X-Ray Free-Electron Lasers: Scientific Goals and Machine Implications

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What is a free-electron laser? How is FEL radiation different from synchrotron radiation?

Why does anyone care? What exciting science can be done with an x-ray FEL?

What x-ray FEL plans are in the works?

Synchrotron radiation and FEL radiation both come from high-energy electrons accelerated by magnetic fields

Conventional synchrotron radiation
Electron density in phase space is low (electron brightness << diffraction limit of emitted radiation)

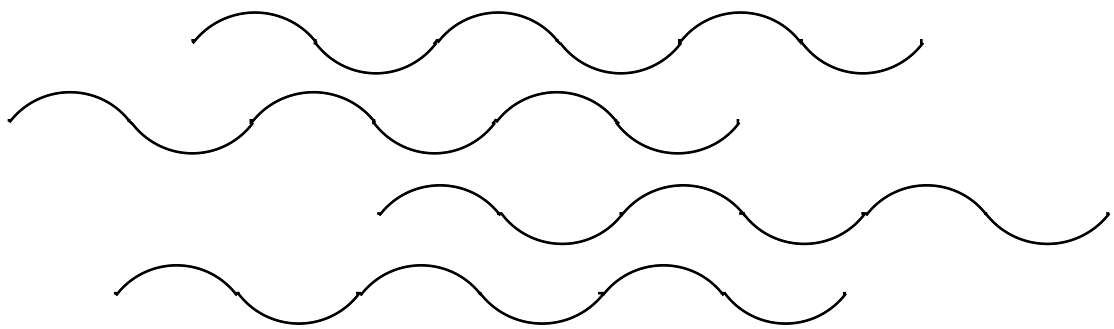
Electromagnetic field effects on the electrons are not significant

Each electron radiates independently, not coherently with others

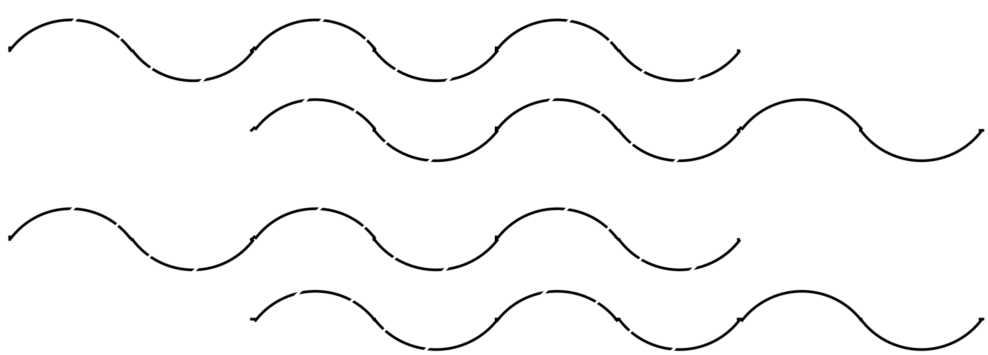
Free Electron Laser radiation
High electron density (electron brightness ~ diffraction limit of radiation)

EM field can cause microbunching of electrons, on scale of radiation wavelength

Electrons radiate collectively, coherently

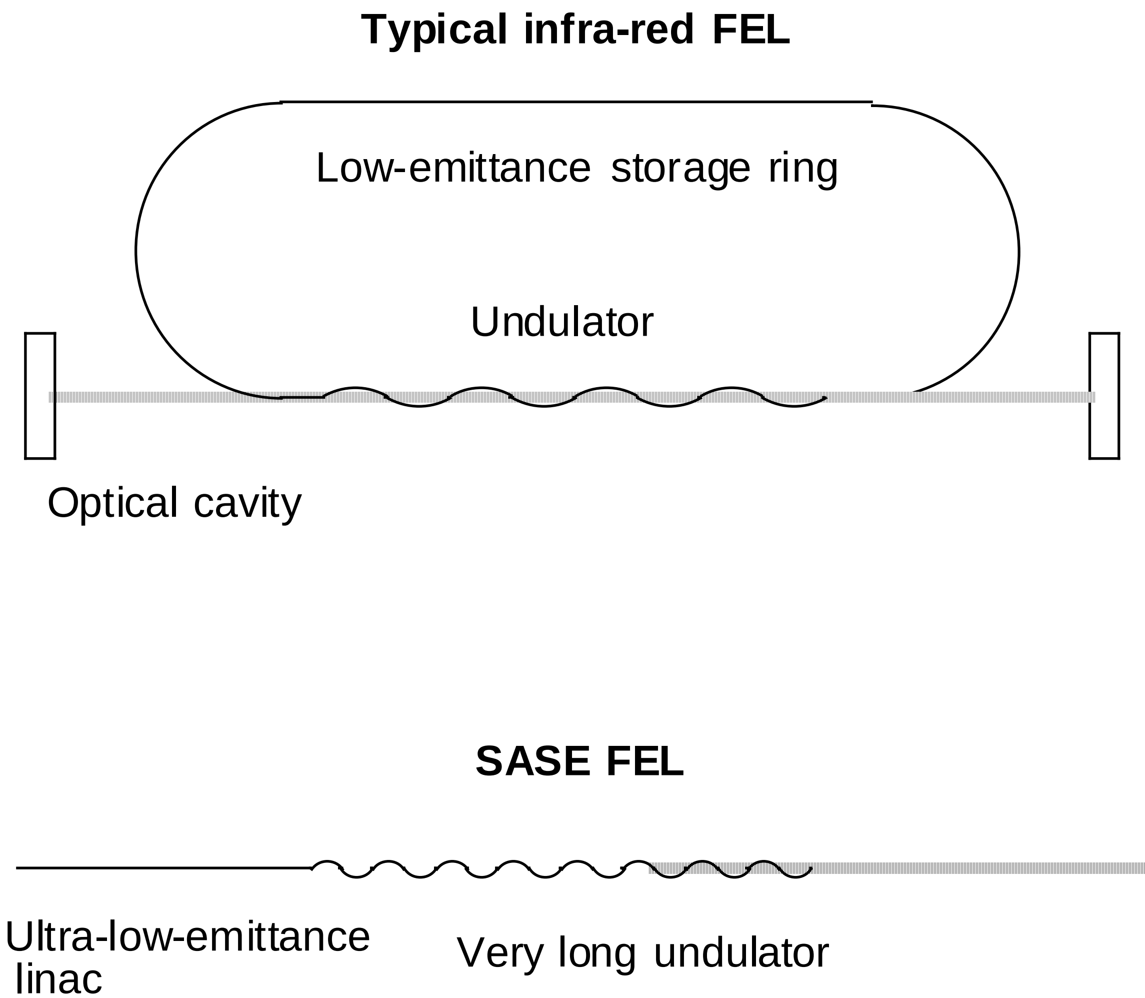


Spontaneous undulator radiation

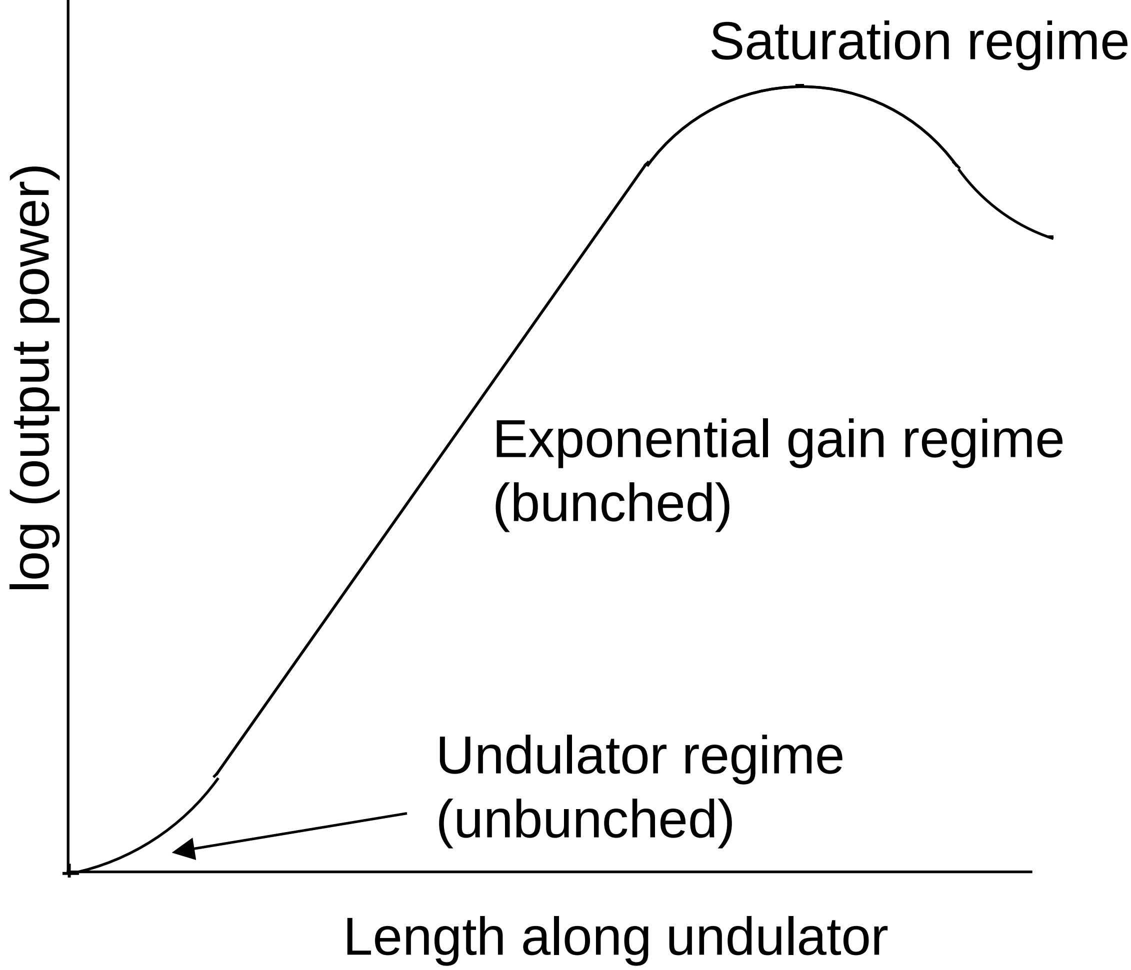


EM field causes bunching, gives

coherent FEL radiation


Typical infra-red FEL
Low-emittance storage ring
Undulator
Optical cavity
SASE FEL
Ultra-low-emittance linac
Very long undulator

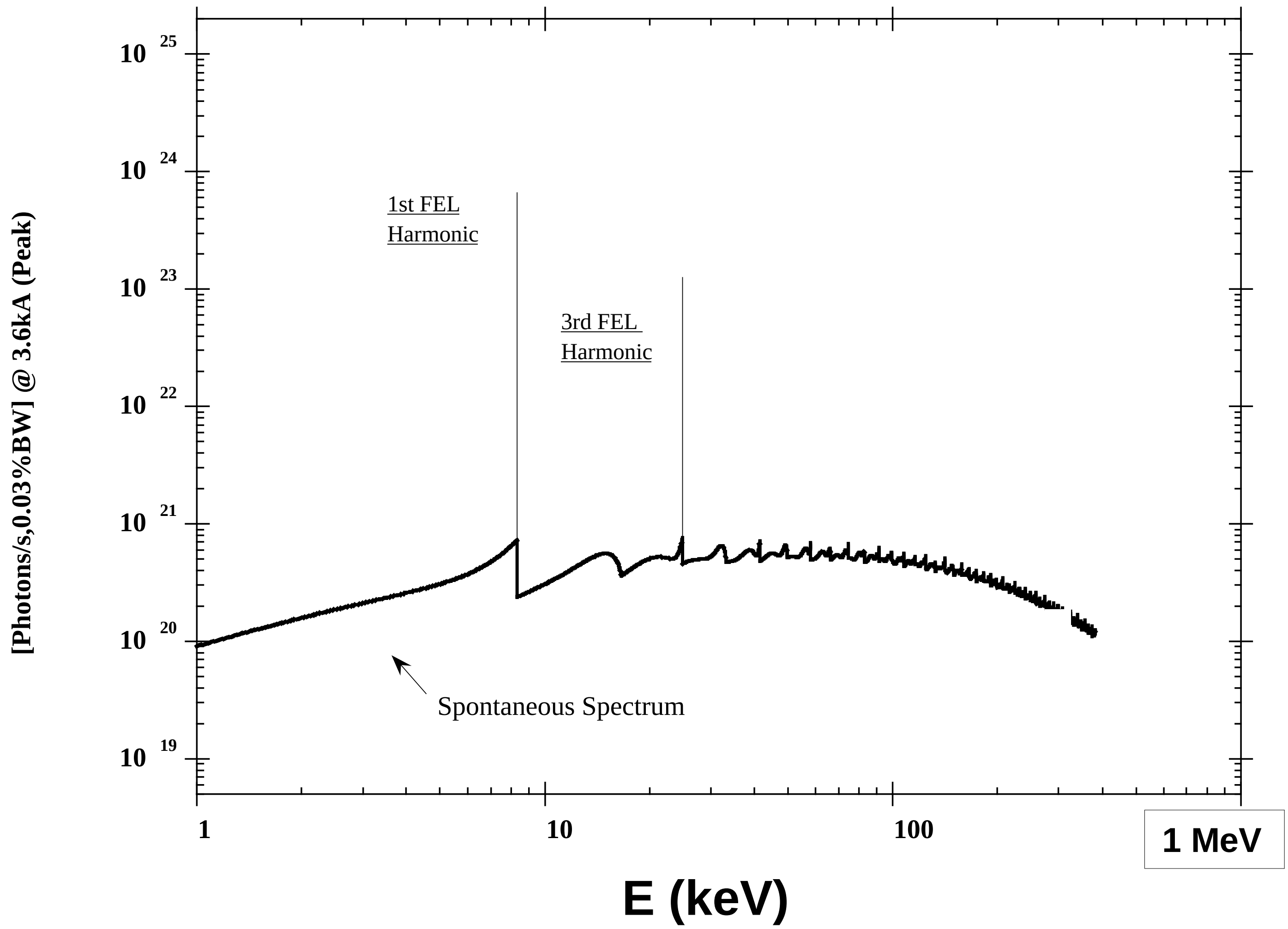
SASE Characteristics

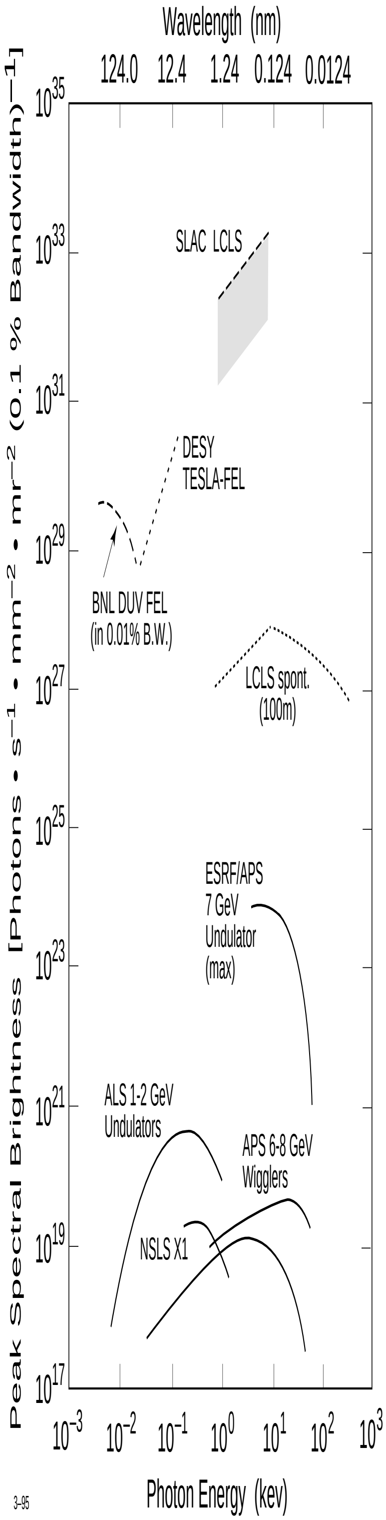


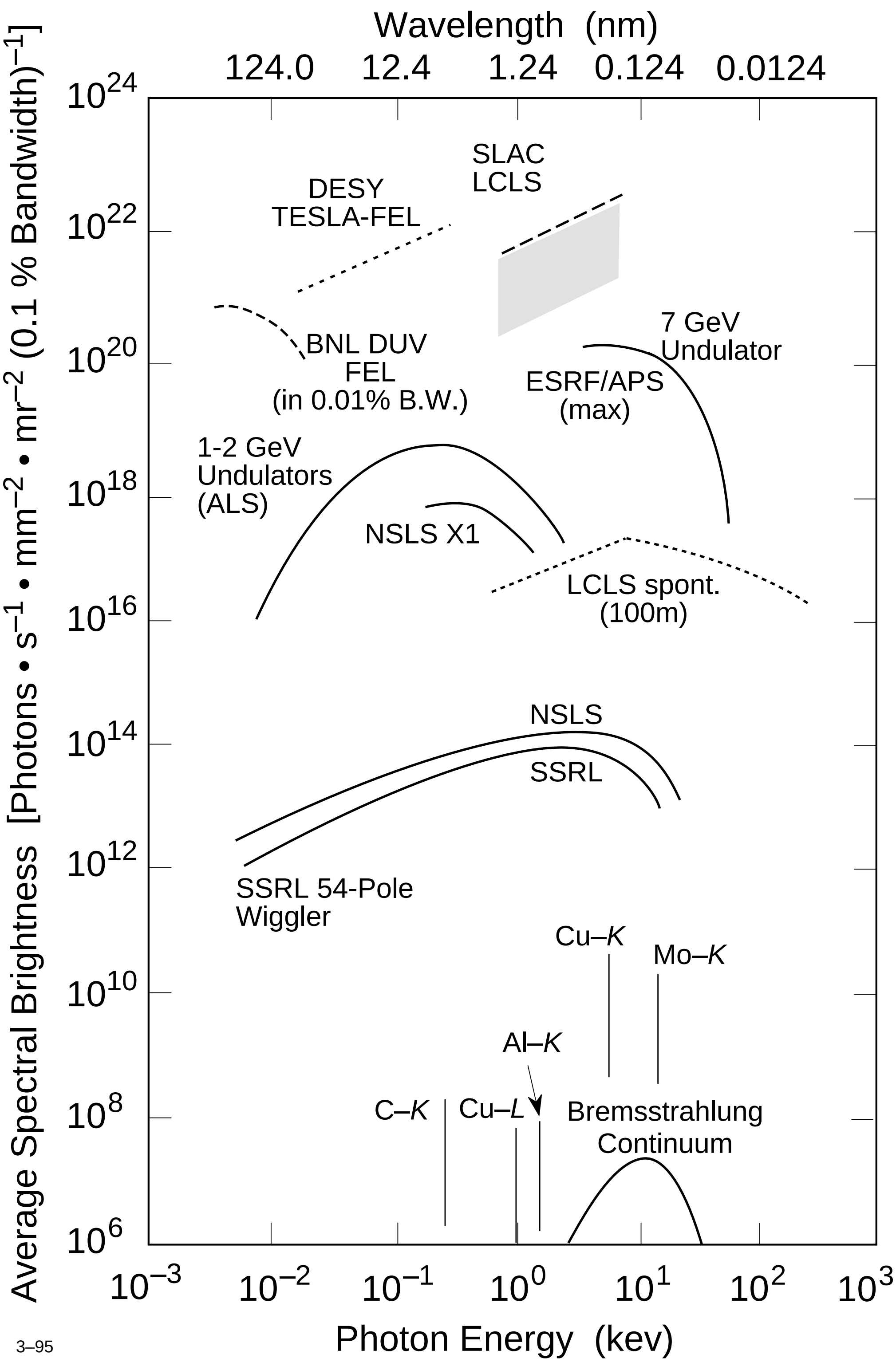
- **Convergence of technologies makes it now possible to construct an x-ray FEL**
  - Photoinjector -> Creation of a bright electron beam
  - SLC experience, Next Linear Collider Studies -> Acceleration with minimum brightness degradation
  - Undulators -> FEL, error control, synchrotron source experience

LCLS Peak Photon Flux Spectrum

3300 periods, K=3.7, E=14.35 GeV, 120 Hz rep rate




Wavelength (nm)
124.0
12.4
1.24
0.124
0.0124
Peak Spectral Brightness [Photons • s^{-1} • mm^{-2} • mr^{-2} (0.1 % Bandwidth)$^{-1}$]
10^{35}
10^{33}
10^{31}
10^{29}
10^{27}
10^{25}
10^{23}
10^{21}
10^{19}
10^{17}
SLAC LCLS
DESY
TESLA-FEL
BNL DUV FEL
(in 0.01% B.W.)
LCLS spont.
(100m)
ESRF/APS
7 GeV
Undulator
(max)
ALS 1-2 GeV
Undulators
APS 6-8 GeV
Wigglers
NSLS X1
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Photon Energy (kev)
3–95


Wavelength (nm)
124.0
12.4
1.24
0.124
0.0124
Average Spectral Brightness [Photons • s^{-1} • mm^{-2} • mr^{-2} (0.1 % Bandwidth)$^{-1}$]
10^{24}
10^{22}
10^{20}
10^{18}
10^{16}
10^{14}
10^{12}
10^{10}
10^{8}
10^{6}
SLAC
LCLS
DESY
TESLA-FEL
BNL DUV
FEL
(in 0.01% B.W.)
7 GeV
Undulator
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(max)
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Undulators
(ALS)
NSLS X1
LCLS spont.
(100m)
NSLS
SSRL
SSRL 54-Pole
Wiggler
Cu–*K*
Mo–*K*
Al–*K*
C–*K*
Cu–*L*
Bremsstrahlung
Continuum
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Photon Energy (kev)
3–95

Key features of X-Ray FEL Radiation

- Sub-picosecond pulse

  230 fs FWHM pulse with 1 fs structure

- Very high peak power and brightness

  More than 10^{12} photons/pulse

  Degeneracy factor greater than 10^{9}
  (APS undulator degen. factor is <1)

- Full spatial coherence

  A diffraction-limited x-ray source

Calculated Characteristics of the LCLS beam

FEL wavelength	1.5	Å
Bandwidth ($\delta E/E$)	0.002	
Pulse duration (FWHM)	233	fs
Pulse length (FWHM)	70	µm
Peak coherent power	9	GW
Energy/pulse	2.6	mJ (2 mJ = 2×10^{16} eV)
Peak coherent power density	2×10^{12}	W/mm^2
Peak brightness	1×10^{33}	$flux/mm^2/mrad^2/0.1\%BW$
Coherent photons/pulse	2×10^{12}	
Coherent photons/second	2×10^{14}	
Degeneracy parameter	10^{9}	
Peak EM field (unfocussed)	3×10^{10}	V/m
Repetition rate	120	Hz
Average coherent power	0.3	W
Average brightness	2×10^{22}	$flux/mm^2/mrad^2/0.1\%BW$
Transverse size of coherent radiation (FWHM)	80	µm
Divergence of coherent radiation (FWHM)	1	µrad
Peak power of spontaneous (wide spectrum) radiation	81	GW

FEL wavelength tuning range: 15-1.5 Å = 0.8-8 keV

Spontaneous radiation spectrum: 0.3-30 x FEL energy
(i.e., 2.4-240 keV for FEL energy of 8 keV)

High Peak Power

Peak power density = $2*10^{14}$ W/cm^2

Focused to 100 nm diameter

=> 10^{20} W/cm^2

Peak electric field = $3*10^{10}$ V/m

Focused => $2*10^{13}$ V/m

High-order atom-photon interactions can not only be studied, they may influence all x-ray FEL experiments

Only very light materials (Be, C) could survive the unfocused beam without damage; Si is on the borderline

Atomic Physics

Atom interactions with x-ray FEL pulse are different from interactions with conventional lasers or weaker x-ray sources

Studying LCLS-atom interactions will advance atomic physics and provide basis for understanding all other LCLS experiments

•Direct observation of multiple core hole formation (MCHF) in an atom

•Direct observation of multiphoton ionization of a K-shell electron (MPIK)

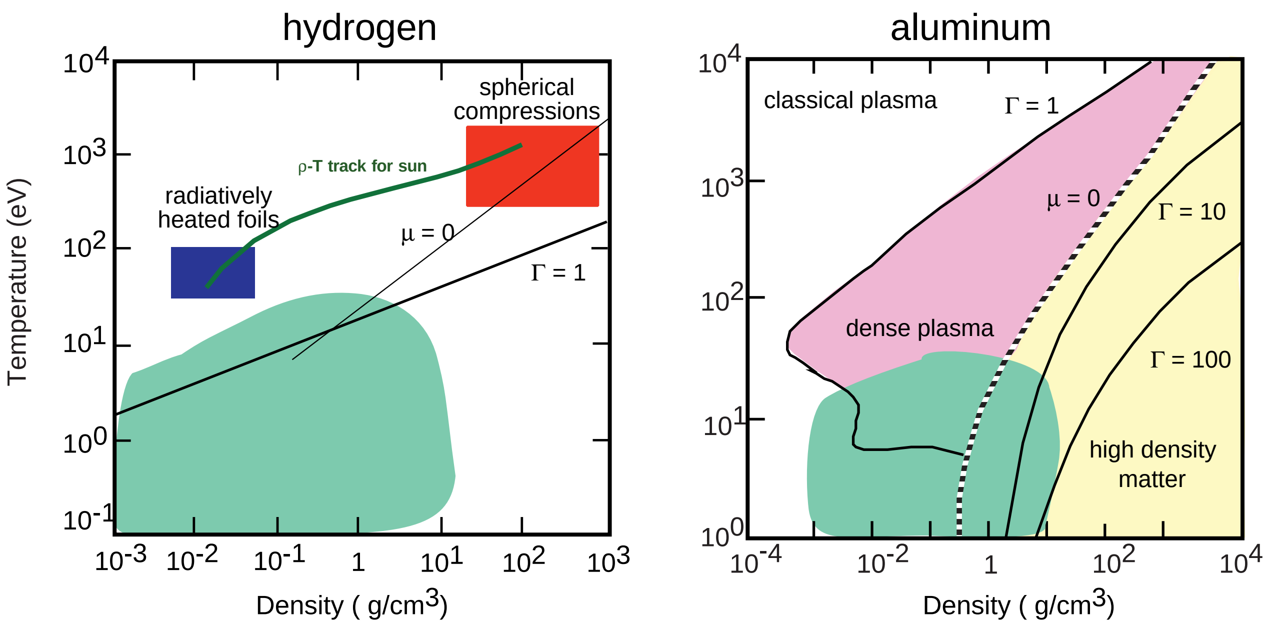
•Observation of giant coulomb explosions in atomic cluster (GCEC)

•Studies of radiation and possibly lasing from XFEL-excited matter

•Formation of highly excited laser plasmas

Studies of Warm Dense Matter

"...that part of the density-temperature phase space where the standard theories of condensed matter physics and/or plasma statistical physics are invalid."



Γ = ratio between electric and thermal potential energy
μ = chemical potential (atom interaction potential)

LCLS will be able, for the first time, to probe the warm dense matter regime

Astrophysical and weapons-related studies come directly into the area of warm dense matter

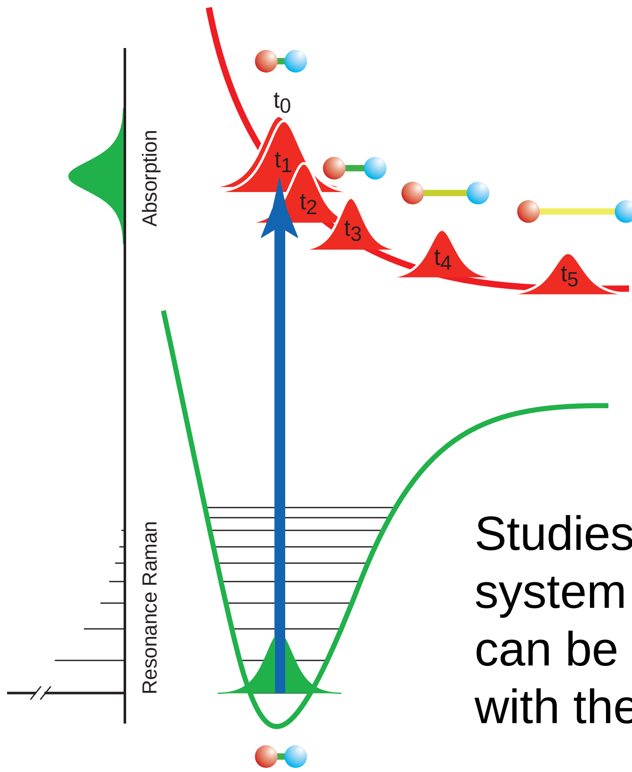
Regions of largest errors and uncertainties in many applied research areas of chemistry and physics come in the warm dense regime

Studies of Warm Dense Matter

- Use LCLS to create warm dense matter state and also (via delayed pulse) to probe it using x-ray scattering or imaging

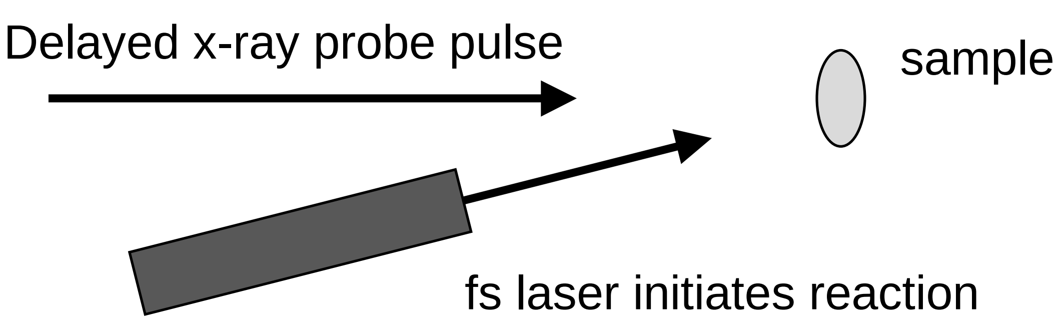
- Use conventional laser to selectively excite certain atomic transitions, creating population inversion which leads to lasing or plasma formation. Study the kinetics of this process using LCLS as probe

Femtosecond Chemistry



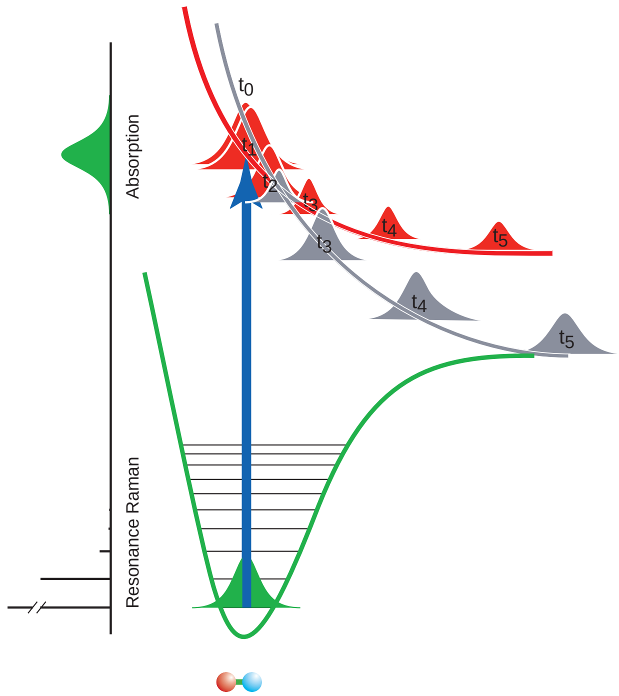
Studies of small system reactions can be compared with theory

Combine single-pulse x-ray diffraction with fast laser excitation



Femtosecond Chemistry

More realistic diatomic system



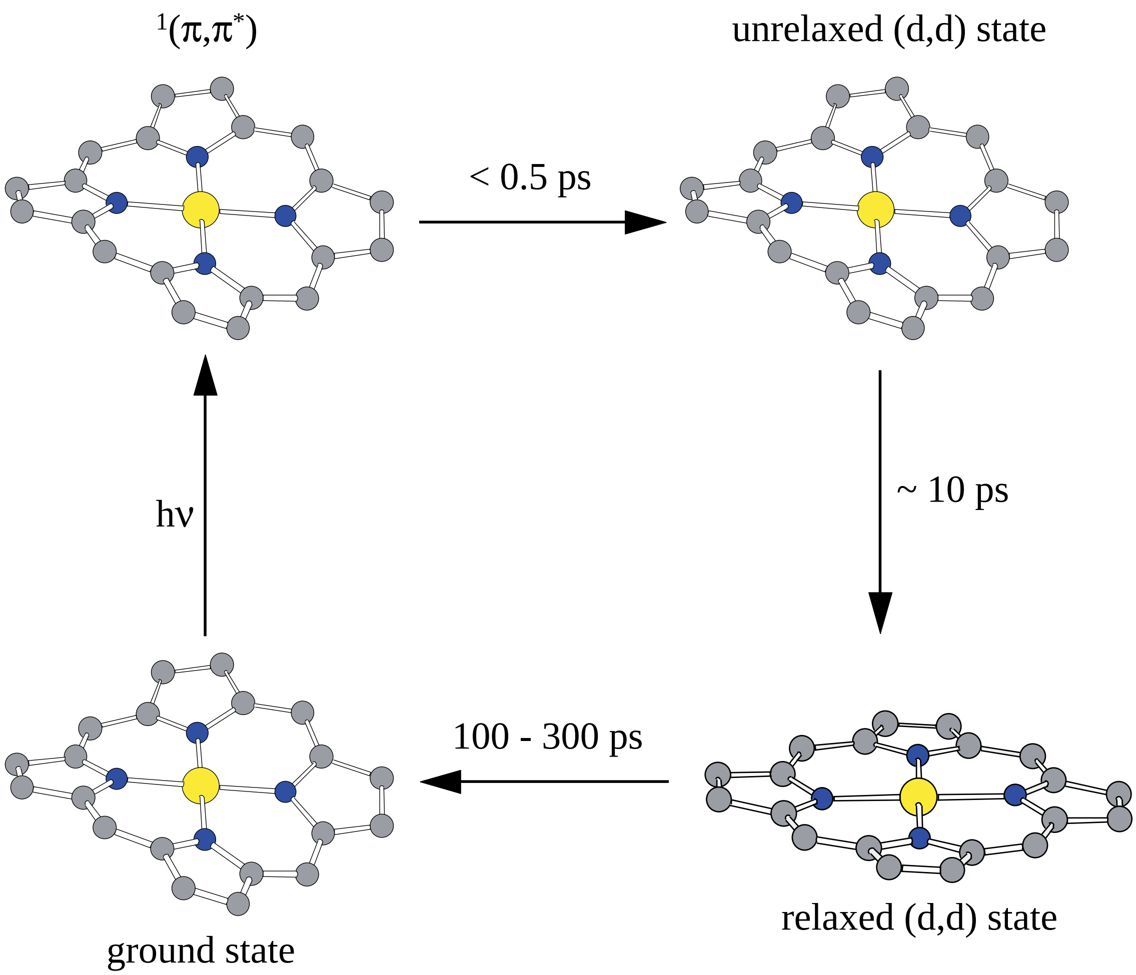
Photodissociation including surface hopping

Initial wavepacket prepared on the optically active red excited state, which is crossed by the dark gray state

As the wavepacket moves to near the crossing point a fraction of its amplitude crosses to the gray state, changing its electronic character in the process

Femtosecond Chemistry

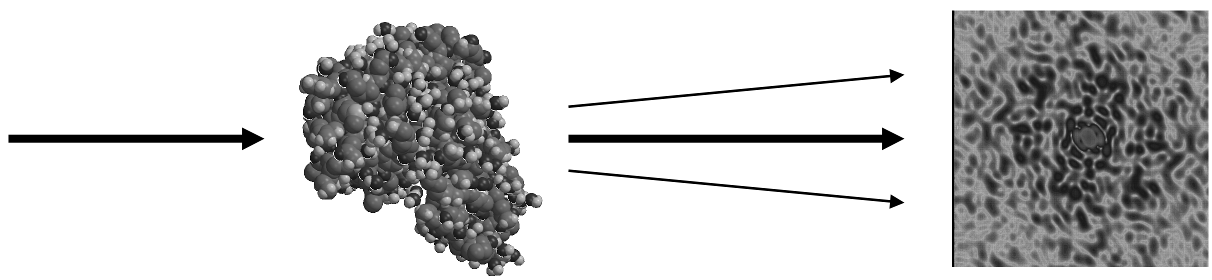
Goal: to study the sequence of structural changes that occur on a sub-ps time scale following an impulse trigger (laser-initiated reaction)



Low-spin (d^8) Nickel(II) Porphyrins deactivation pathway

X-Ray Diffraction from a Single Protein Molecule

Diffuse x-ray scattering from single protein molecule can be used to solve the protein structure



Lysozyme

Calculated scattering pattern from single lysozyme molecule

For 2Å resolution, need 10^{14} photons on protein
-> 10^{10} photons/Å^2, radiation dose ~ 10^{15} Gy

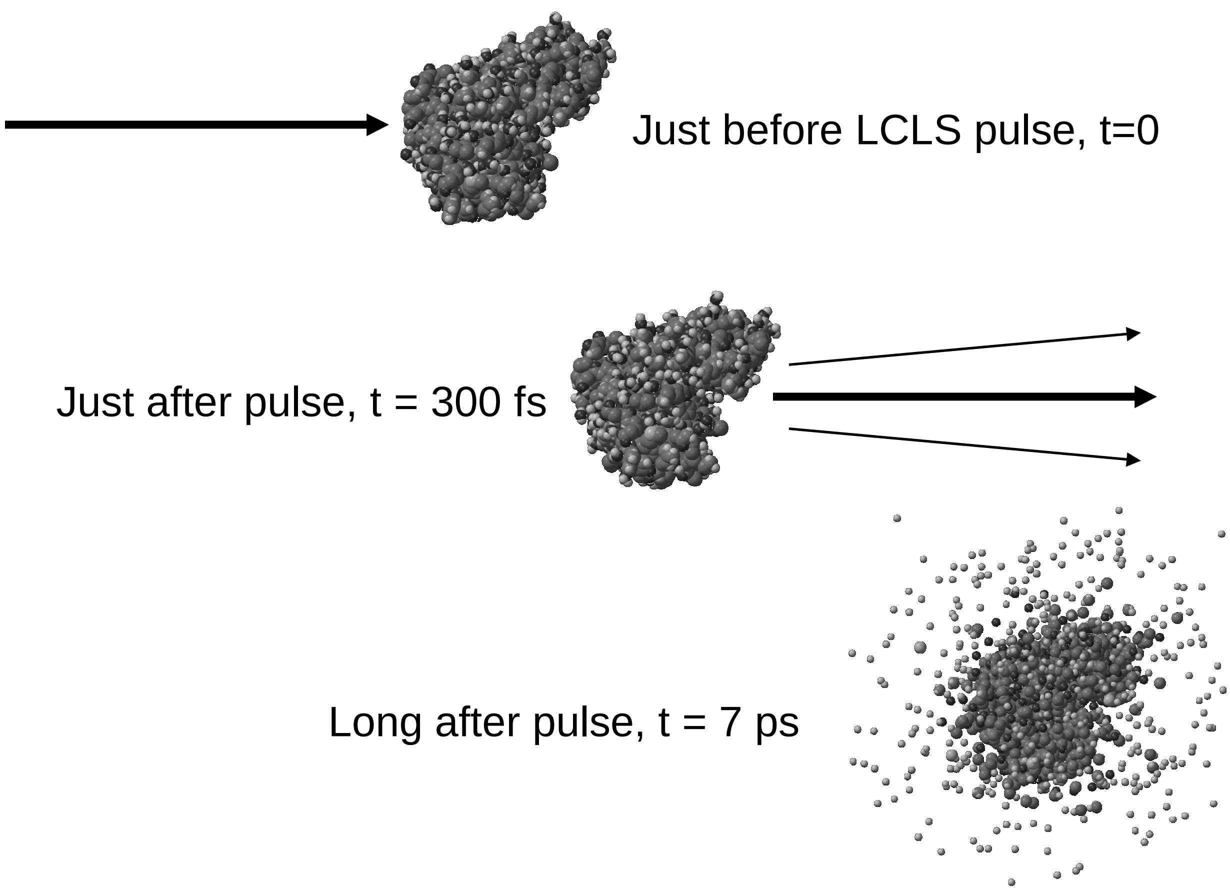
At 3rd gen. synchrotron source, 10^5 Gy destroys sample
10^7 Gy pulse will cause the sample to explode (~1 eV/atom)

X-Ray Diffraction from a Single Protein Molecule

A bright idea: A very short, intense x-ray pulse could produce a diffraction pattern before the molecule explodes

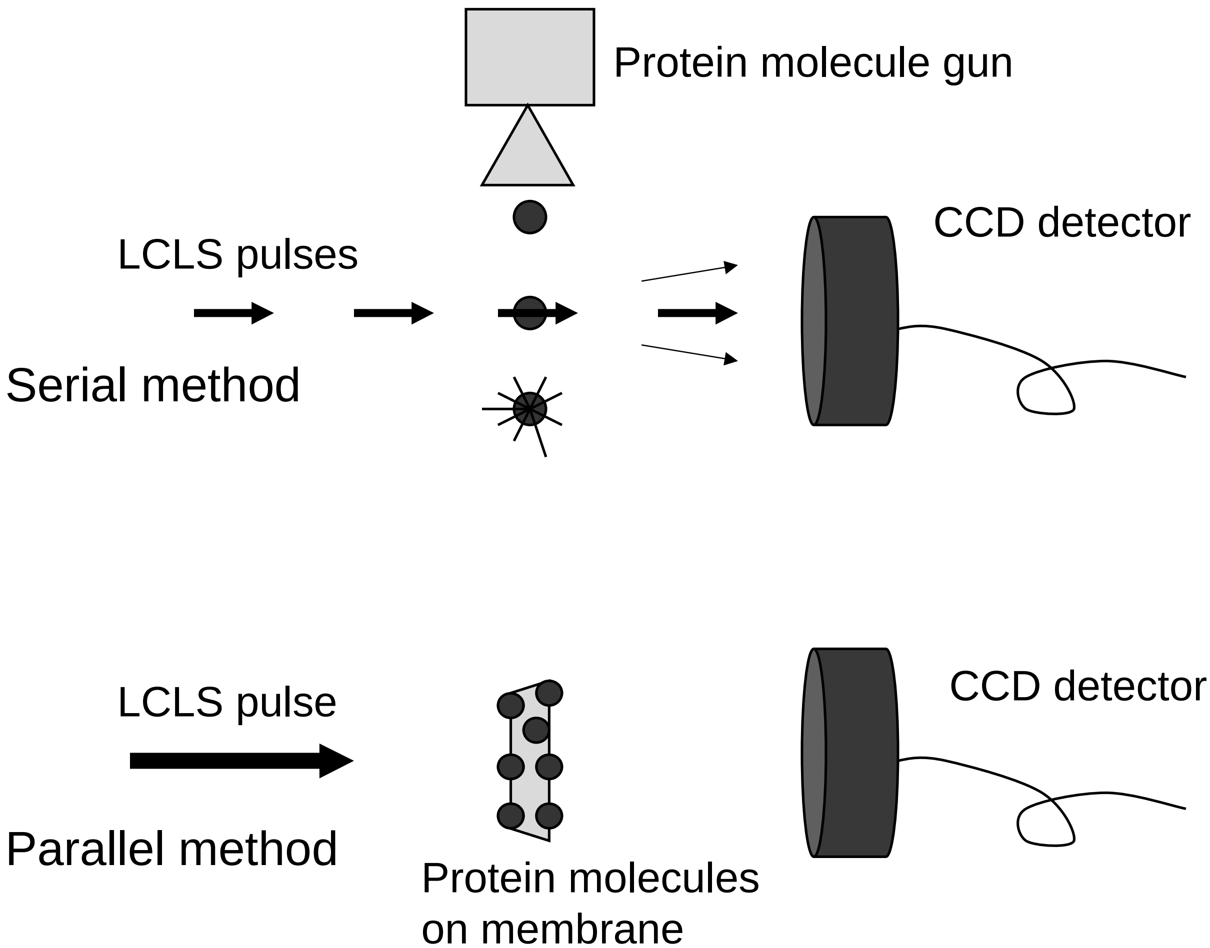
Janos Hajdu (Uppsala Univ.) and collaborators have used molecular dynamics calculations to study this idea. An important result:

- Lysozyme would survive LCLS pulse intensity for much longer than the 300 fs pulse length.



X-Ray Diffraction from a Single Protein Molecule

Complete 2Å structure would require multiple samples, orientations

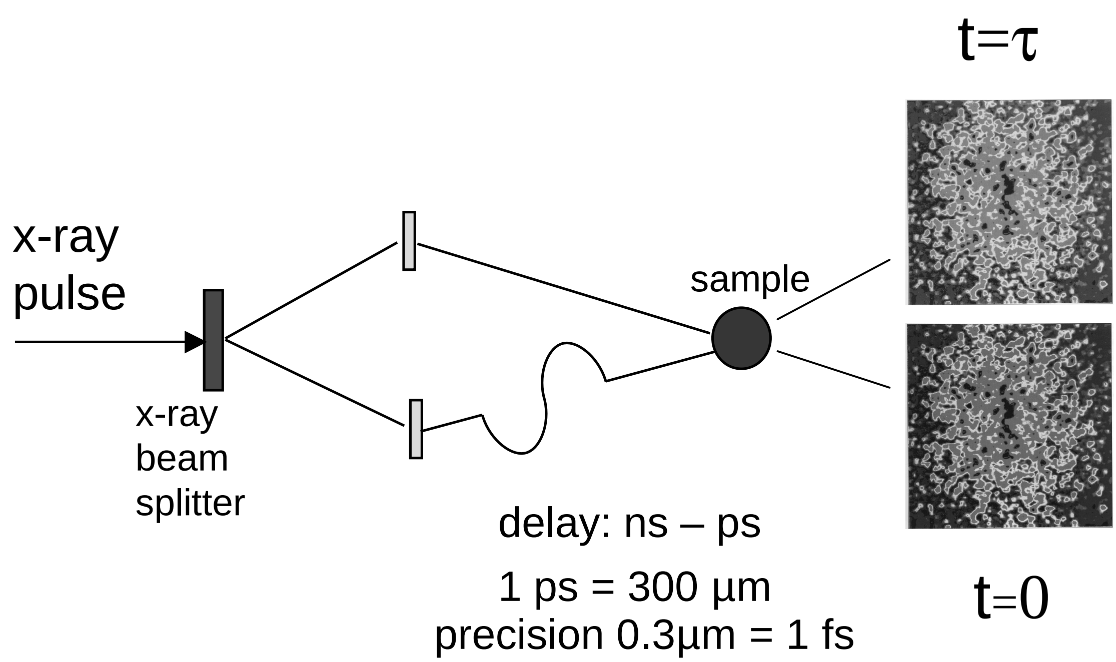


Nanoscale Dynamics in Condensed Matter

Study fast, atomic-scale motions in condensed systems using FEL pulse in various roles:

•X-ray probe followed by delayed x-ray probe studies equilibrium fluctuations

•X-ray or optical laser pump followed by x-ray probe studies relaxation dynamics

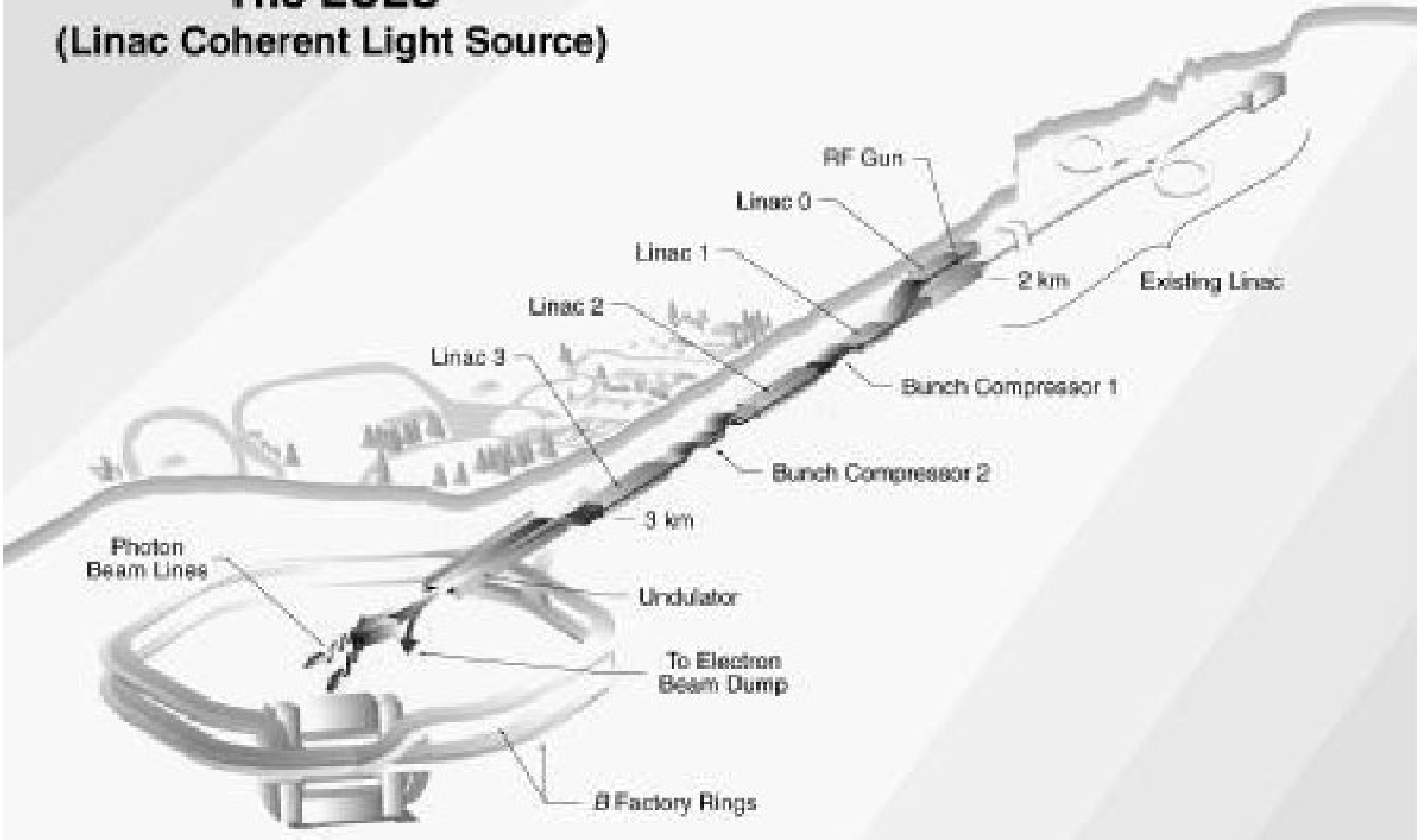


Nanoscale Dynamics in Condensed Matter

Possible areas of study

Simple Liquids – Transition from hydrodynamic to kinetic regime.
Complex Liquids – Effect of local structure on collective dynamics.
Polymers – Entanglement and reptative dynamics.
Glasses – Vibrational and relaxational modes in mesoscopic space-time region.
Dynamic Critical Phenomena – Order fluctuations in alloys, liquid crystals, etc.
Charge Density Waves – Direct observation of sliding dynamics.
Quasicrystals – Nature of phason and phonon dynamics.
Surfaces – Dynamics of adatoms, islands, and steps during growth and etching.
Defects in Crystals – Diffusion, dislocation glide, domain dynamics.
Ferroelectrics – Order-disorder vs. displacive nature; anisotropic correlations and size effects.

The LCLS
(Linac Coherent Light Source)



Linac Coherent Light Source Project Goals

Find ways to meet the technical challenges

Demonstrate SASE at x-ray wavelengths, eventually at 1.5 Å

Pioneer the use of x-ray FEL radiation for materials science, plasma physics, chemistry, and biology

Schedule:

R&D funded since 1999

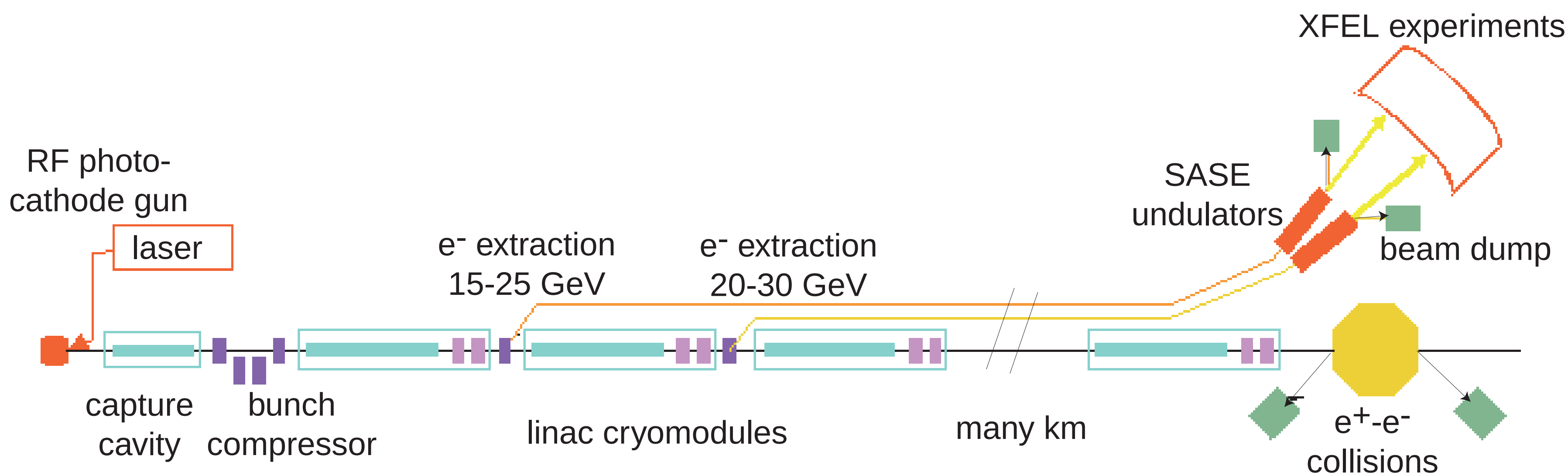
SASE visible and UV experiments at ANL, BNL

LCLS CDR goes to DOE in spring of 2001

Hope for construction funding in 2003

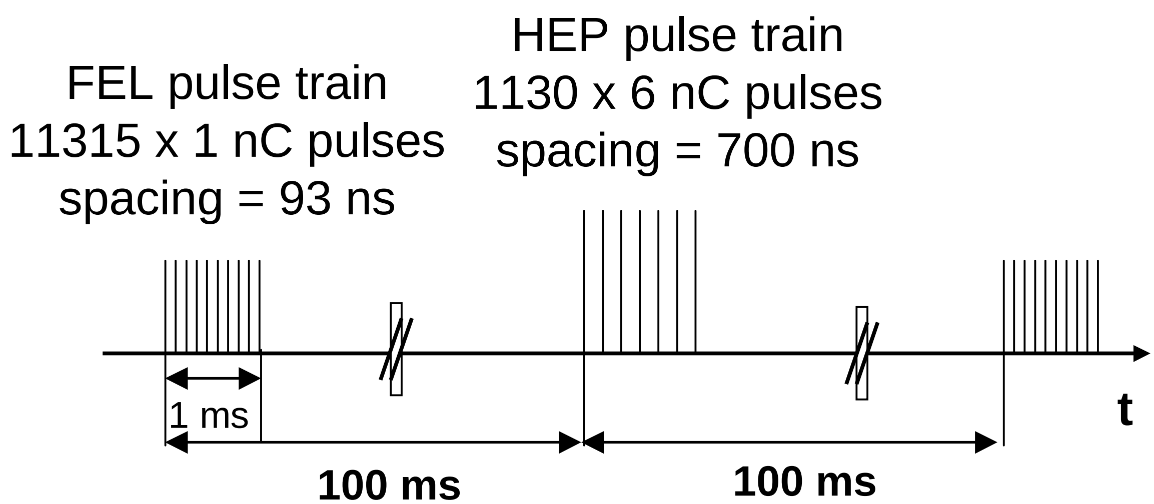
FEL operation in 2006

The XFEL user facility at TESLA



TESLA electron pulse pattern

Each pulse = 100 fs
Pulse train length ~ 1 ms
Train repetition rate = 0.1 Hz
Alternating FEL and HEP pulse trains



The XFEL user facility at TESLA

Conclusions

X-ray free-electron lasers have the potential to facilitate exciting new science in several disciplines.

X-ray FELs will require extremely bright high-energy electron beams, requirements that are very similar to those of linear colliders.

The US DOE is supporting R&D on SASE FEL physics, with the goal of building an x-ray FEL within 5-10 years. An FEL user facility may follow.

DESY is already preparing a plan for an x-ray FEL user facility, associated with a 500 GeV linear collider.