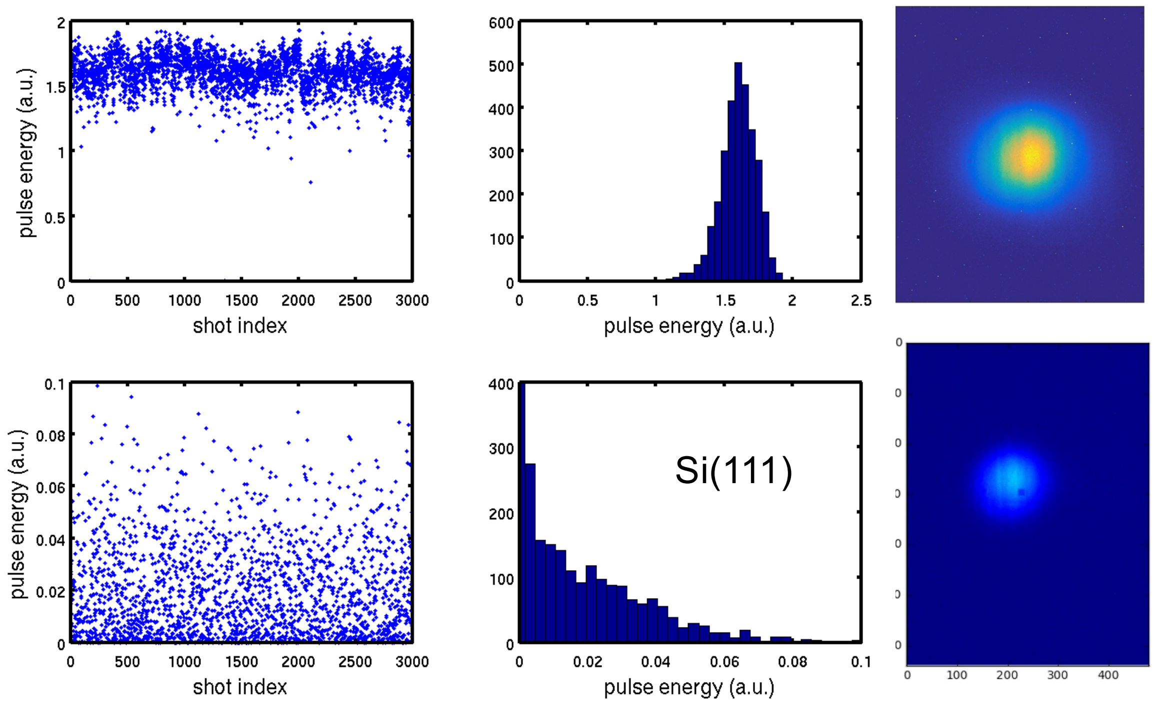
SLAC

Storage Ring

Rock Stable !

With
Or
Without
Top-up

Free Electron Laser



Pink Beam

Drastic difference between and

Mono Beam

Courtesy of XPP

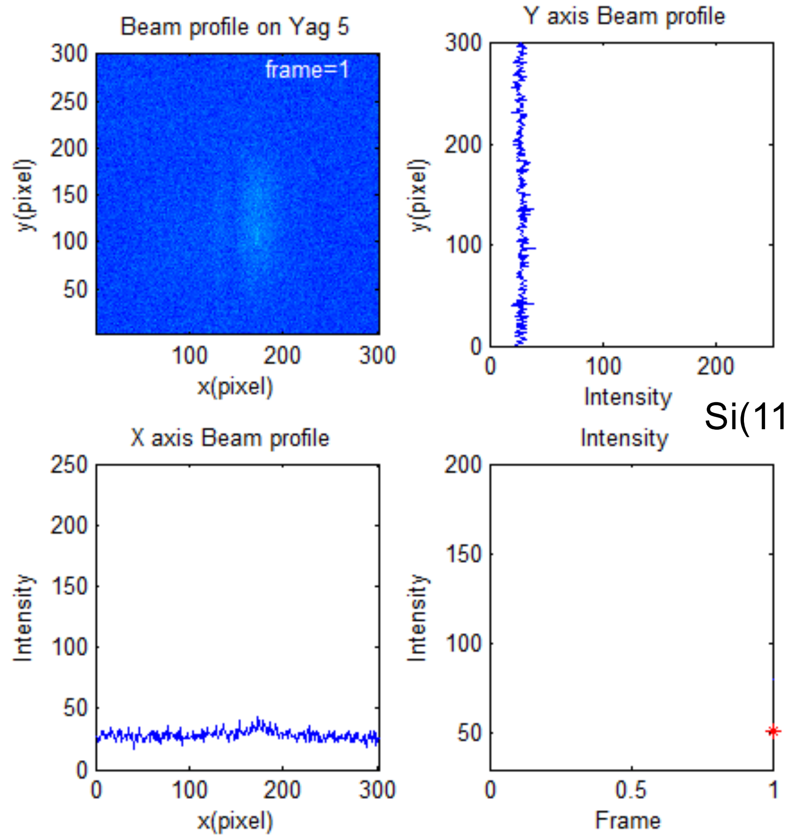
(4) INTENSITY

FEL

Storage Ring

Rock Stable !

With
Or
Without
Top-up



Si(111)

Intensity fluctuations come intrinsically from the SASE process.

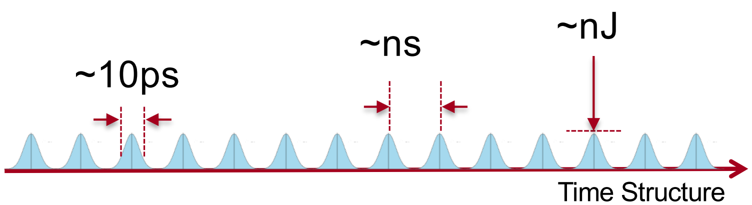
In addition, machine instabilities and special behavior when using a monochromator.

(5) PULSE DURATION & (6) TIMING

Storage Ring

Pulse duration : typ. 50-100ps

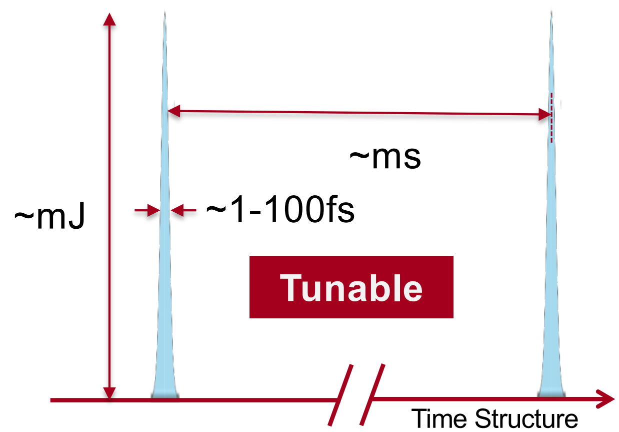
High repetition rate (100sMHz)

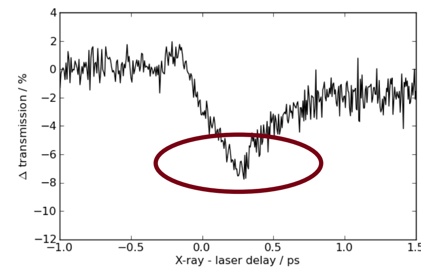


FEL : LCLS

Pulse duration : typ. < 100fs

Repetition rate ~50-100Hz





Step position indicates arrival time

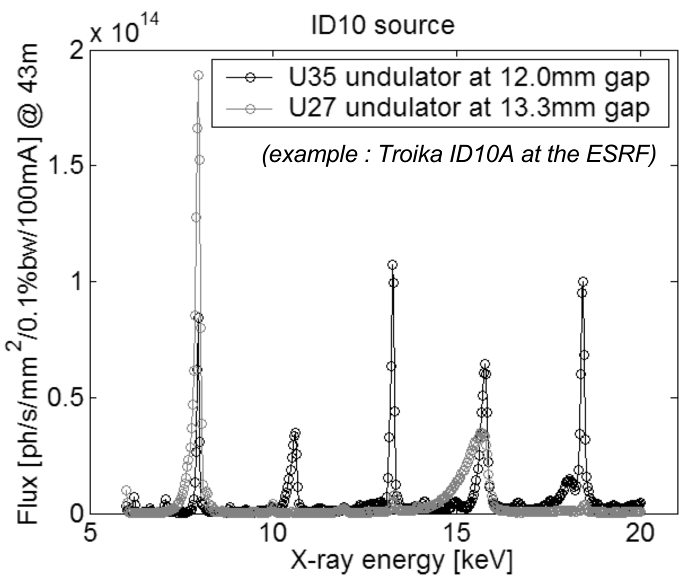
(7) E-spectrum

Storage Ring

Access to high Energies with 3rd harmonic

Stable and well define energy spectrum

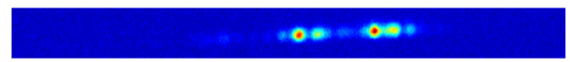
1st harmonic width : 1-4%



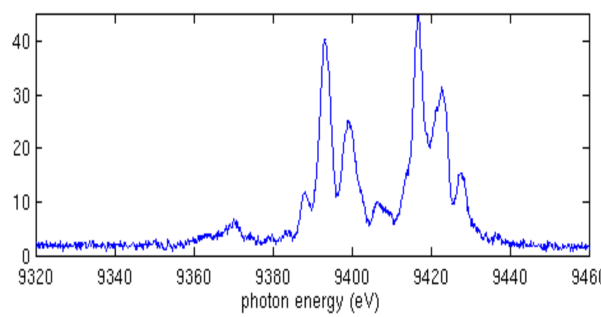
Free Electron Laser

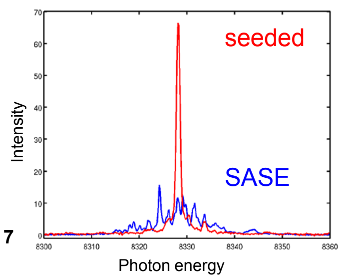
Access to high Energies with 3rd harmonic

1st harmonic width : 0.1-0.2% (<dE/E>=0.7%)



Fluctuating spectrum from e-beam jitter and structure





“seeding” will fix this

(8) Degree of Coherence

Storage Ring

Limited Coherence

Slit down the beam to typ. 20x20 micron beams to extract the coherent fraction of the beam.

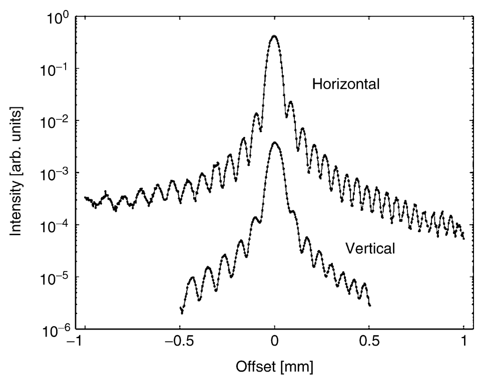
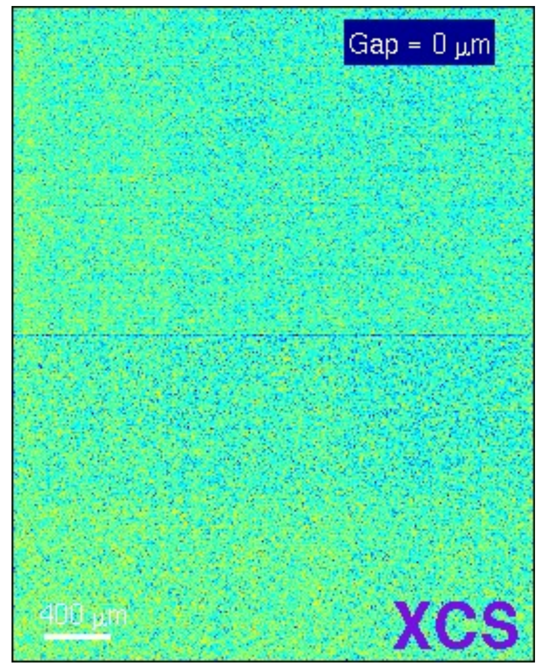


Figure 18-2
Airy fringes from a 5 × 5 μm² slit, recorded with λ = 1.54 Å radiation at 1.5 m from the slit. The visibility V of the fringes can be quantified by $V = (I_{max} - I_{min})/(I_{max} + I_{min})$, where I_{max} is a fringe maximum and I_{min} is an adjacent minimum

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

Free Electron Laser

The beam is fully transversely coherent



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

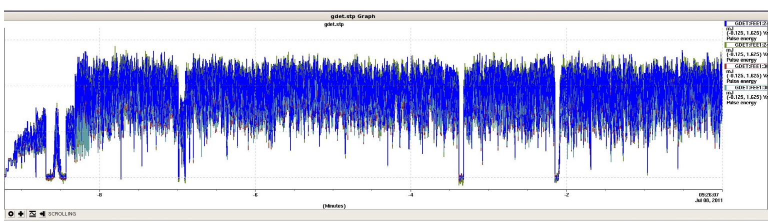
Day to day operation

Something very different from storage ring sources, we have :

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

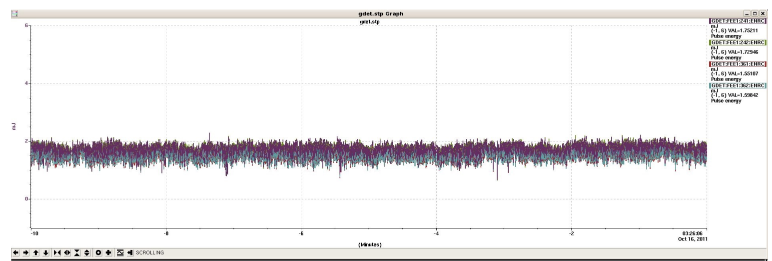
" BAD" days

- Less than 1mJ per pulse
- Very large intensity fluctuations



"GOOD" days

- more than 1.5mJ up to 5 mJ
- 10-15% intensity fluctuation and no loss at all



Remember, FELs are in their infancy, this behavior is reminiscent of storage ring performance in the late 1970's and early 1980's when they were infants

FEL Experimental Strategies

So, you want to do an experiment at an FEL.

Where do you start?

First, talk to the instrument scientists. They really want to help. But what follows is my two cents.

Understand the Detectors

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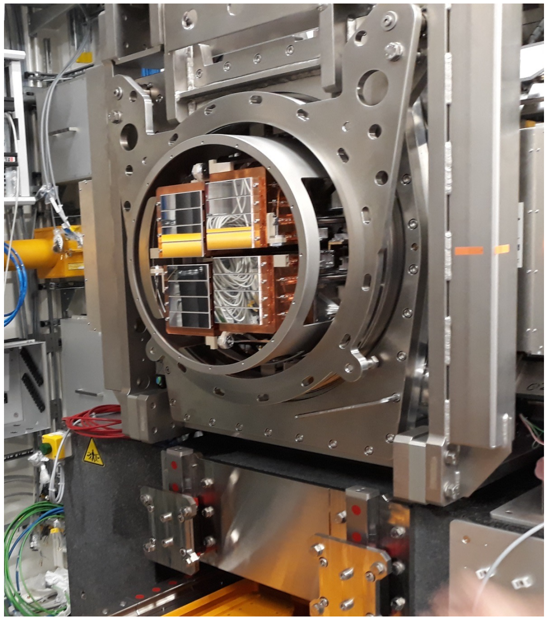
Almost every FEL has detectors that are optimized for their facility. This is totally unlike the case for storage ring experiments.

Also, because of the nature of FELs, one cannot in general either:

- Use signal averaging on the detector
- Do single photon analysis

Since the detectors are all developed locally, all have different software, and all have different idiosyncrasies.

Most likely your experiment will fail if you don't pay careful attention to the detector.



If you are coming to LCLS, ask for help. We have detector experts standing by.

Develop a Data Analysis Strategy

An experiment, successful or not, will deluge you with data.

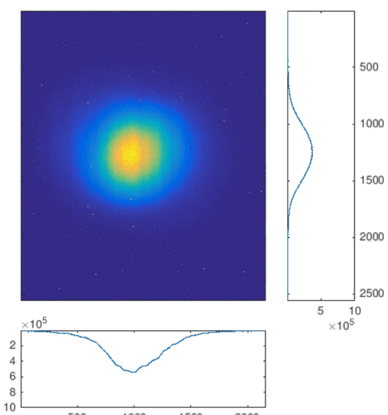
- Probably a hundred parameters are recorded for every x-ray pulse.
- The detector will produce 5 megabytes of data for every pulse.
- And the data acquisition system will do that 120 times a second for hours.

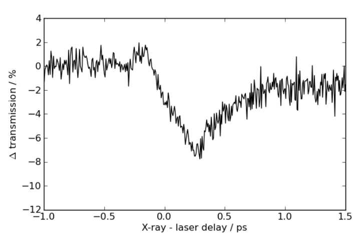
That's a lot of data. You need a plan.

If you are coming to LCLS, ask for help. We have data analysis experts standing by.

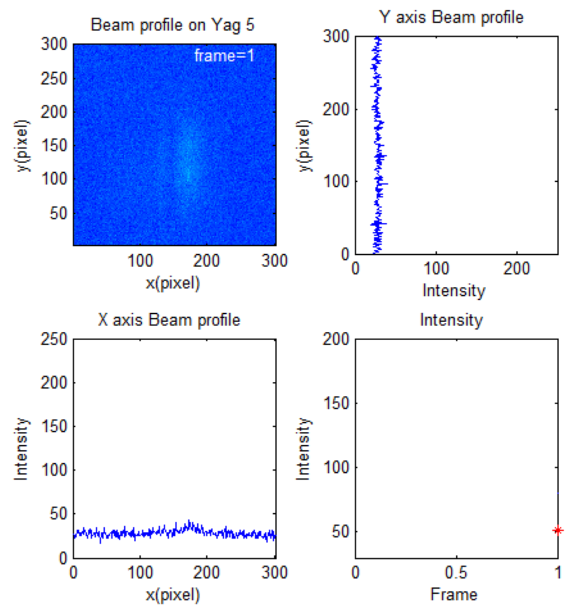
Normalizing, Filtering, Binning

- Each X-ray Pulse is UNIQUE
- Each X-ray pulse fluctuates in many way

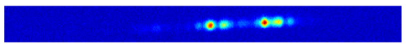


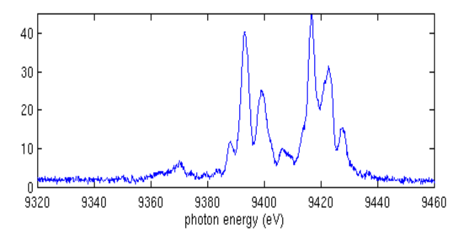


- It is critical to characterize every pulse with precision to the extent possible
- Diagnostics are critical



- Filtering
- Normalizing
- Binning
- Averaging



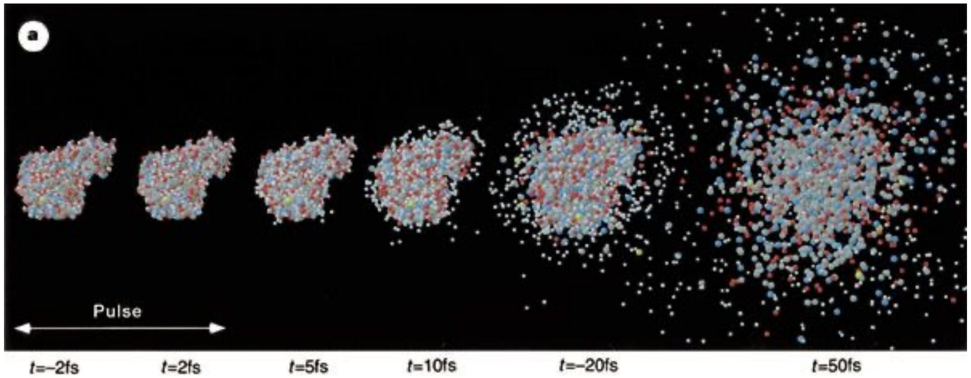


Diffract before destroy

SLAC

Let's correct a misconception !
Most samples survive a single shot FEL beam

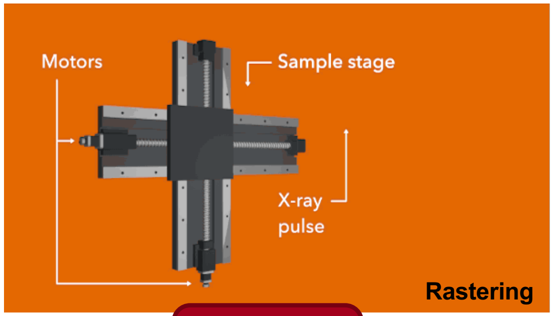
If all photons are focused in a very small spot size (<2-5 micron) nothing survives a single shot



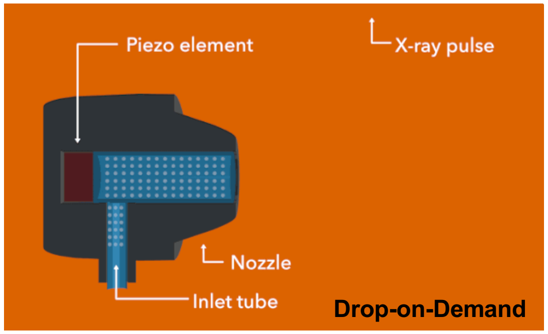
Neutze et al., Nature **406**, pp752 (2000)

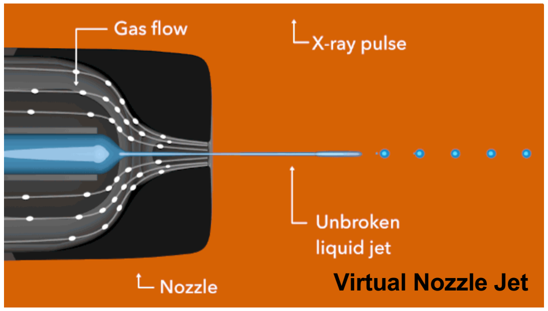
"Diffract-Before-Destroy" take advantage of the peak power to obtain information before the systems reacts to the X-ray probe

Sample Delivery to support "Diffract and Destroy"



SOLIDS



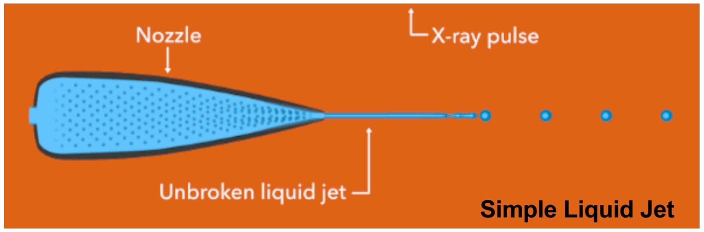


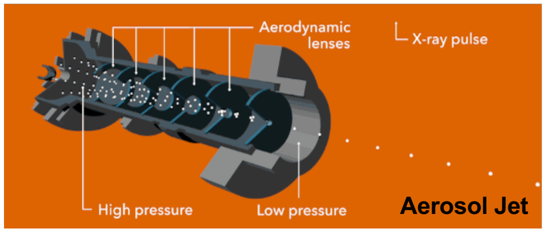
Ability to change the sample when damage by the FEL

LIQUIDS

Delivery must be optimized for each sample.

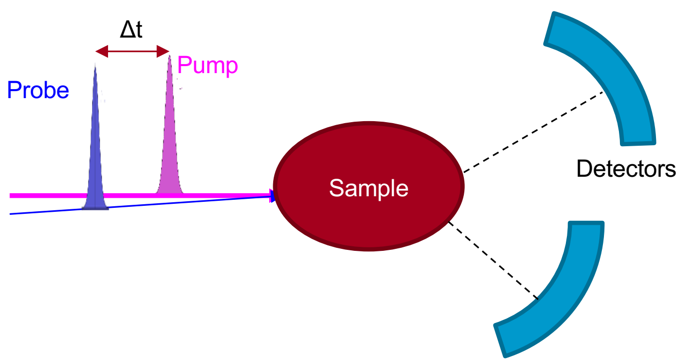
LCLS has dedicated staff to help users with this critical task.





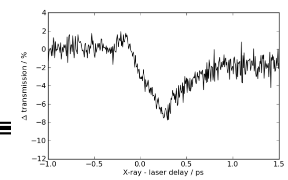
https://www6.slac.stanford.edu/news/2015-02-02-5-ways-put-tiny-targets-front-x-ray-laser.aspx

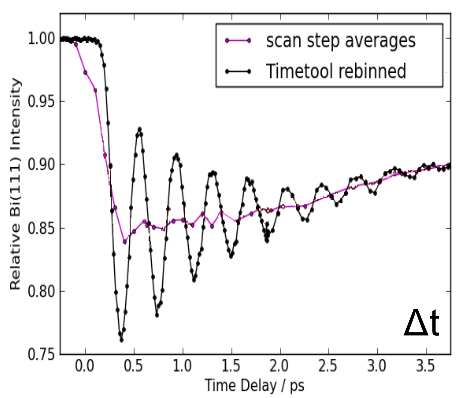
Typical Pump- Probe Experiment

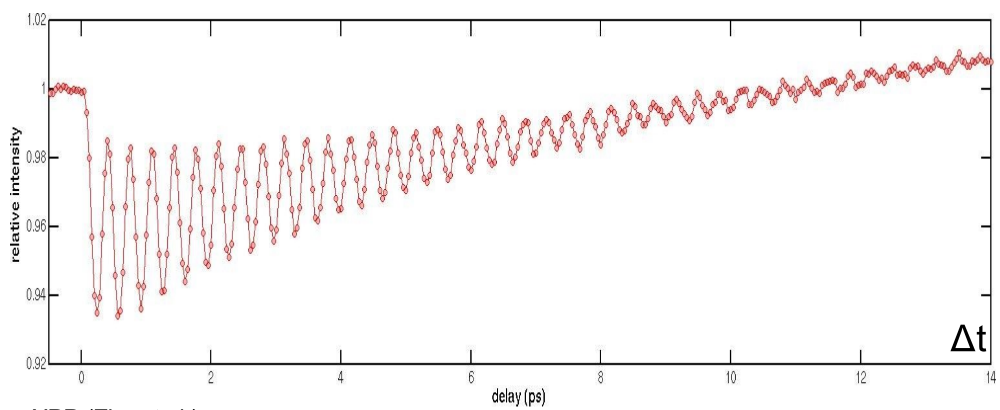


Pump-Probe : evolution of relative signal with X-ray probe at different time delays Δt after excitation (probe)

- **Reproducibility of the excited state**
- **Reproducibility of the sample if damaged**
- **Ability to synchronize two short pulses**
- **Correct for timing jitter**





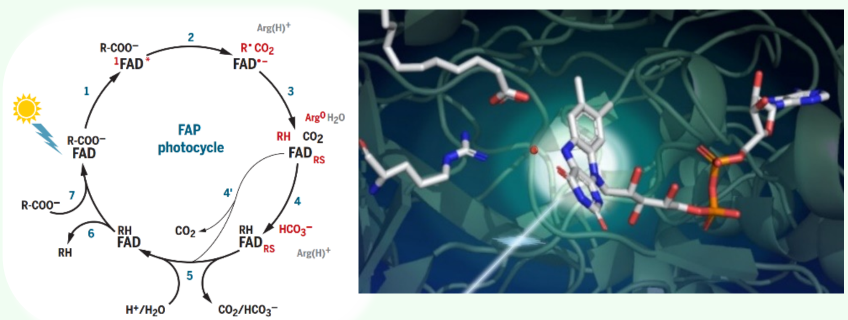


Courtesy XPP (Zhu et al.)

LCLS Structural Biology

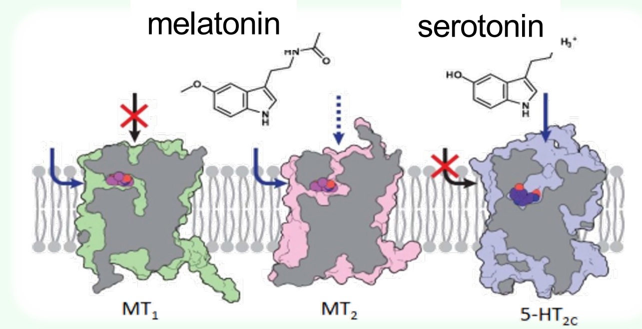
SLAC

Photo-enzyme: Fatty Acids to Hydrocarbons



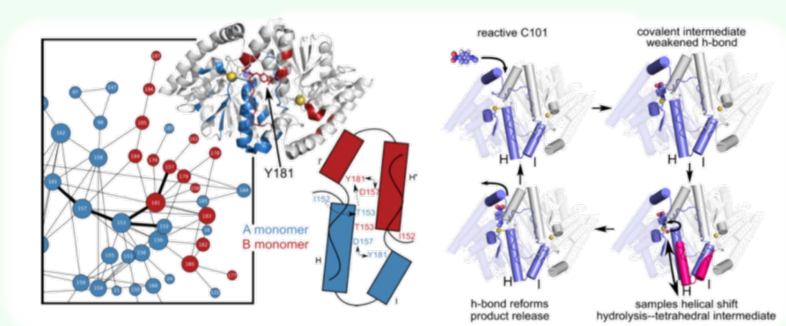
D. Sorigué, et al., Science 372, eabd5687 (2021)

Structure of Human Melatonin Receptors



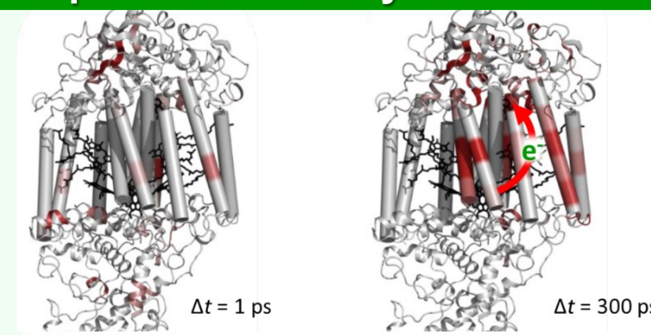
Stauch B. et al., Nature (2019); Johansson L. C. et al., Nature (2019)

Conformational Dynamics – Enzyme Catalysis



M. Dasgupta, *et al.*, *PNAS* 116, 25634 (2019)

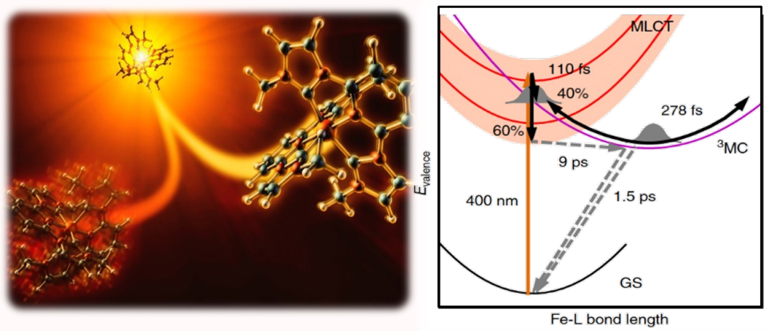
Light Response of Photosynthetic Protein



R. Dods, *et al.*, *Nature*, 589, 310 (2021)

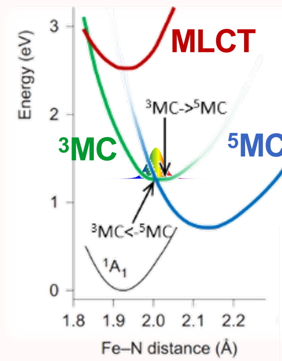
LCLS Chemistry

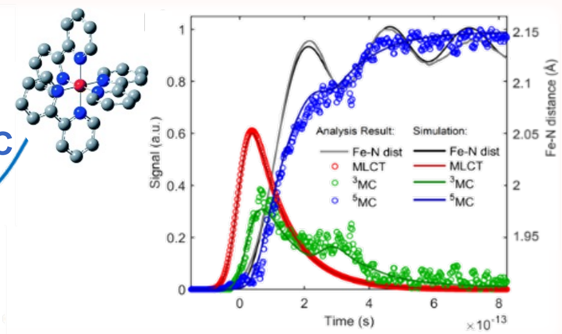
Photosensitizer Charge Relaxation Pathways



K. Kunnus, K.J. Gaffney, et al., Nature Comm. 11, 634 (2020)

Electronic Excited-state Conical Intersections

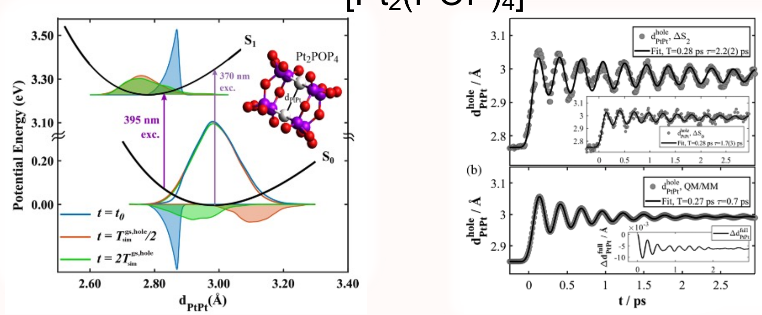




K.S. Kjaer et al., Chem. Sci., 10, 5729 (2019)

Molecular Ground-state Structural Dynamics

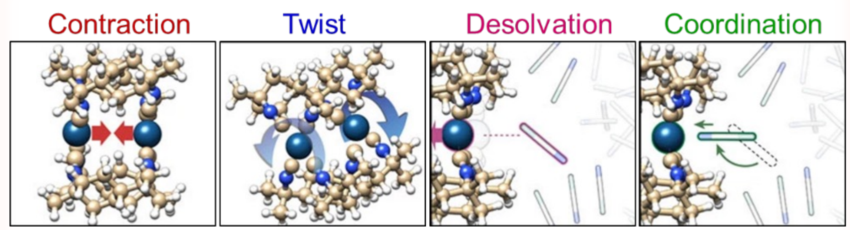
$[Pt_2(POP)_4]^{2+}$



K. Haldrup, et al., Phys. Rev. Lett. 122, 063001 (2019).

Solvation Dynamics of a Model Photocatalyst

$[Ir_2(dimen)_4]^{2+}$

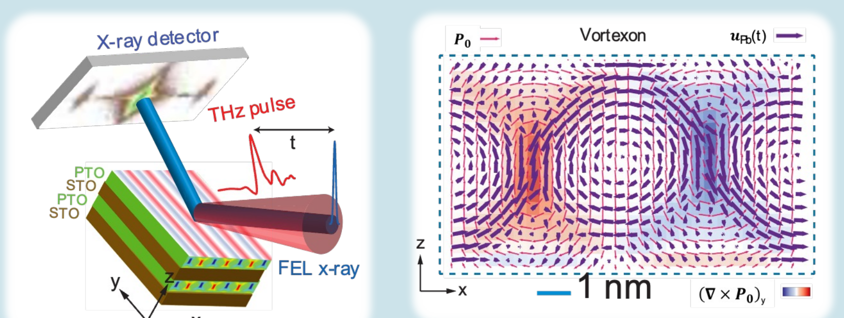


T.B. van Driel, et al., Nature Comm. 7, 13678 (2016)

LCLS Materials Science

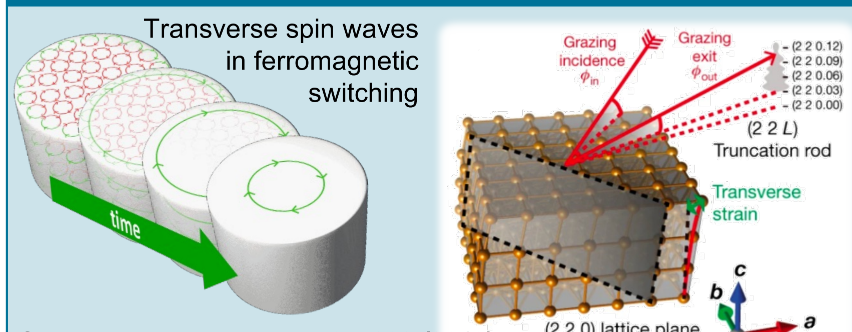
SLAC

Ultrafast Collective Dynamics of Polar Vortices



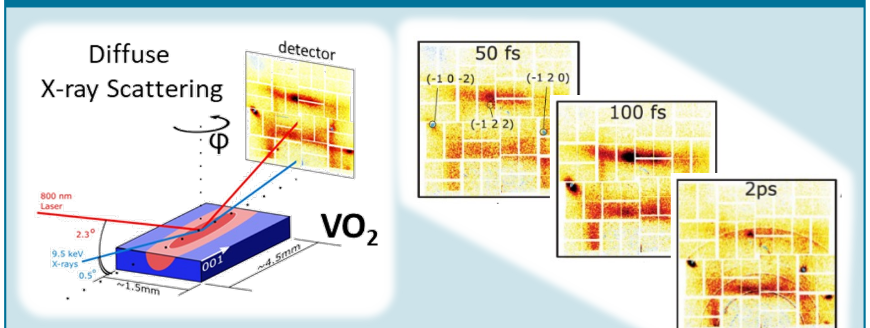
Q. Li et al., Nature (2021)

Ultrafast Einstein - de Haas Effect



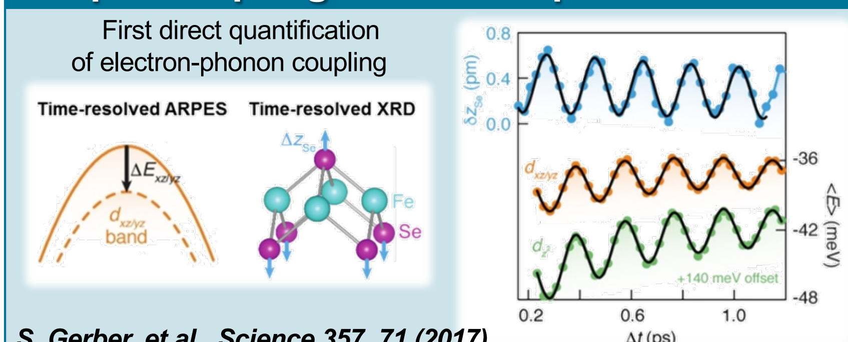
C. Dornes, et al., Nature 565, 209 (2019)

Ultrafast Disorder in Insulator-Metal Transition



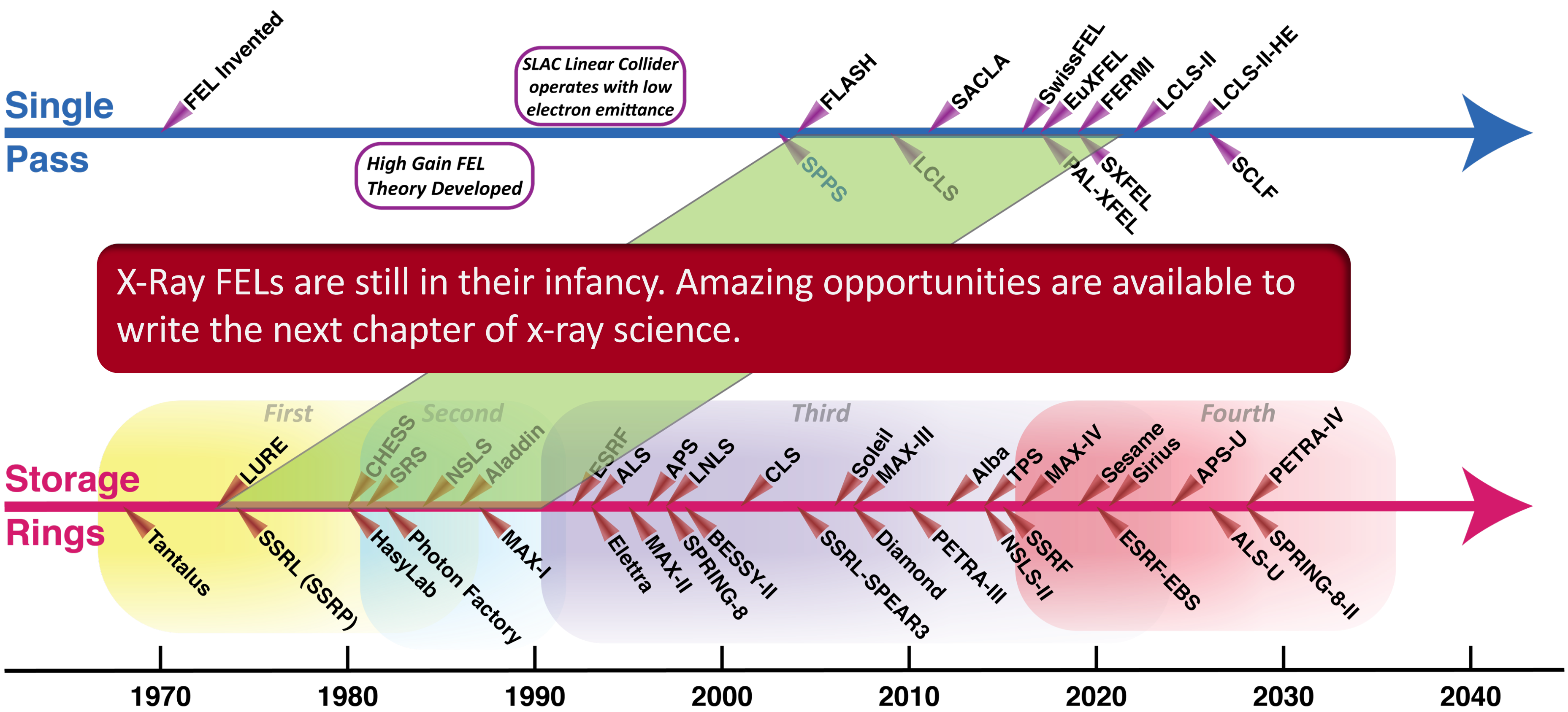
S. Wall, M. Trigo. et al., Science, (2019)

e-ph Coupling in FeSe Superconductor



S. Gerber, et al., Science 357, 71 (2017)

Evolution of Hard X-Ray Sources



Opportunities to Pursue Research

LCLS is a user facility

- Operated by SLAC for the Department of Energy, Office of Science, Office of Basic Energy Science

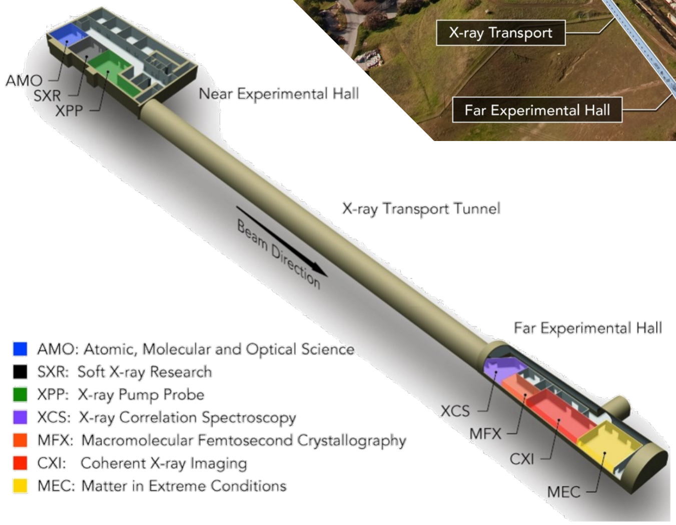
Scientific access via beamtime proposal

- Open to all
- Scientific merit evaluation
- Free of charge for non-proprietary research

Scientific staff is available to provide proposal advice

Details at:

http://LCLS.SLAC.Stanford.edu



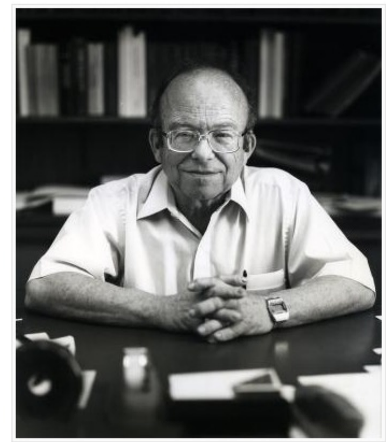
Opportunities for Early Career Scientists

In addition to normal graduate and post-graduate research positions, there are also a few highly competitive prestigious early-career fellowships awarded each year.

Details can be found on the SLAC website:

https://careers.slac.stanford.edu/

Panofsky Fellowship Overview



The Panofsky Fellowship honors SLAC National Accelerator Laboratory's founder and first Director, Wolfgang K. H. Panofsky. It is intended to recognize exceptional and promising early career scientists who would most benefit from the unique opportunity to conduct their research at SLAC National Accelerator Laboratory. While the scientific direction of the candidates is expected to have some overlap with existing programs, an emphasis will also be placed on the potential for innovation and growth of new opportunities, aligned with the overall mission and values of the laboratory, as their career develops. The intent is to foster the creativity and high achievement to which W.K.H. Panofsky devoted himself both as a researcher and as a visionary leader in enabling fundamental science research.

The Fellowship celebrates **W.K.H. Panofsky's breadth of activities** and is awarded without regard to a candidate's particular specialty within our programs. The candidate's research plan should encompass one or more areas within the general scope of the **science program at SLAC**:

- Accelerator science & advanced accelerator research
- Applied Energy research
- Biosciences
- Chemical science
- Computer science
- Elementary particle physics
- High energy density matter
- Material and condensed matter science
- Particle astrophysics and cosmology
- X-ray science, including ultrafast science and advanced X-ray instrumentation, at LCLS and SSRL

Applicants are encouraged to contact **OCRO@slac.stanford.edu** to find out the leads of a program to find out more details about the program and the context for developing their proposed research plan as a Panofsky Fellow.

The End

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Feedback

Lecture – 2:15 – 3:15
General introduction to FELs - Paul Fuoss
https://forms.office.com/g/ADmyv5Bynr