New Directions in X-Ray Light Sources

or

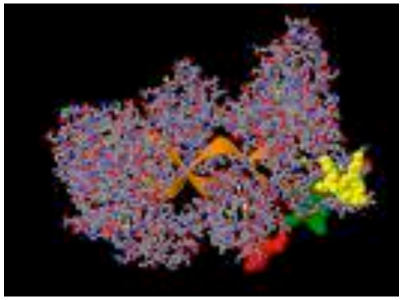
Fiat Lux: what's under the dome & watching atoms with x-rays

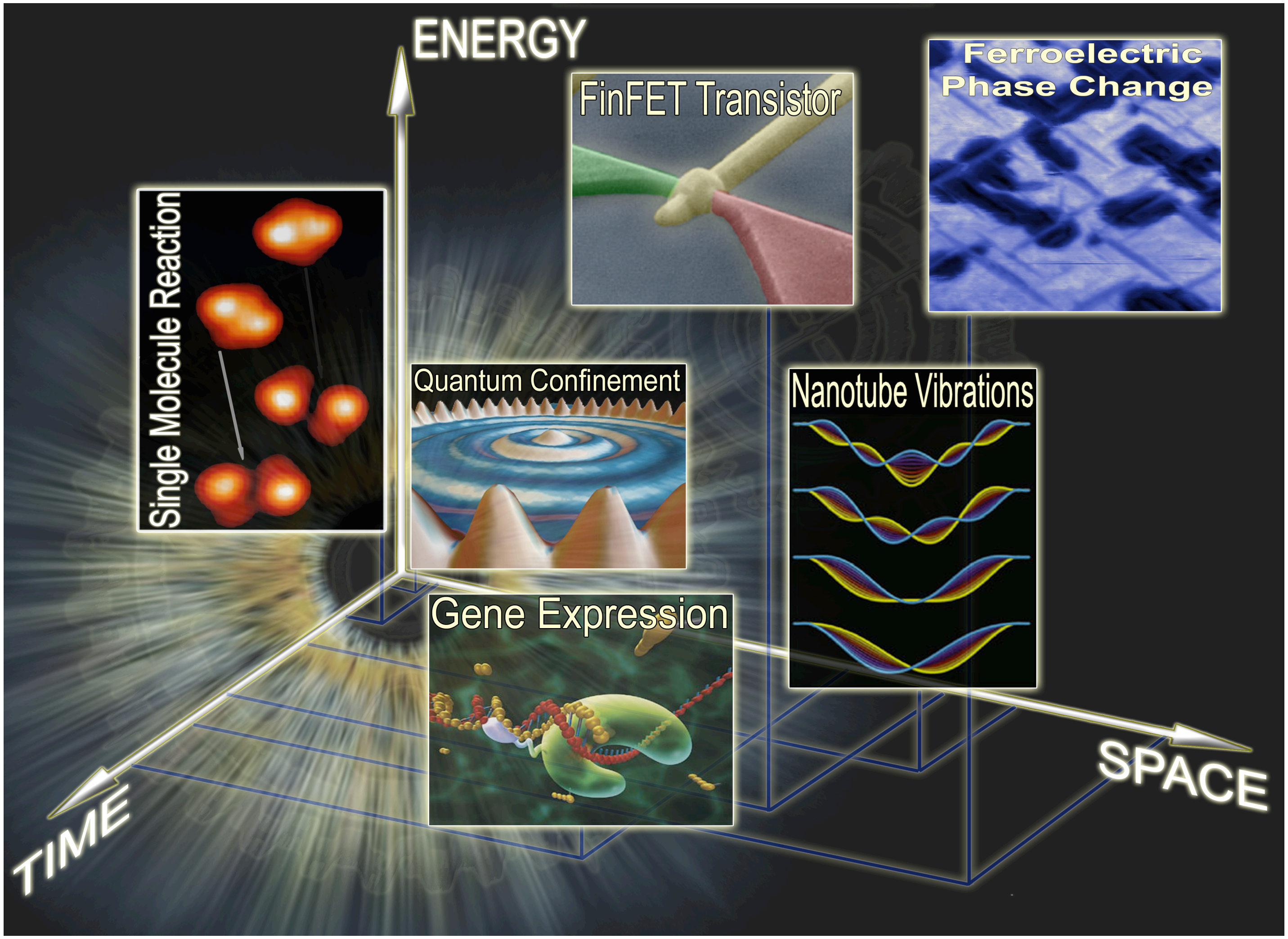
Roger Falcone

Physics Department, UC Berkeley
Advanced Light Source, LBNL

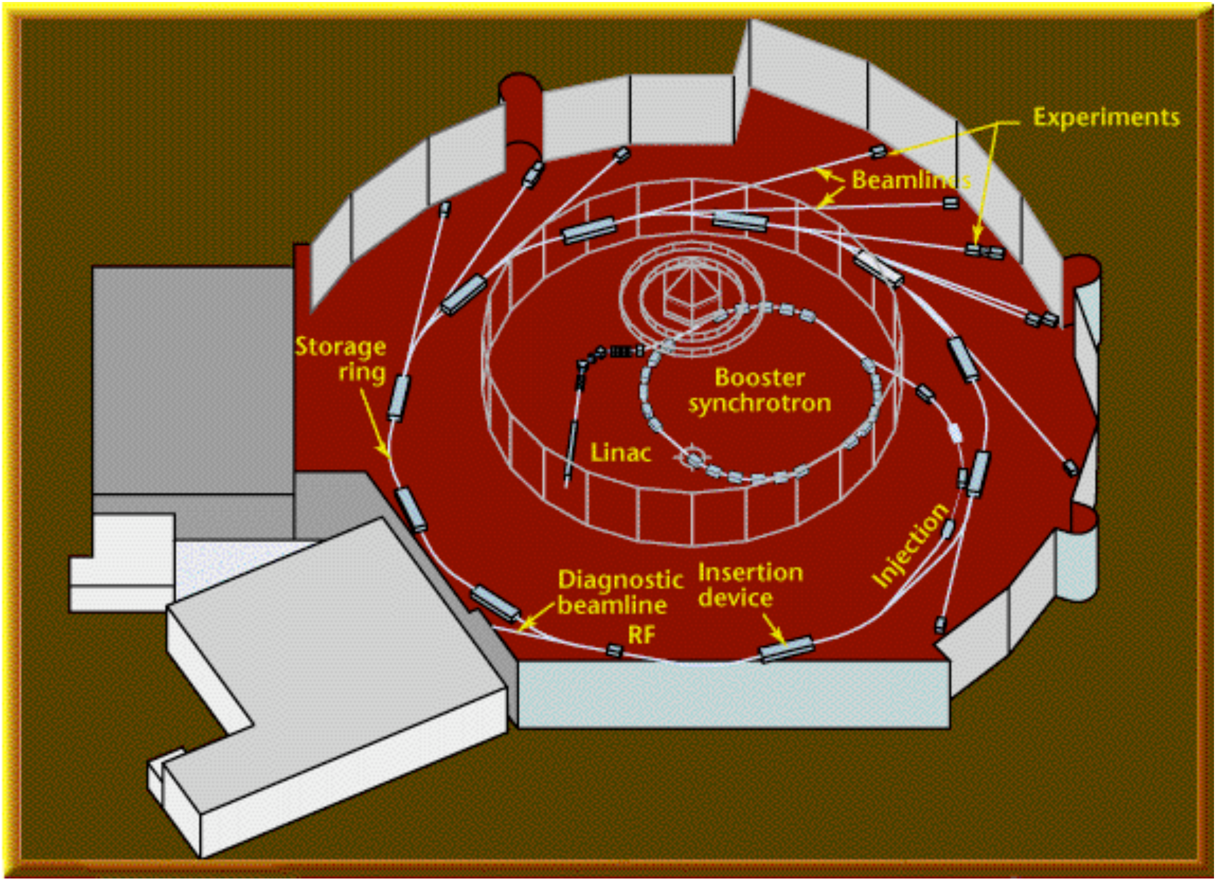
LBNL July 15, 2008

jc/ALSaerial/11-96

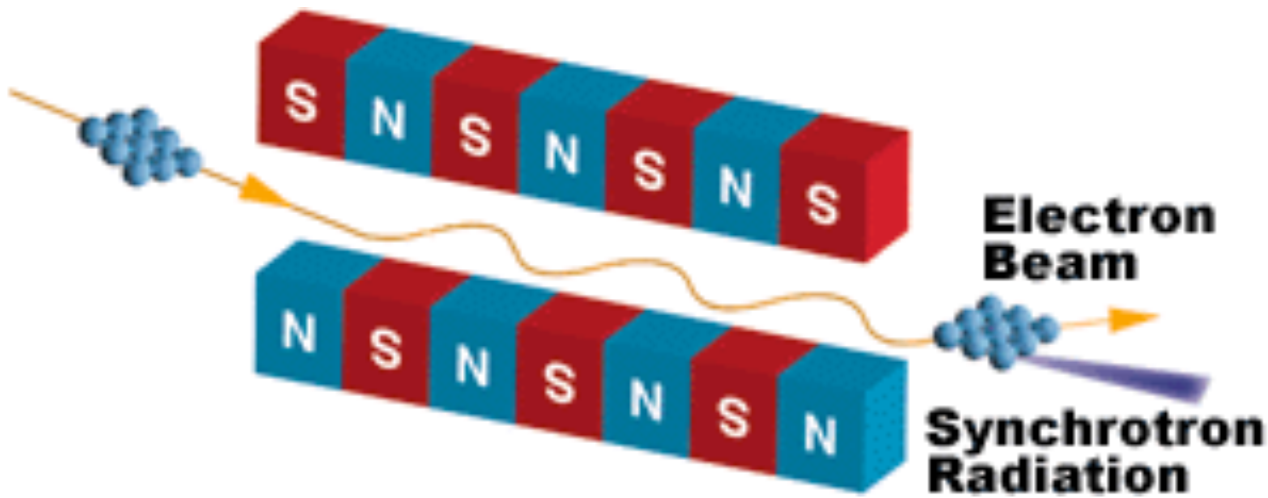



ENERGY
FinFET Transistor
Ferroelectric Phase Change
Single Molecule Reaction
Quantum Confinement
Nanotube Vibrations
Gene Expression
TIME
SPACE

Storage ring x-ray sources

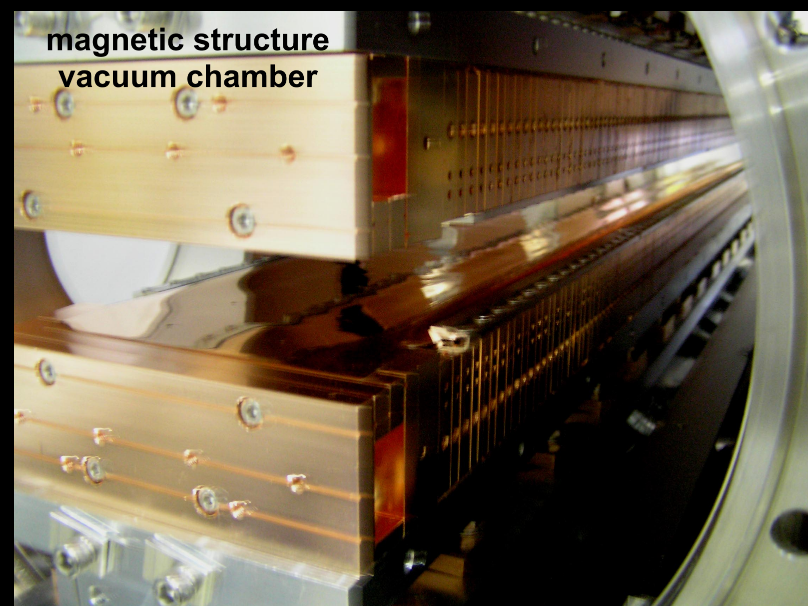


“synchrotron” x-ray pulses are produced by relativistic electron bunches in accelerators when the electrons pass through periodic magnetic fields

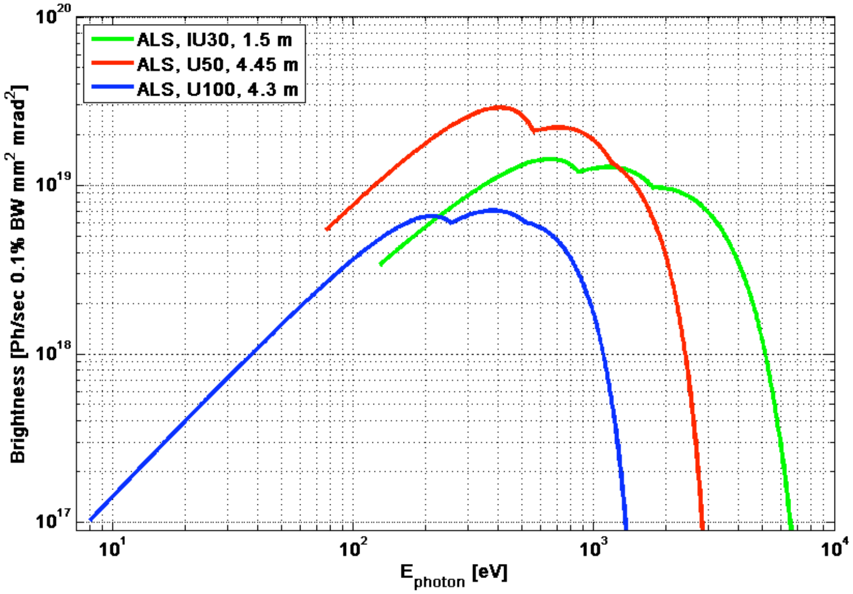


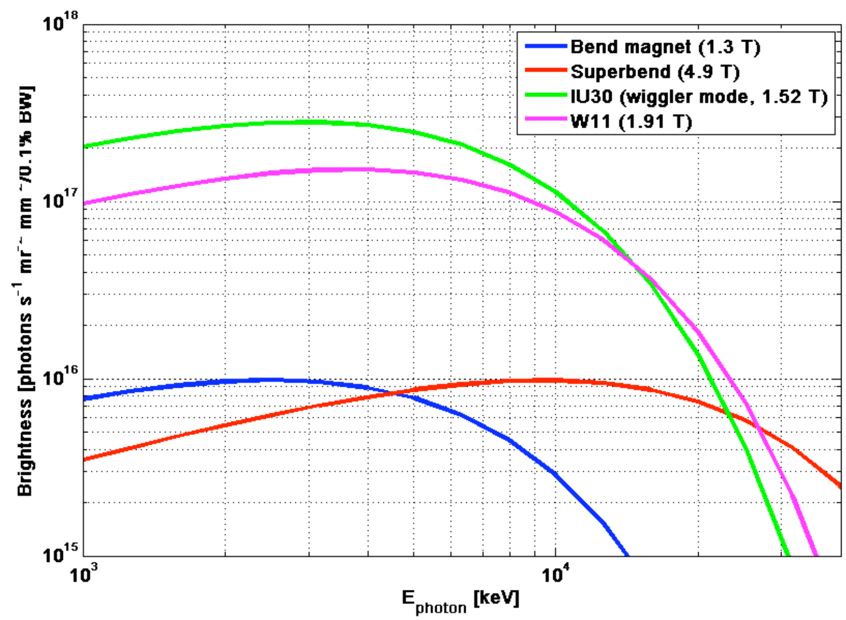
Undulator / Wiggler

Specifications	
Magnetic gap	5.5 mm
Period	30 mm
No. periods	50
Vacuum gap	>5 mm
B_o	1.45 T

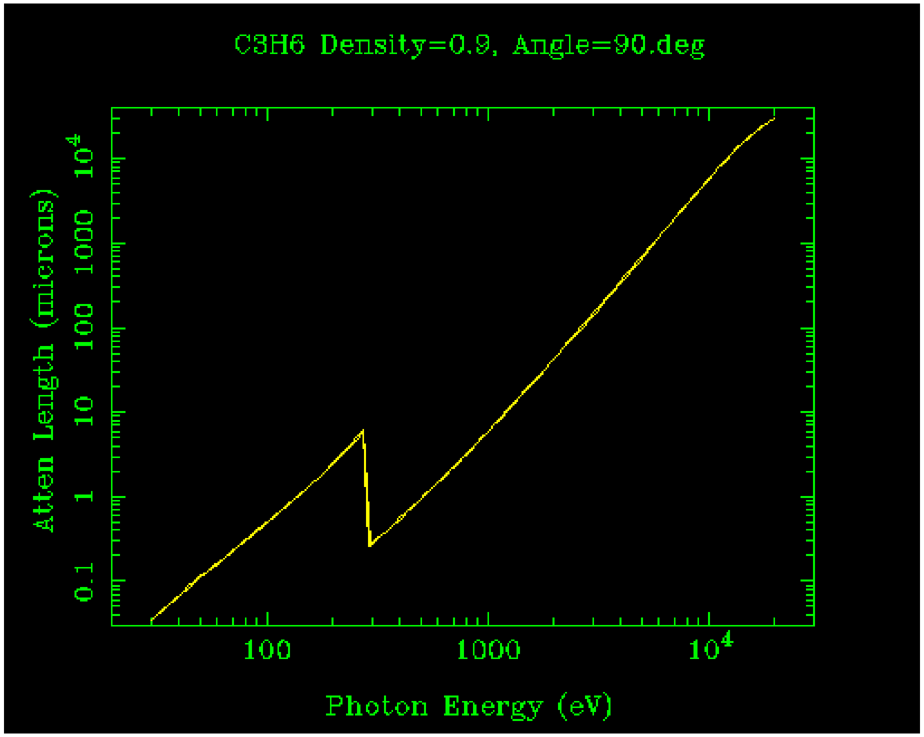


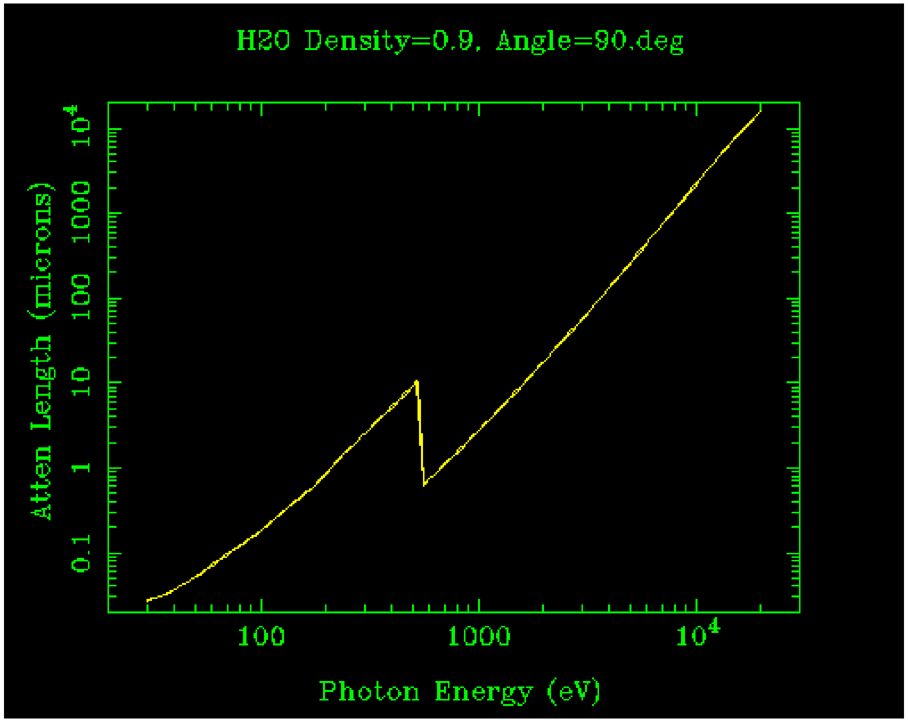
The ALS is a broad spectrum source



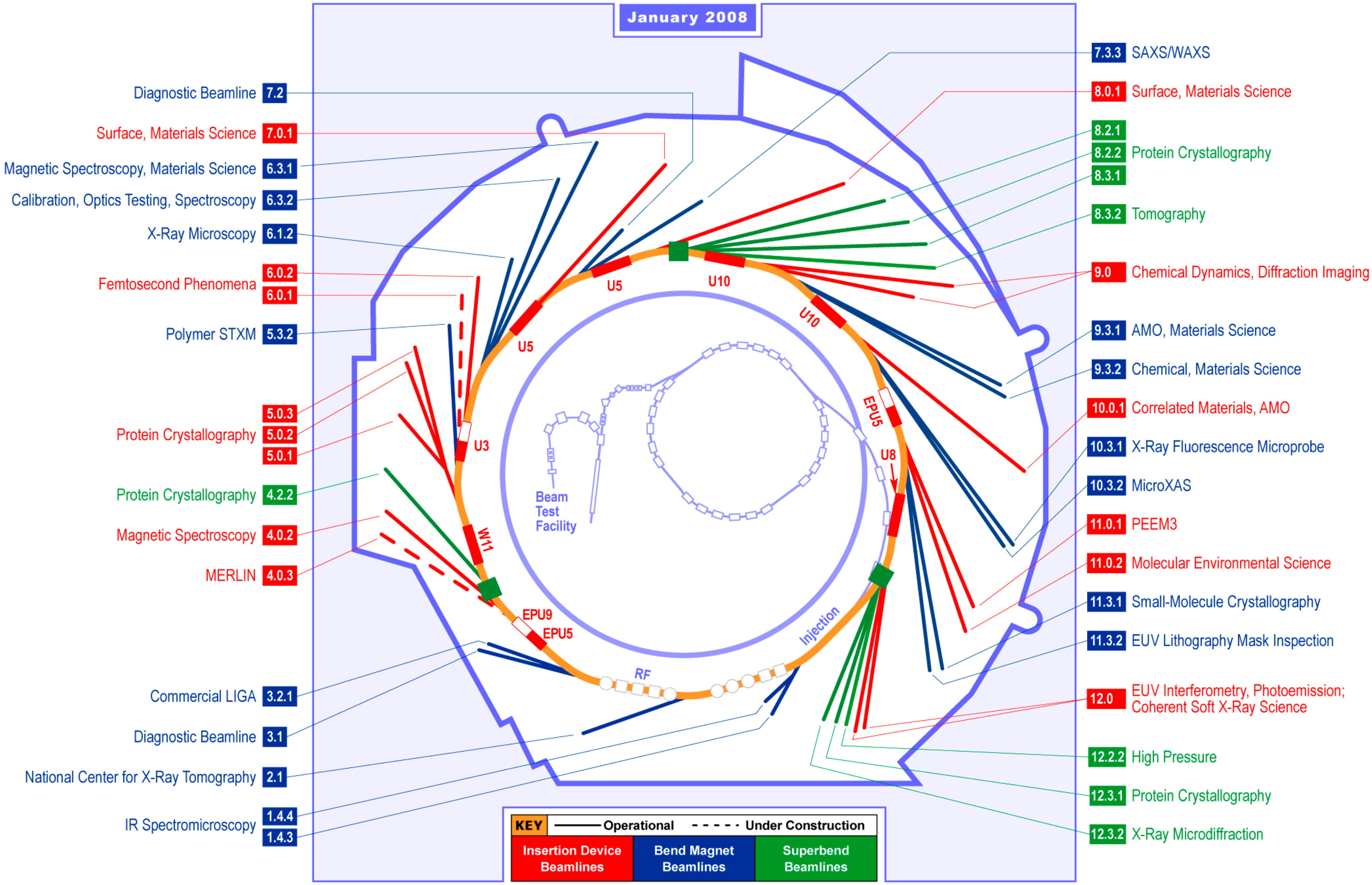


Material transmission limits on imaging





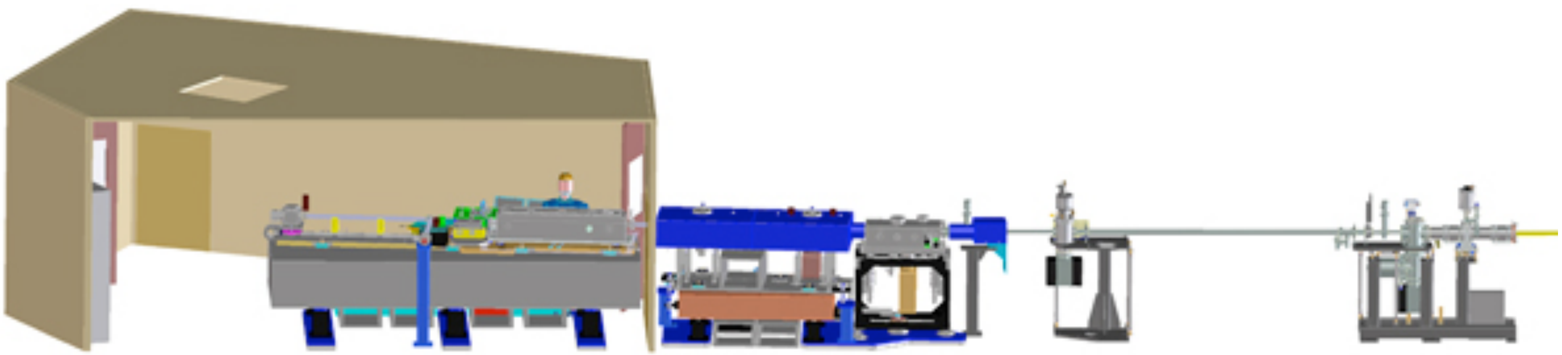
Beamlines at the ALS 2008



New biomedical imaging facility at the ALS

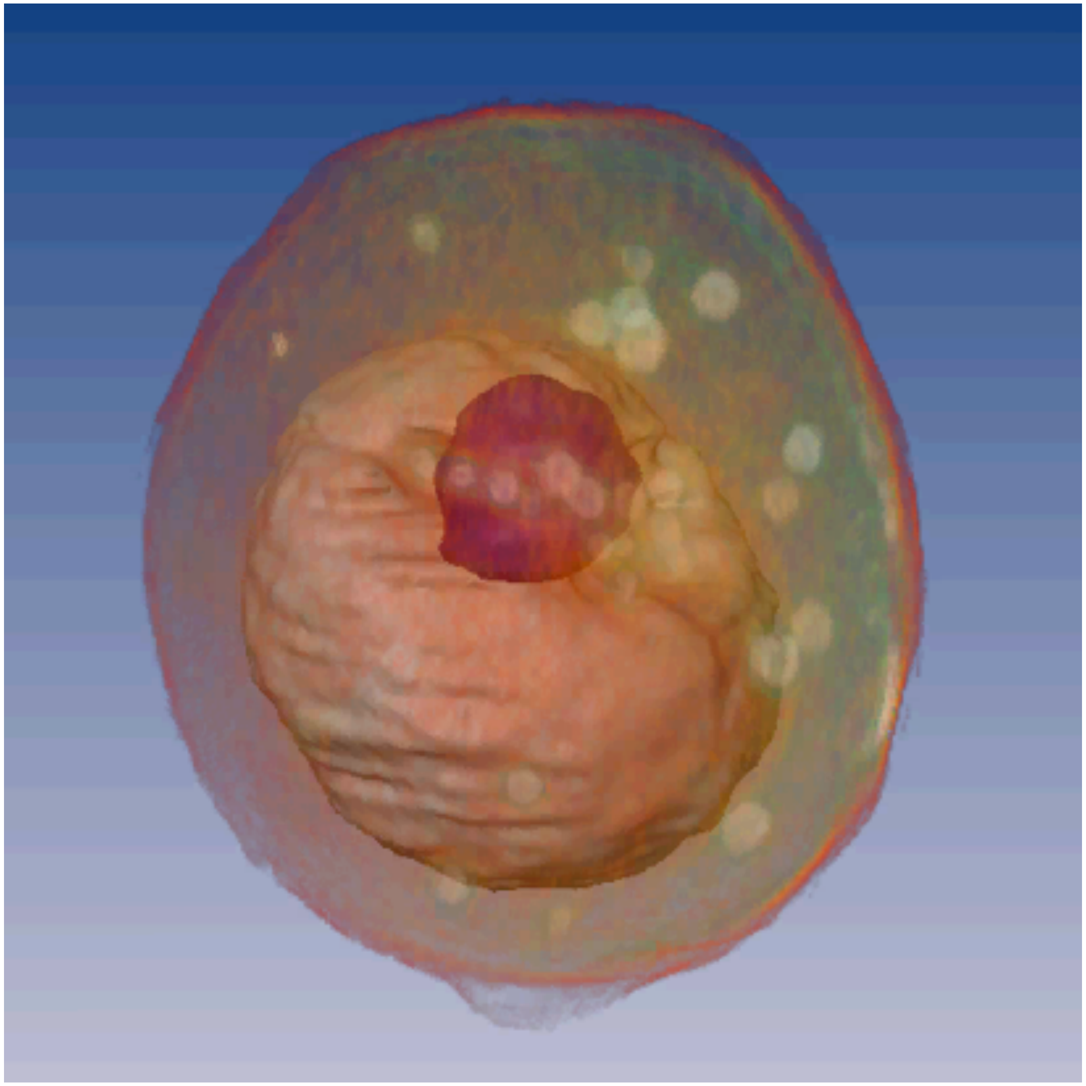
The National Center for X-Ray Tomography

Director: Carolyn Larabell (UCSF/LBNL)

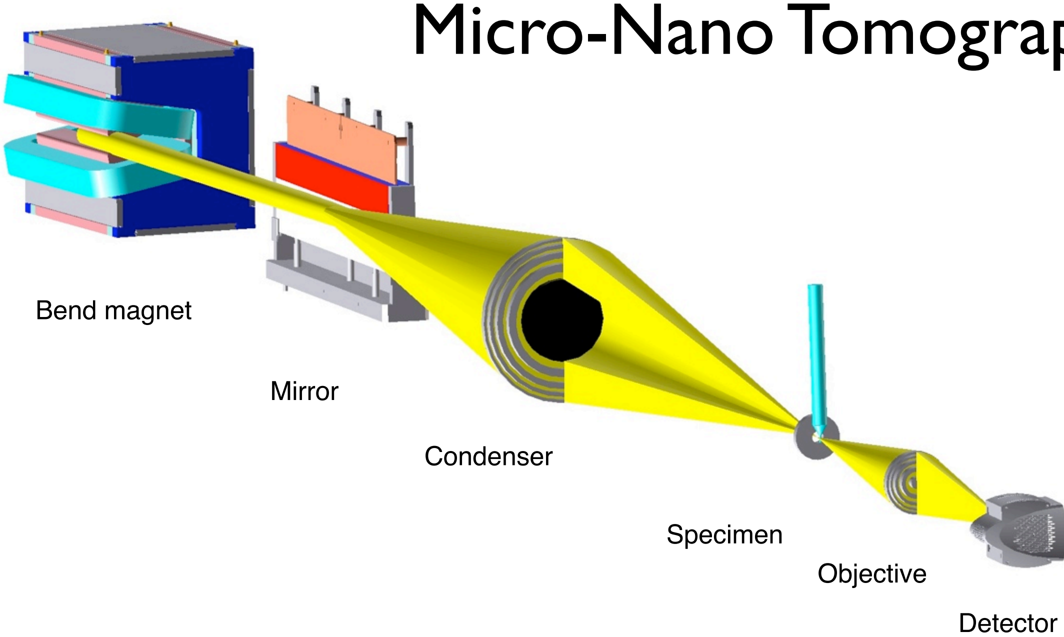


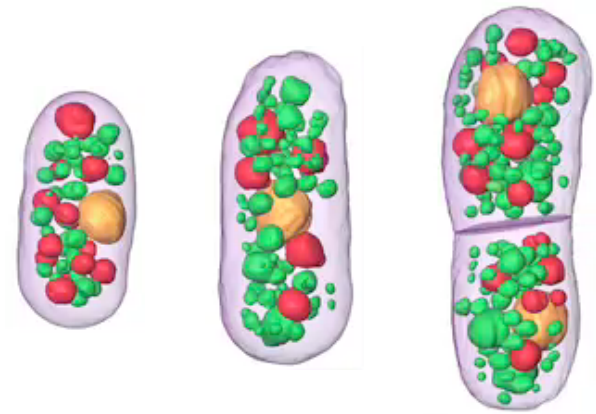
- Cellular imaging at the nanoscale
- Joint funding from DOE and NIH
- An NIH National Center for Research Resource

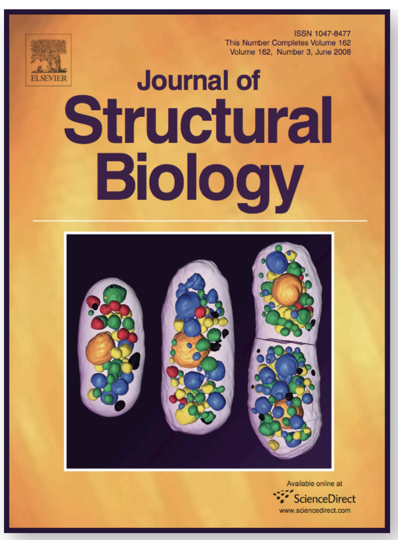
3-d x-ray tomography of a cell

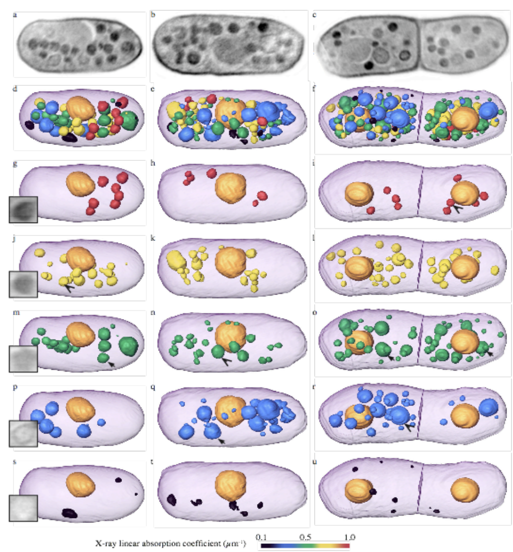


Micro-Nano Tomography / Radiography









Segmented using organelle appearance:

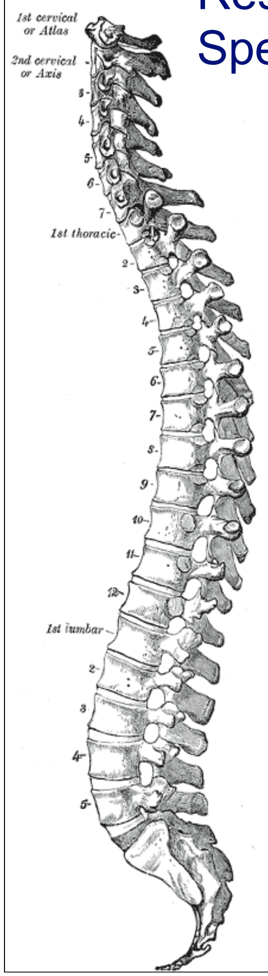
Mitochondria

Other organelles

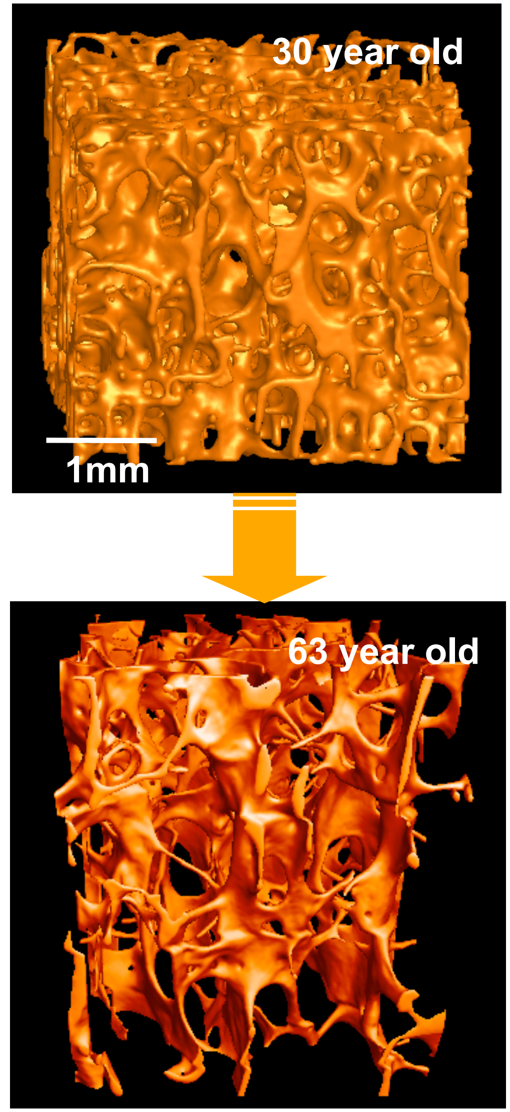
D.Y. Parkinson, G. McDermott, L.D. Etkin, M.A. Le Gros & C.A. Larabell (2008) J. Structural Biology 162:380-386.

Micro X-ray Tomography of Trabecular bone decay in vertebrae

Photon energy 10-40KeV
Full field imaging with scintillator and visible light magnification optics.
Resolution 3um (achievable 0.5um)
Specimen in natural condition



The internal structure of vertebra is Trabecular bone (spongy bone) – carries 90% of the force
Osteoporis is the weakening and collapse of this structure.



Osteoporosis studies

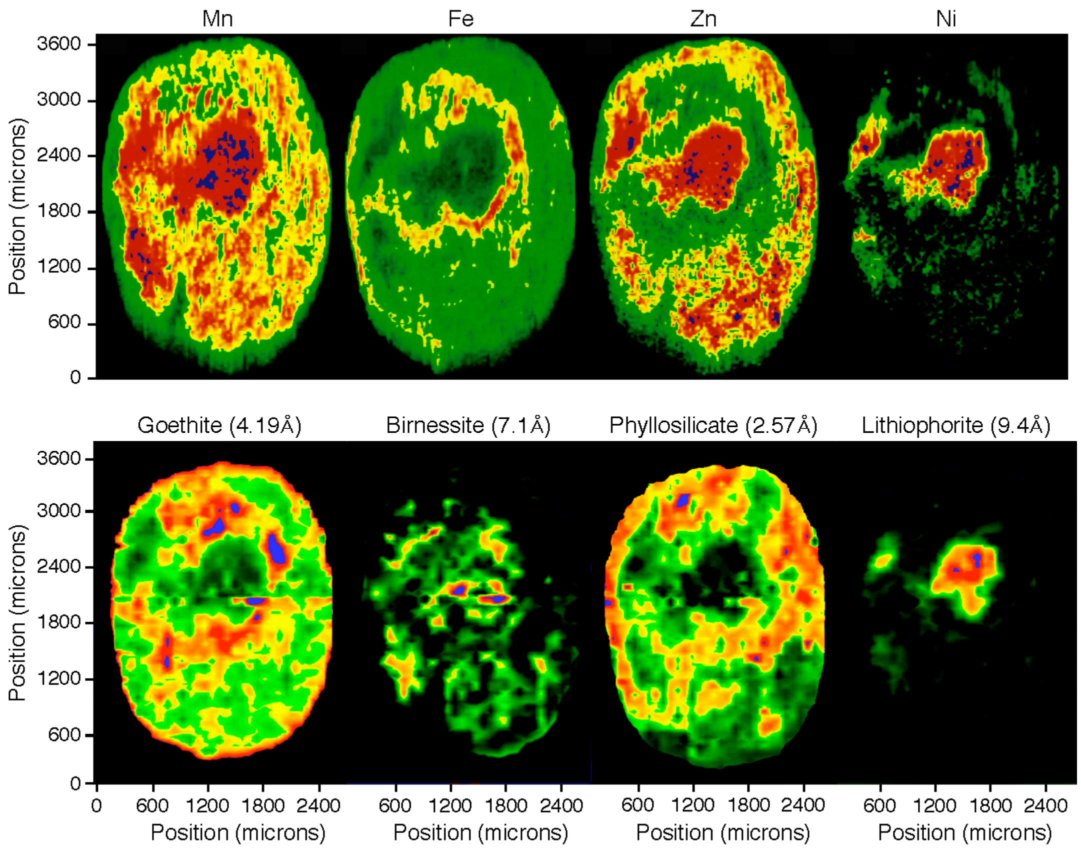
Osteoporosis is not entirely explained by loss of bone mass. Some people loose bone mass and do not gets fractures – others are the opposite.

Local architecture and local bone density tissue needs to be understood for accurate diagnosis of what is going on.

J.Kinney et al.Bone, **36**, 193-201 (2005)

TRACE METALS IN SOILS AND SEDIMENTS

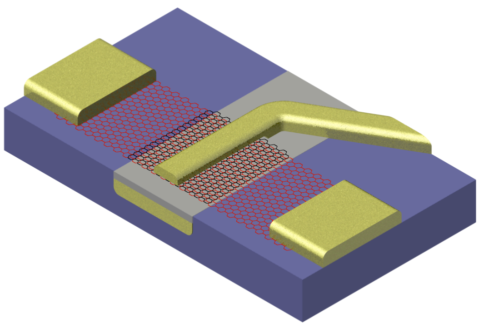
Three X-Ray Micro Techniques Focus on Nickel and Zinc Sequestration

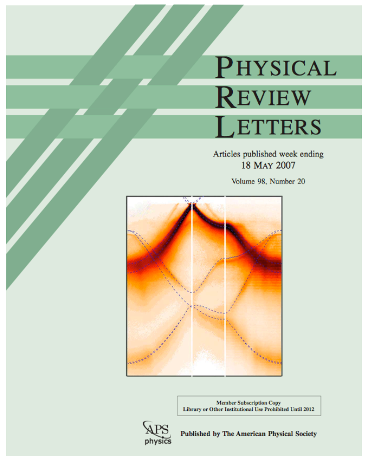


Combined μSXRF–μSXRD measurements recorded on a soil iron–manganese nodule. The four images on the top are elemental maps obtained by μSXRF, and the four images on the bottom are mineral species maps obtained by rastering the sample in an XY pattern and analyzing the diffraction patterns.

A. Manceau (Université Joseph Fourier and CNRS, France, and ALS); N. Tamura, M.A. Marcus, A.A. MacDowell, R.S. Celestre, R.E. Sublett, and H.A. Padmore (ALS); and G. Sposito (Berkeley Lab). [*American Mineralogist* **87**, 1494 (2002)]

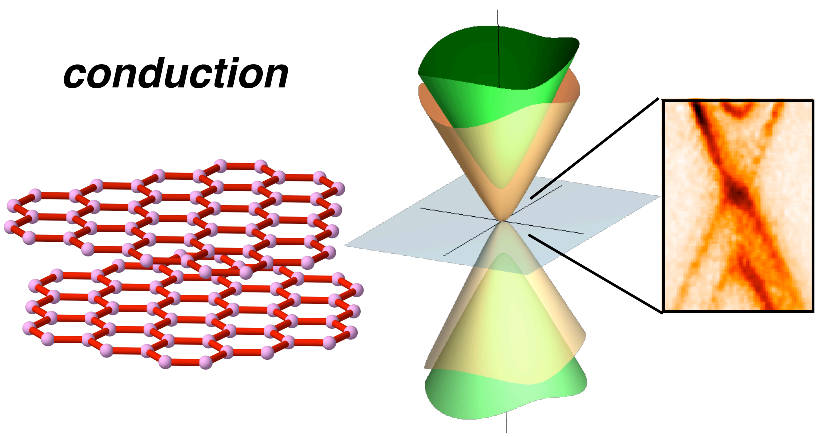
Graphene: a new material for high performance electronics- more tomorrow



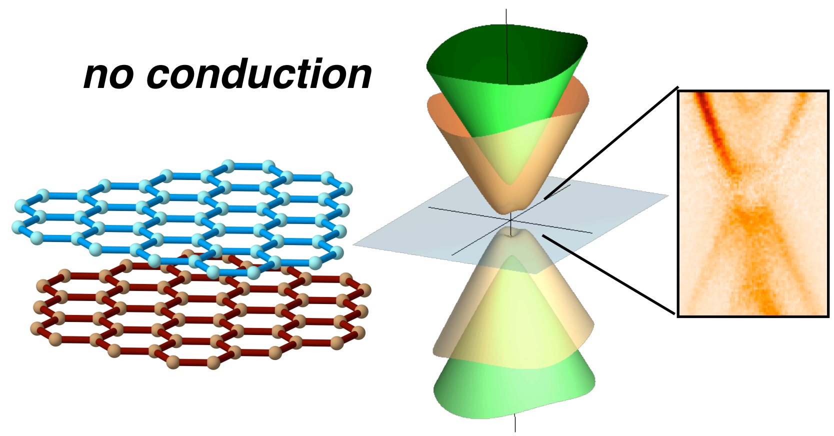


- Graphene, a single layer of carbon, is the building block of graphite, nanotubes, buckyballs.
- A bilayer of graphene can be a switch <1 nm thick for high current densities (~10^8 A/cm^2).
- Angle-resolved photoemission measurements validate this concept by demonstrating control over the current-carrying electronic states.

Unbiased



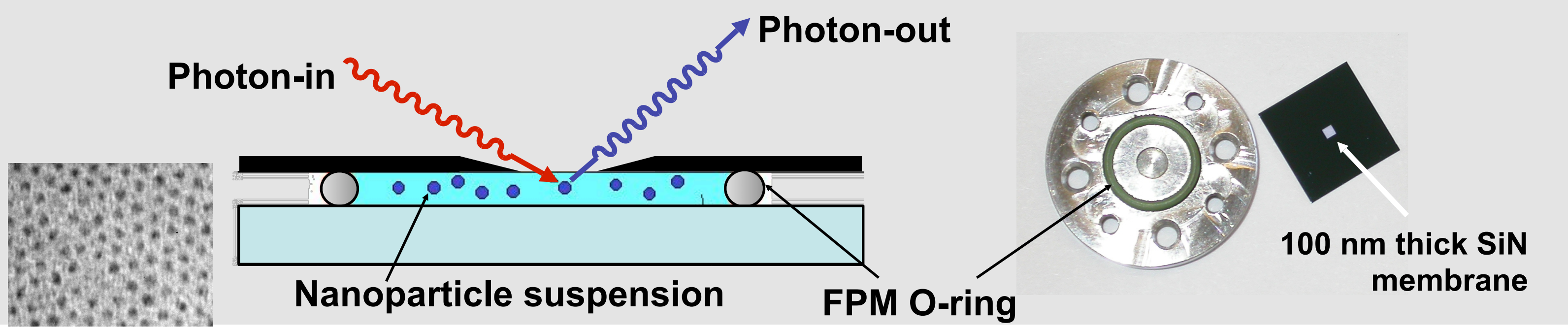
Biased

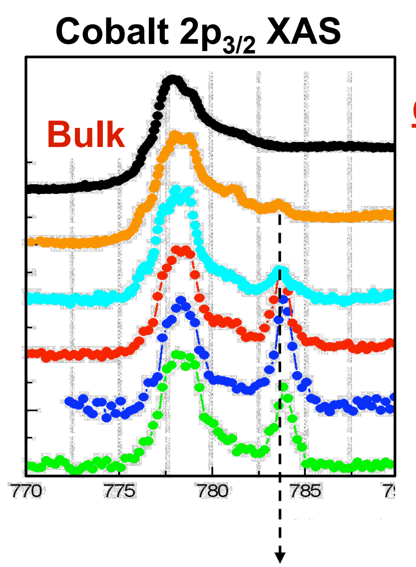


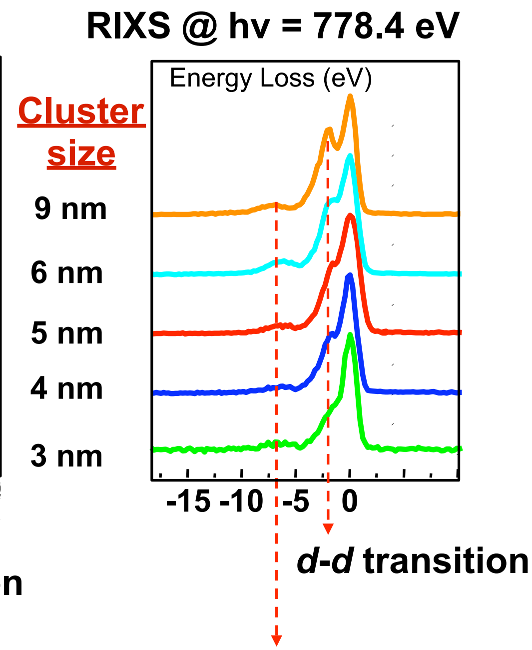
T. Ohta, A. Bostwick, Th. Seyller, K. Horn, E. Rotenberg, Science, 2006. 313: p. 951-954.

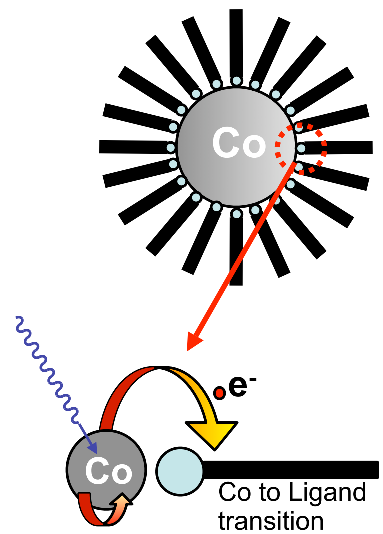
Size Dependent Electronic Structure of Co Nanoparticles with Ligand Molecules

Cell for photon-in/photon-out studies of clusters in gas or liquid environments





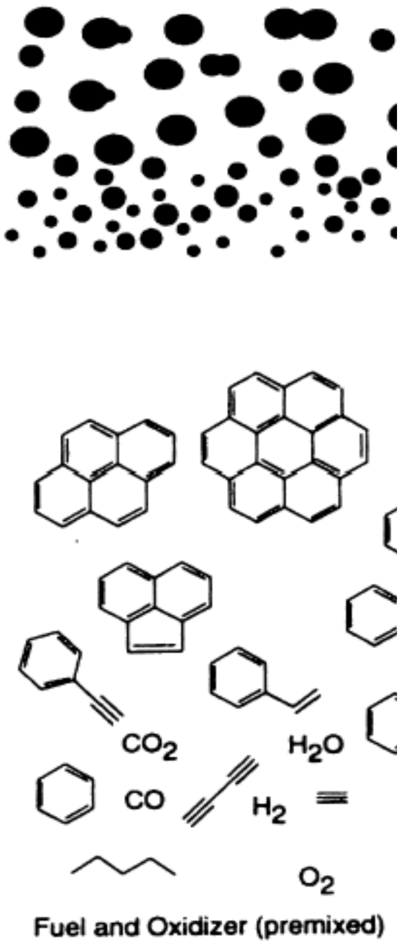


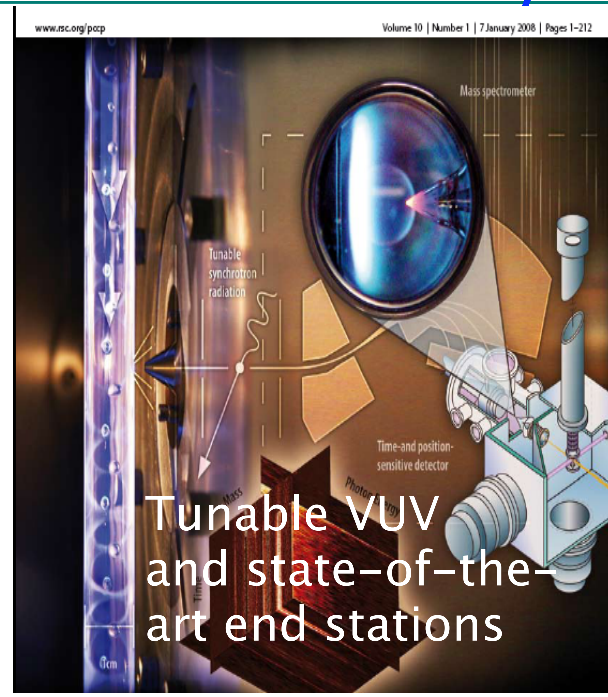


Nano Letters 7, 1919 (2007)

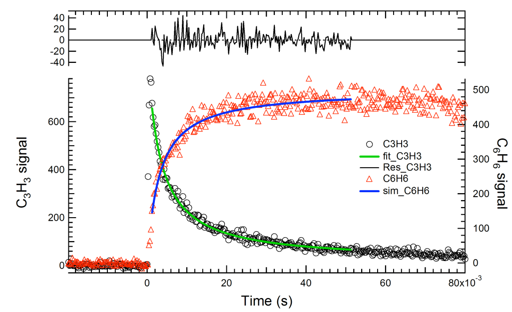
P. Alivisatos & M. Salmeron (MF)
J. Guo (BL7, ALS)

Combustion Chemistry at the Chemical Dynamics Beamline

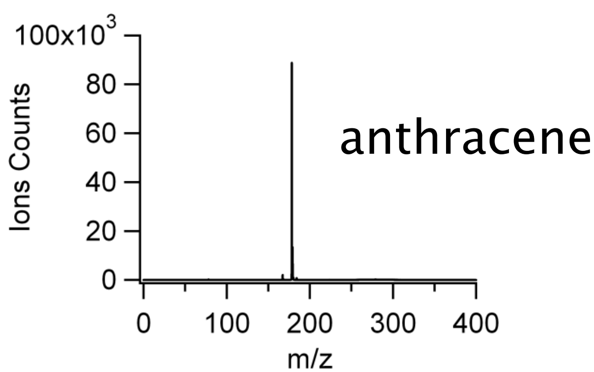




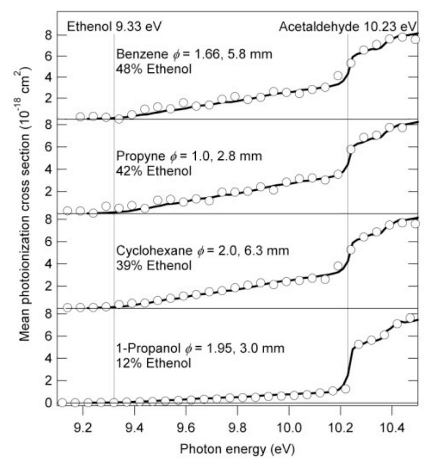
$C_3H_3 + C_3H_3 \rightarrow C_6H_6$



Multiplexing and universal detection



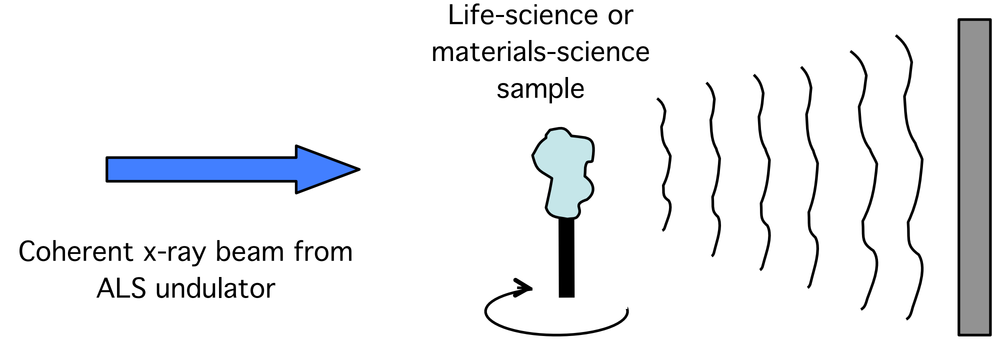
Fragment free mass spectrometry



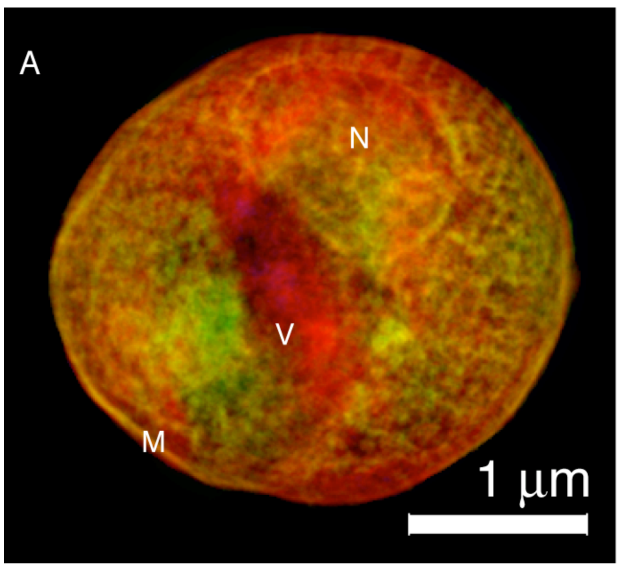
Enol formation in flames

Isomer selectivity

Diffraction Microscopy at Beamline 9.0.1

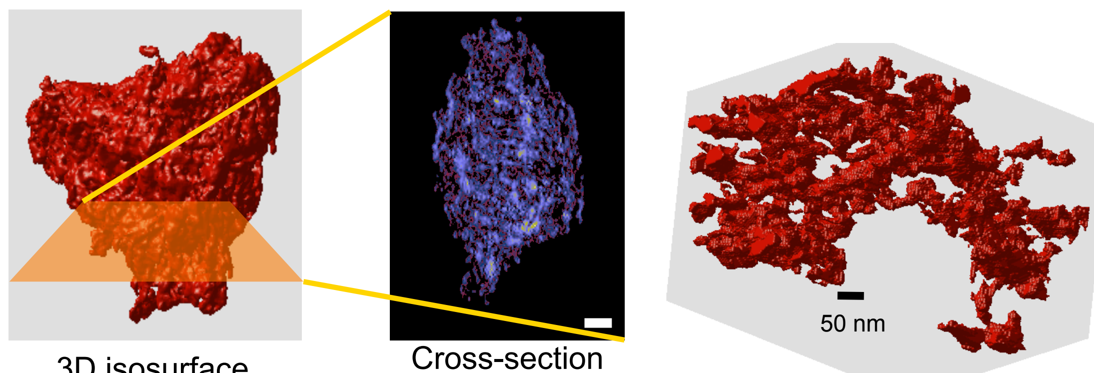


Freeze dried yeast cell



D. Shapiro et al, PNAS 2005

Tantalum oxide foam



3D isosurface

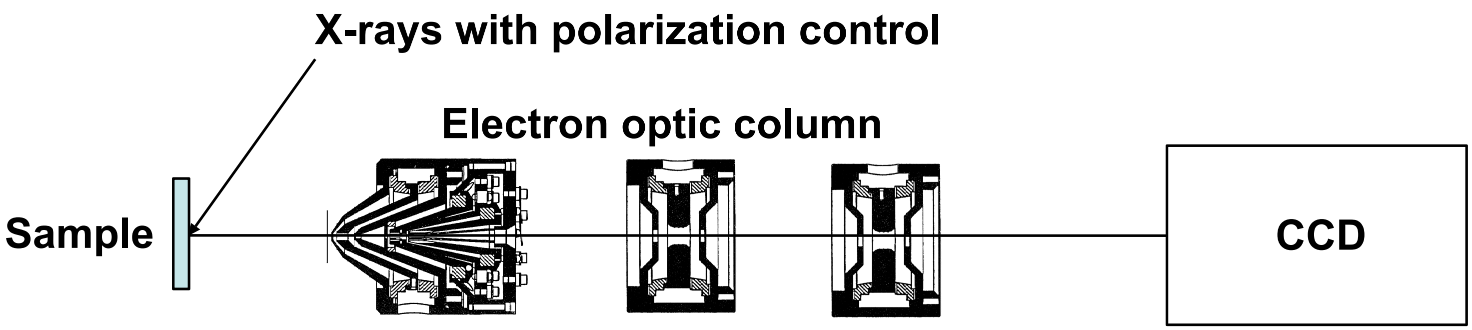
Cross-section (bar = 200nm)

Res’n 20-30 nm

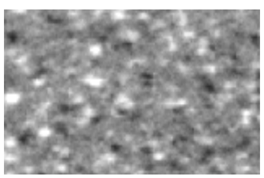
H. Chapman, M. Howells, A. Barty, S. Marchesini

Photoemission Electron Microscopy **PEEM**

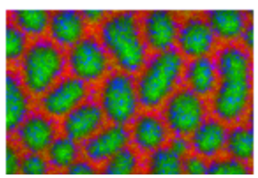
ALS PEEM allows measurements of composition, chemistry, and magnetic properties of surfaces and thin films at nanometer spatial and picosecond temporal resolution.



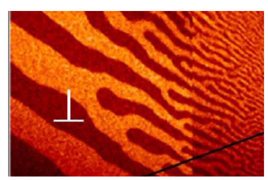
Examples



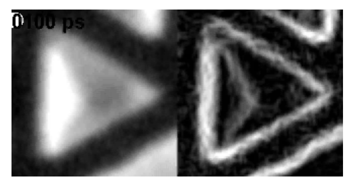
Sub 100 nm size magnetic pillars in a ferroelectric matrix
T. Zhao et al., Appl. Phys. Lett. 90, 123104 (2007)



Protein adsorption on two segregated polymers
C. Morin et al., JES&RP 137-140, 785 (2004).



Magnetic phase transition in Fe
Y. Wu et al., Phys. Rev. Lett. 93, 117205 (2004)

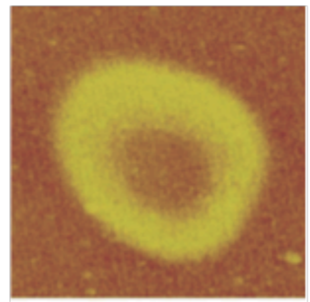


Vortex dynamics
S.B. Choe et al., ALS, Science 304, 420 (2004)

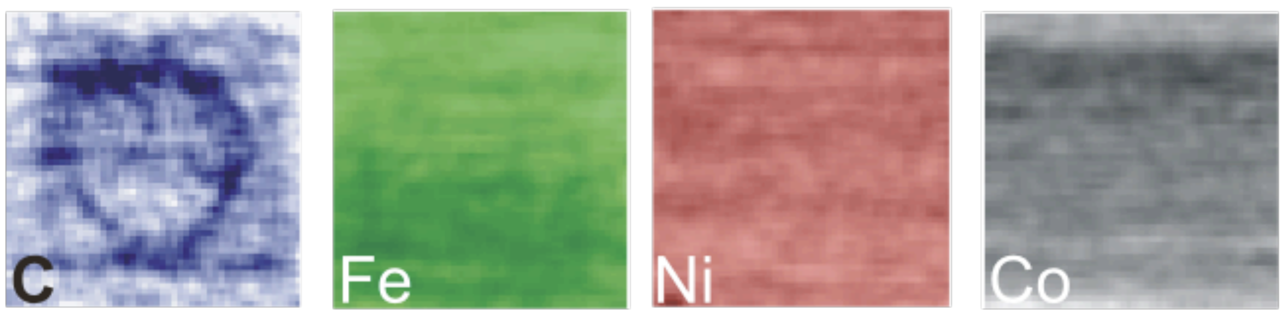
Magnetic XMCD STXM at 11.0.2

Reveals That ONLY Carbon is Magnetic

The area around the proton beam impact shows a magnetic signal in the AFM



AFM image -Field of view~4μm



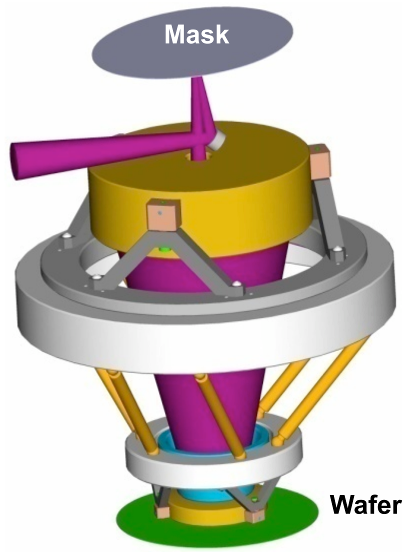
Element specific magnetic STXM images of the identical area

STXM images at BL11.0.2 reveals the “magnetic ring” is caused by long range magnetic order of carbon atoms only

H. Ohldag, T. Tyliszczak, R. Höhne, D. Spemann, et al, PRL 98, 187204 (2007)

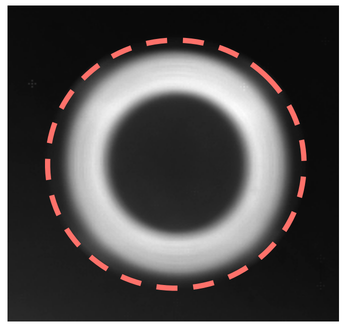
Center for X-Ray Optics: EUV Lithography

Two-bounce, 0.3 NA, MET at ALS Beamline 12.0



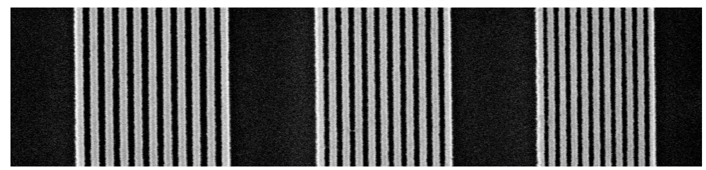
Patrick Naulleau, CXRO/MSD

Programmable illumination

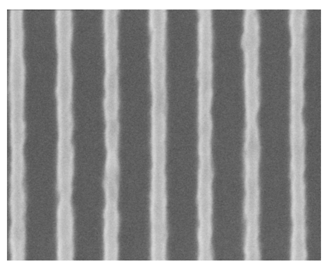


Addressing critical EUV lithography issues for Sematech at the ALS: testing state-of-the-art EUV resists

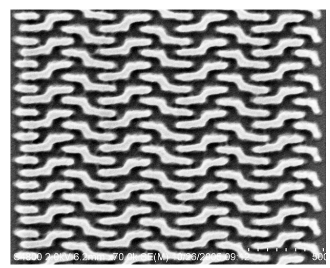
45 nm **40 nm** **35 nm**



27 nm



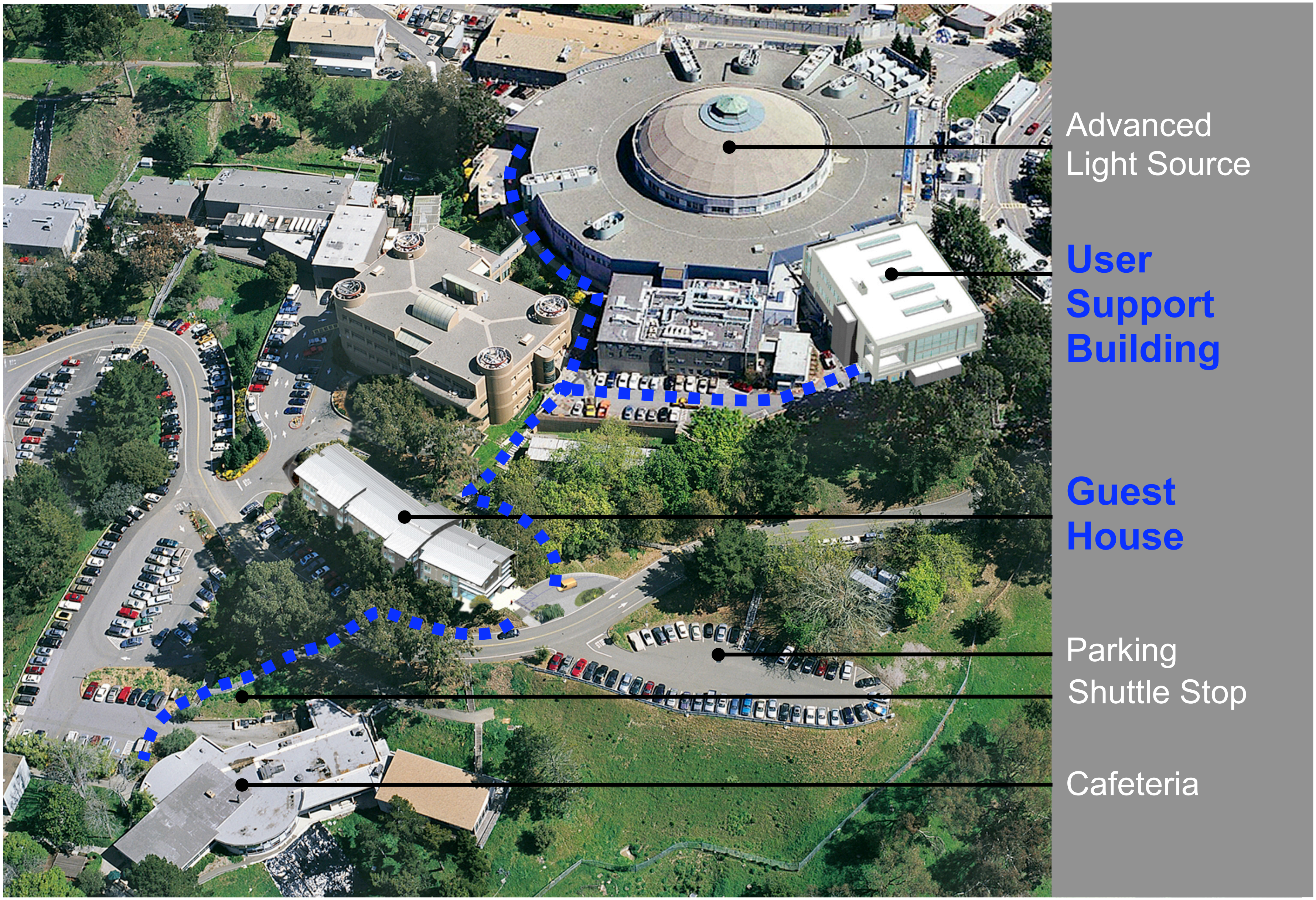
35 nm



Significant issue for EUV lithography

When will EUV resists be available with combined high spatial resolution (20 nm), high sensitivity (10 mj/cm^2), and low line edge roughness (LER, 1.2 nm)?

Major support and collaborators include Sematech, Intel, AMD, IBM, Samsung and others



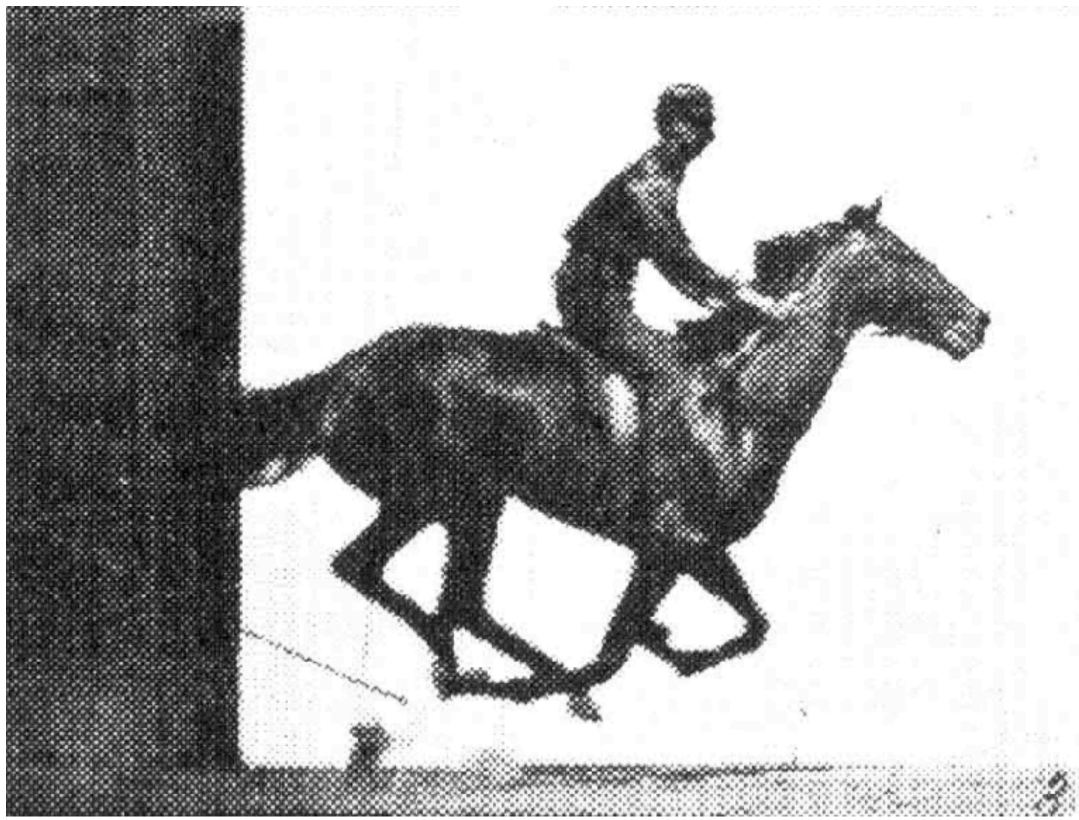
Advanced Light Source
User Support Building
Guest House
Parking
Shuttle Stop
Cafeteria

Berkeley Lab Guest House

E. Muybridge

Muybridge's "ultrafast" movie using spark photography Stanford University, 1878

L. Stanford

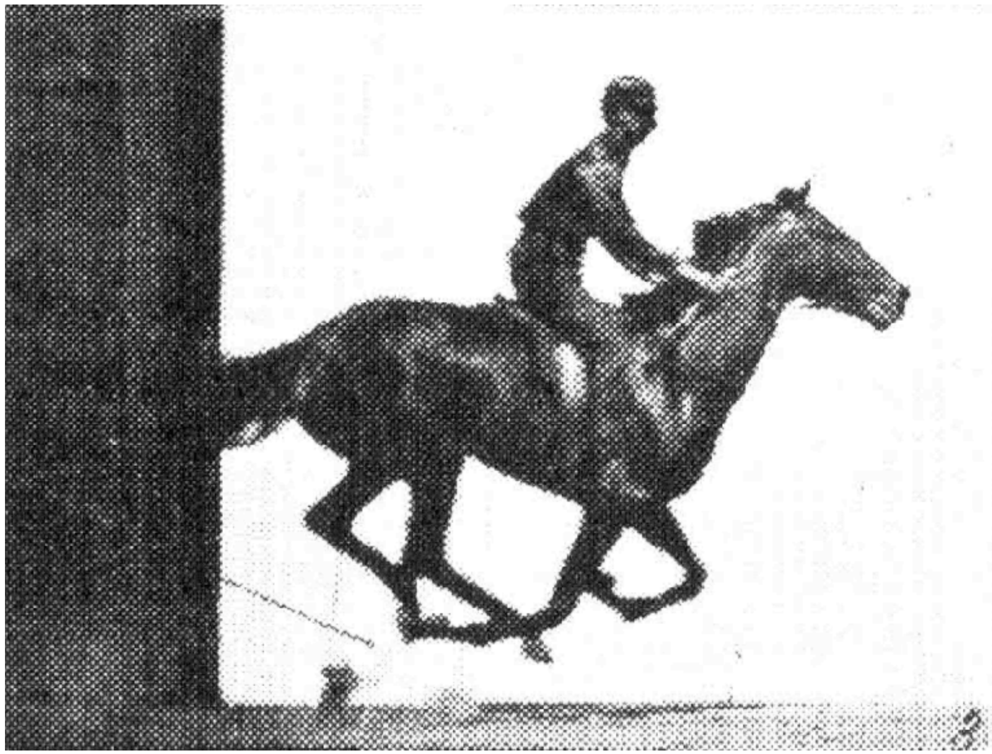


E. Muybridge, *Animals in Motion*, ed. by L. S. Brown (Dover Pub. Co., New York 1957).

E. Muybridge

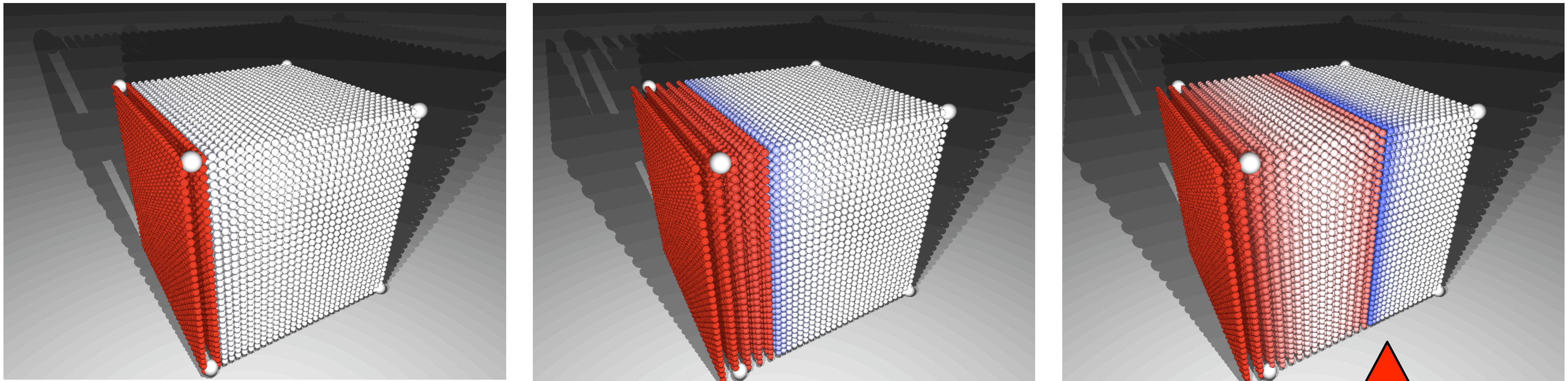
Muybridge's "ultrafast" movie using spark photography Stanford University, 1878

L. Stanford



To see atomic motion, we need to shorten the wavelength by 10^4 and the time scale by 10^{13}

Absorbed energy
generates "coherent" atomic motion in solids



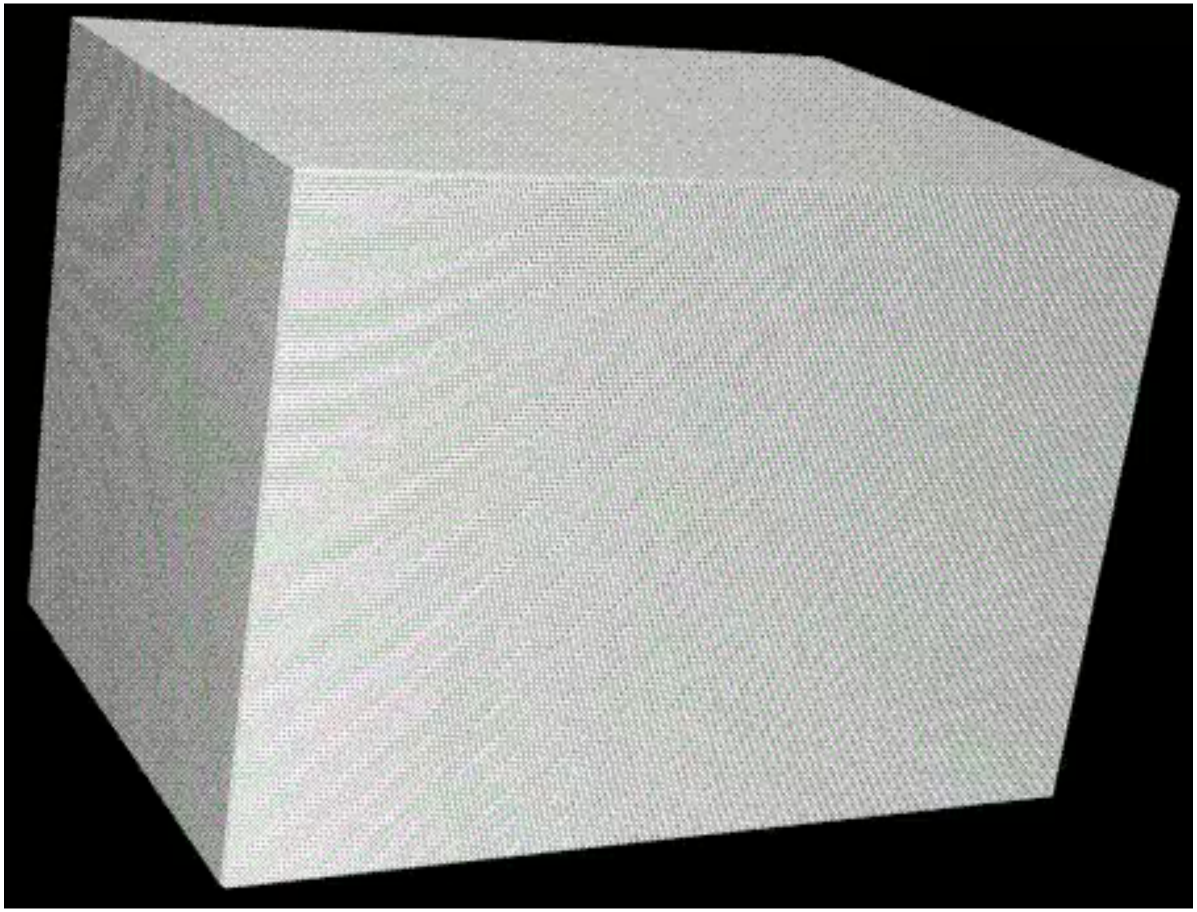
Fast heating at constant Volume — *Surface expansion* — *Newton's 3rd Law*

Stress → **Strain** → **Acoustic Pulse**

Phys Rev. B 34, 4129 (1986)

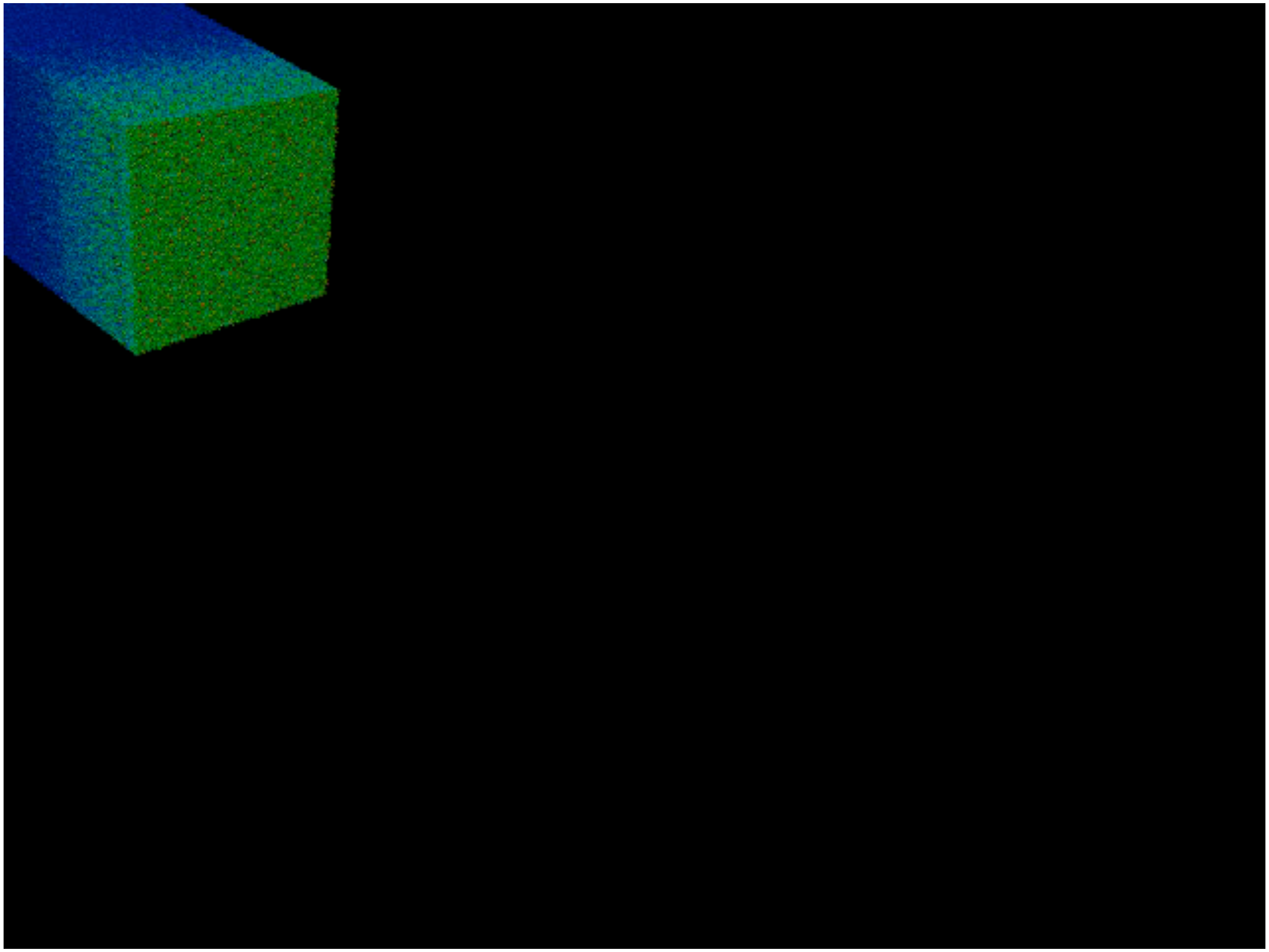
Molecular Dynamics simulations indicates shock-driven phase transitions take ~ 1 ps

Grey = static BCC Blue = compressed BCC Red = HCP



- 8 million atoms, total run time 10 ps (K. Kadau LANL)
- Require LCLS to time-resolve kinetics of the transition

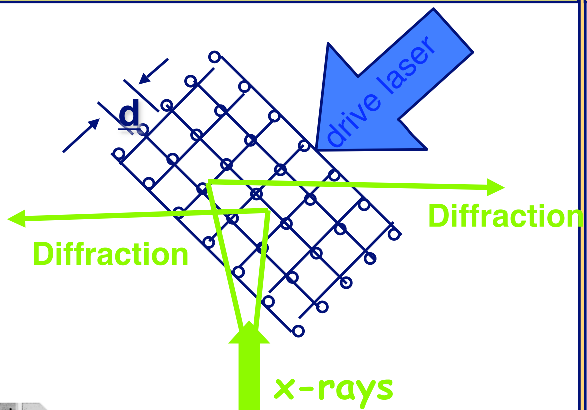
Ablation of a surface under high energy flux

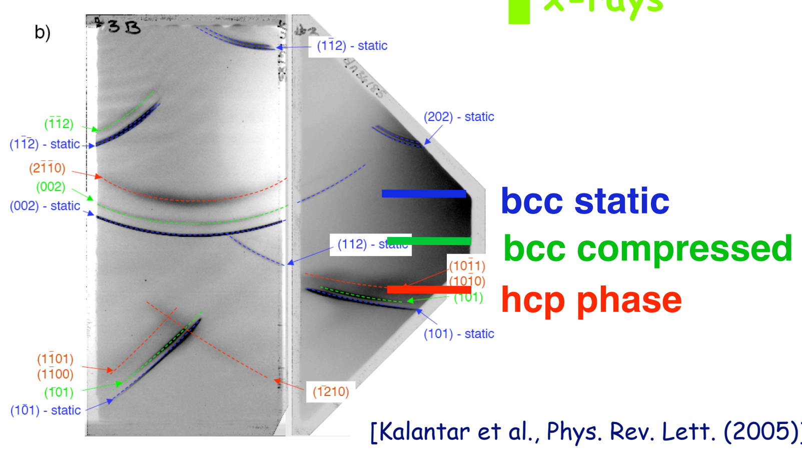


Intense x-ray fluxes from x-ray sources will enable real-time, in-situ measurements of microstructure evolution at high pressure

What is the timescale of the bcc-hcp phase transformation in Fe?

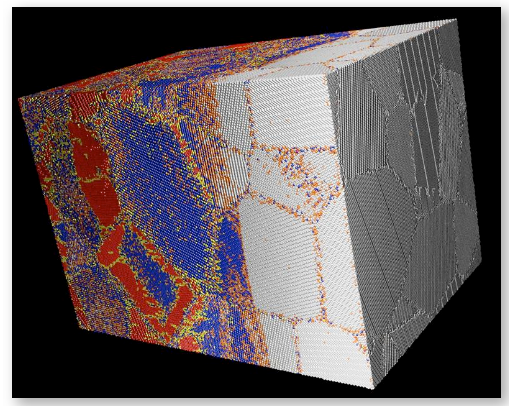
Current measurement limited to timescales >> psec



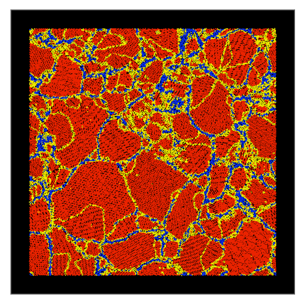


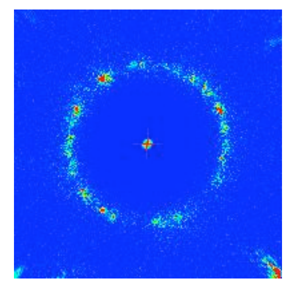
[Kalantar et al., Phys. Rev. Lett. (2005)]

Simulations predict subpicosecond phenomena observable using LCLS



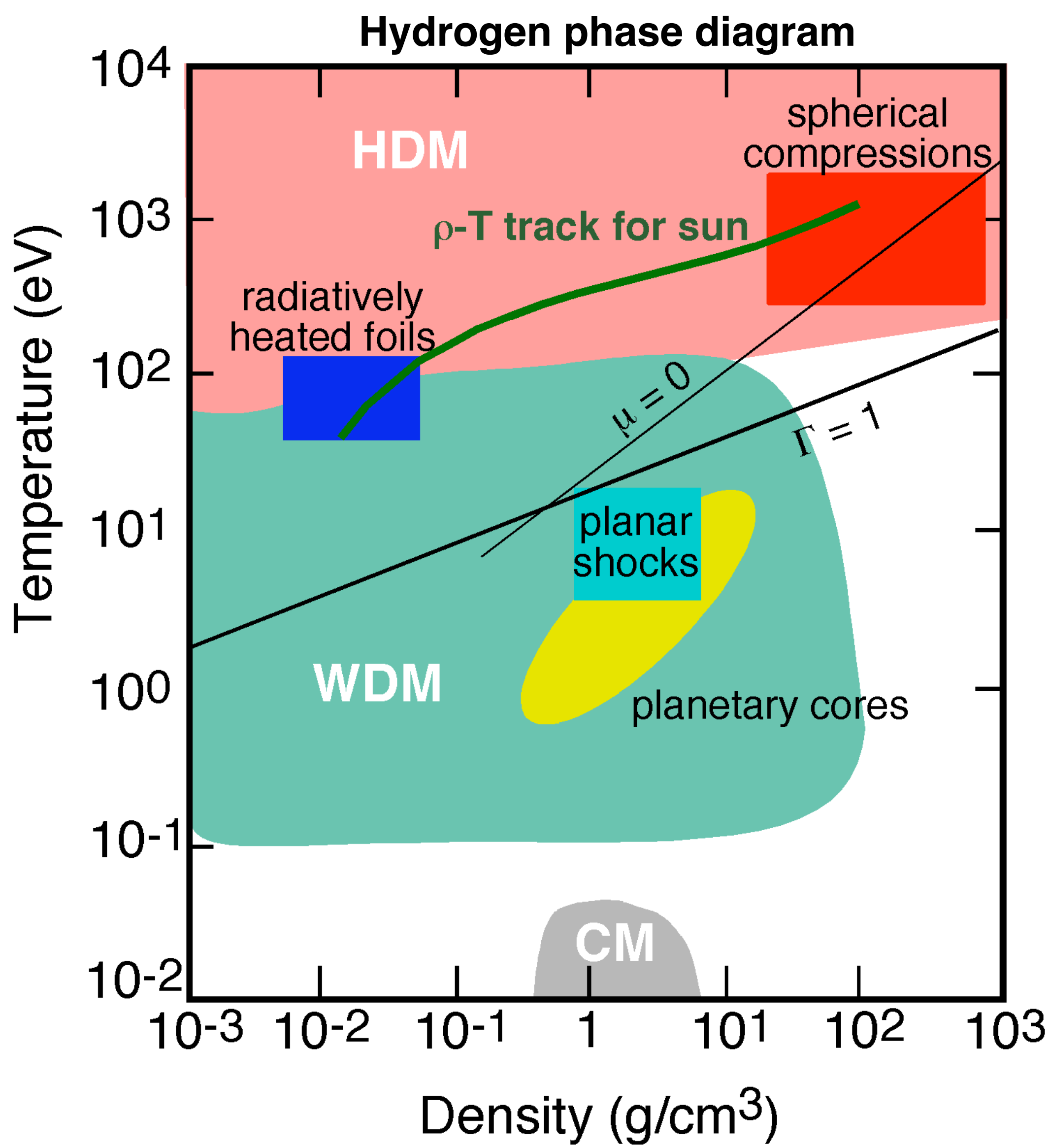
Kadau et al., Science (2002).



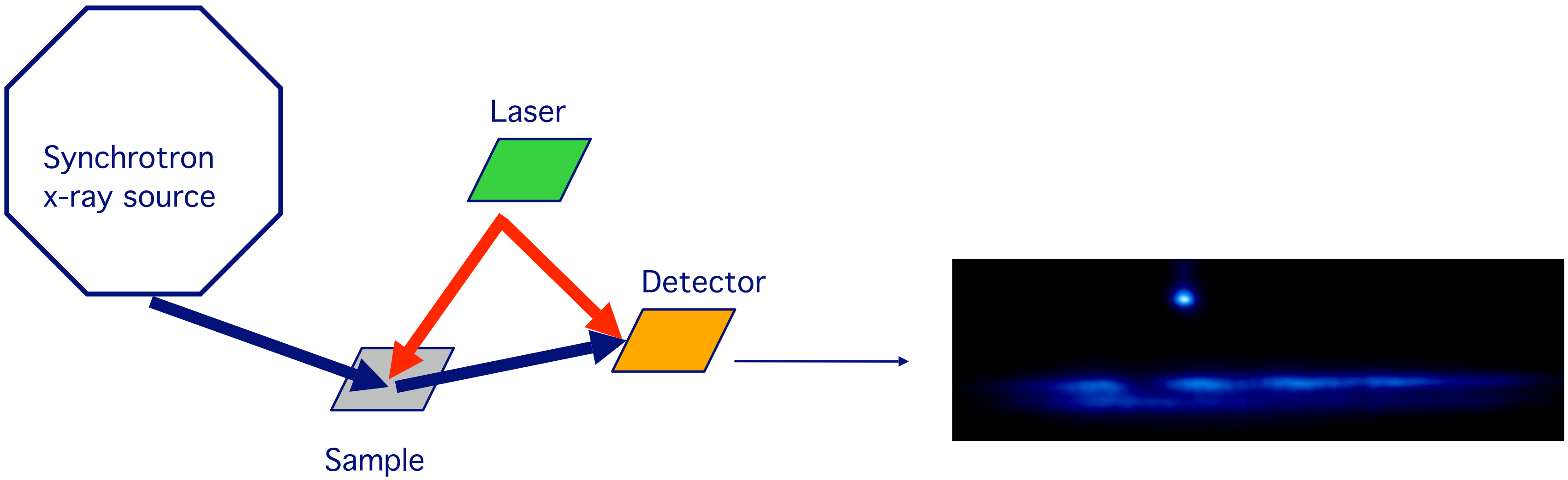


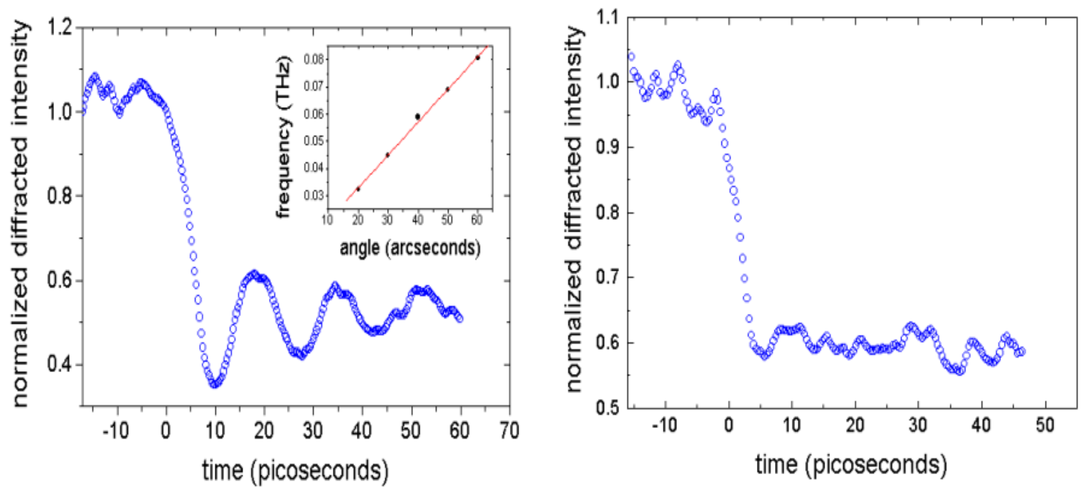
High Energy Density Matter
is interesting because it occurs widely

- **Hot Dense Matter (HDM) occurs in:**
  - Supernova, stellar interiors, accretion disks
  - Plasma devices: laser produced plasmas, Z-pinches
  - Directly and indirectly driven inertial fusion experiments
- **Warm Dense Matter (WDM) occurs in:**
  - Cores of large planets
  - X-ray driven inertial fusion experiments



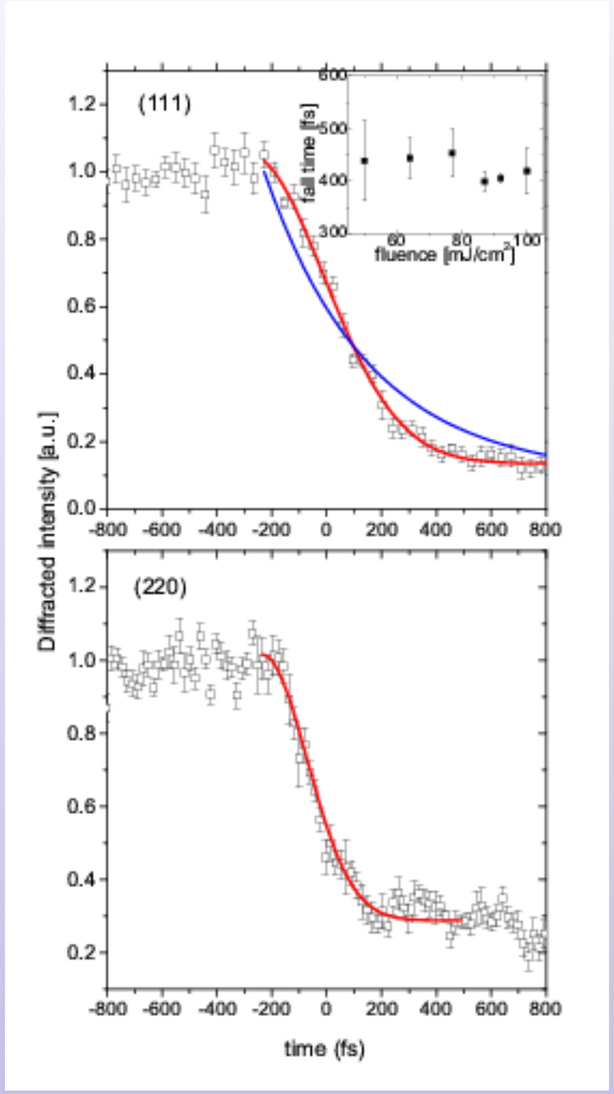
Laser-generated strain, bond-breaking, and hot electron-phonon coupling can initiate a solid-to-liquid phase transition which can be probed by ultrafast x-ray scattering





Lindenberg et al., Phys Rev. Lett. 84, 111 (2000)

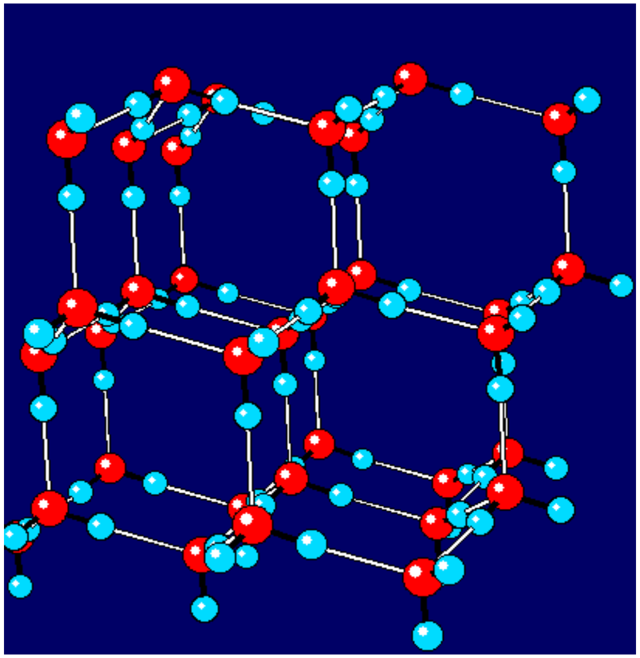
Observation of disordering of an atomic lattice indicates bond-breaking processes



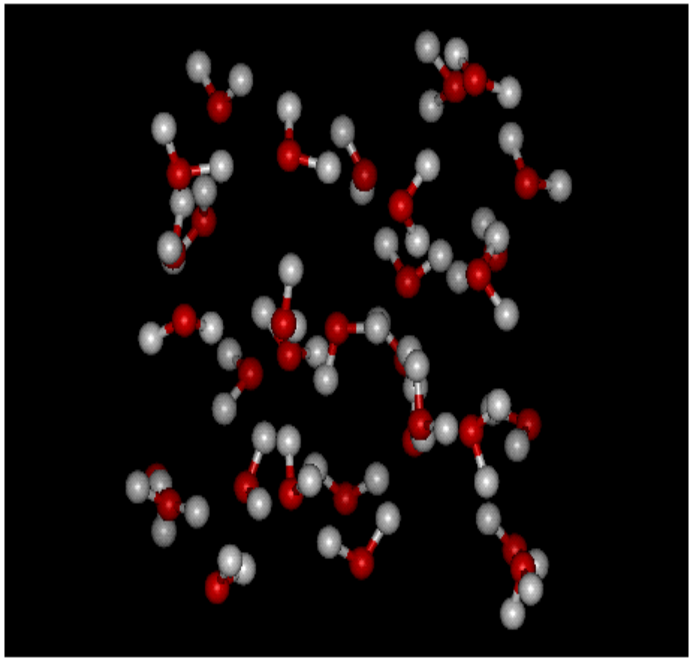
Non-thermal melting of solids observed !

The structure of water: probe by diffuse x-ray scattering

Ice



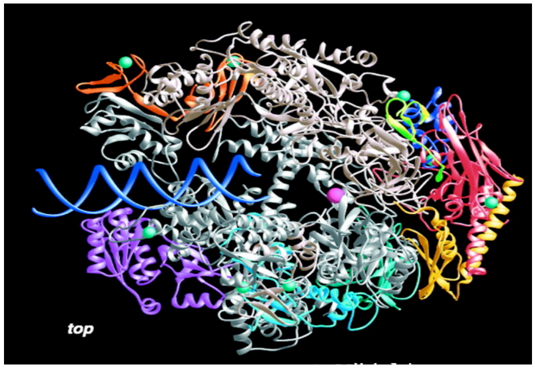
Water



Intrinsic fluctuations
on ~ 1 ps timescale

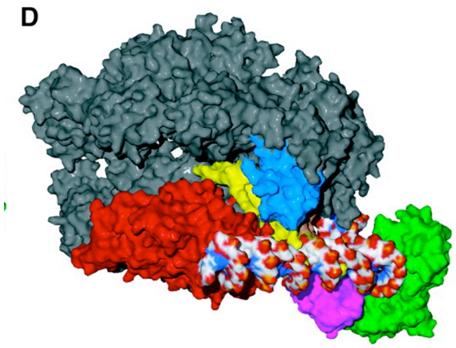
Macromolecular Crystallography: Eukaryotic Transcription

Transcription of the genetic code is essential to life. The genetic information is copied from DNA into messenger-RNA. This messenger carries the information out of the cell nucleus so that it can be translated into proteins. Crystallography has been vital in understanding the detailed mechanism of transcription.



2006 Nobel Laureate for Chemistry
Roger Kornberg

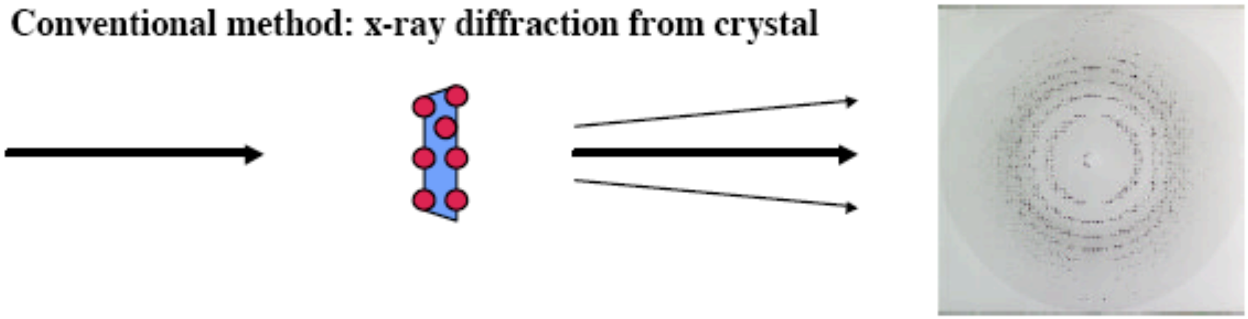
Kornberg used beamlines at the ALS as well as SSRL to determine the structure of RNA Polymerase II



Bushnell, D.A., K.D. Westover, R.E. Davis, and R.D. Kornberg, "Structural basis of transcription: an RNA polymerase II-TFIIB cocrystal at 4.5 Angstroms," Science 303, 983 (2004). (5.0.2, 8.2.1)

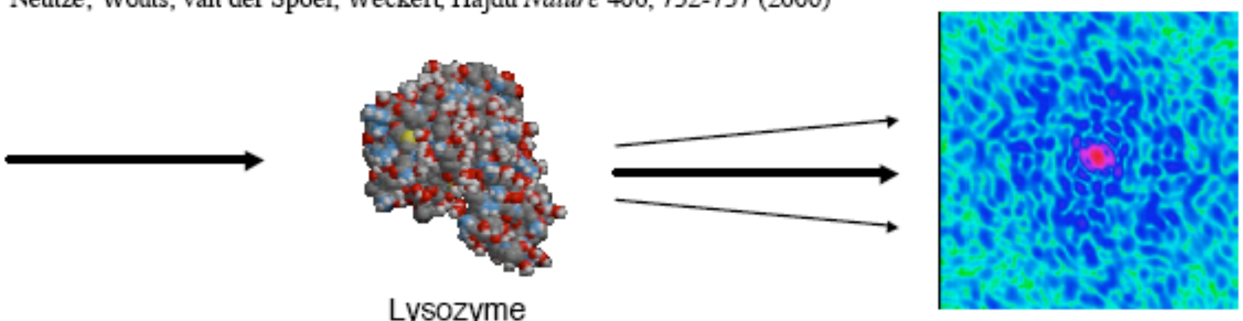
Macromolecular crystallography yields atomic structure of proteins

Conventional method: x-ray diffraction from crystal



Proposed method: diffuse x-ray scattering from single protein molecule

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

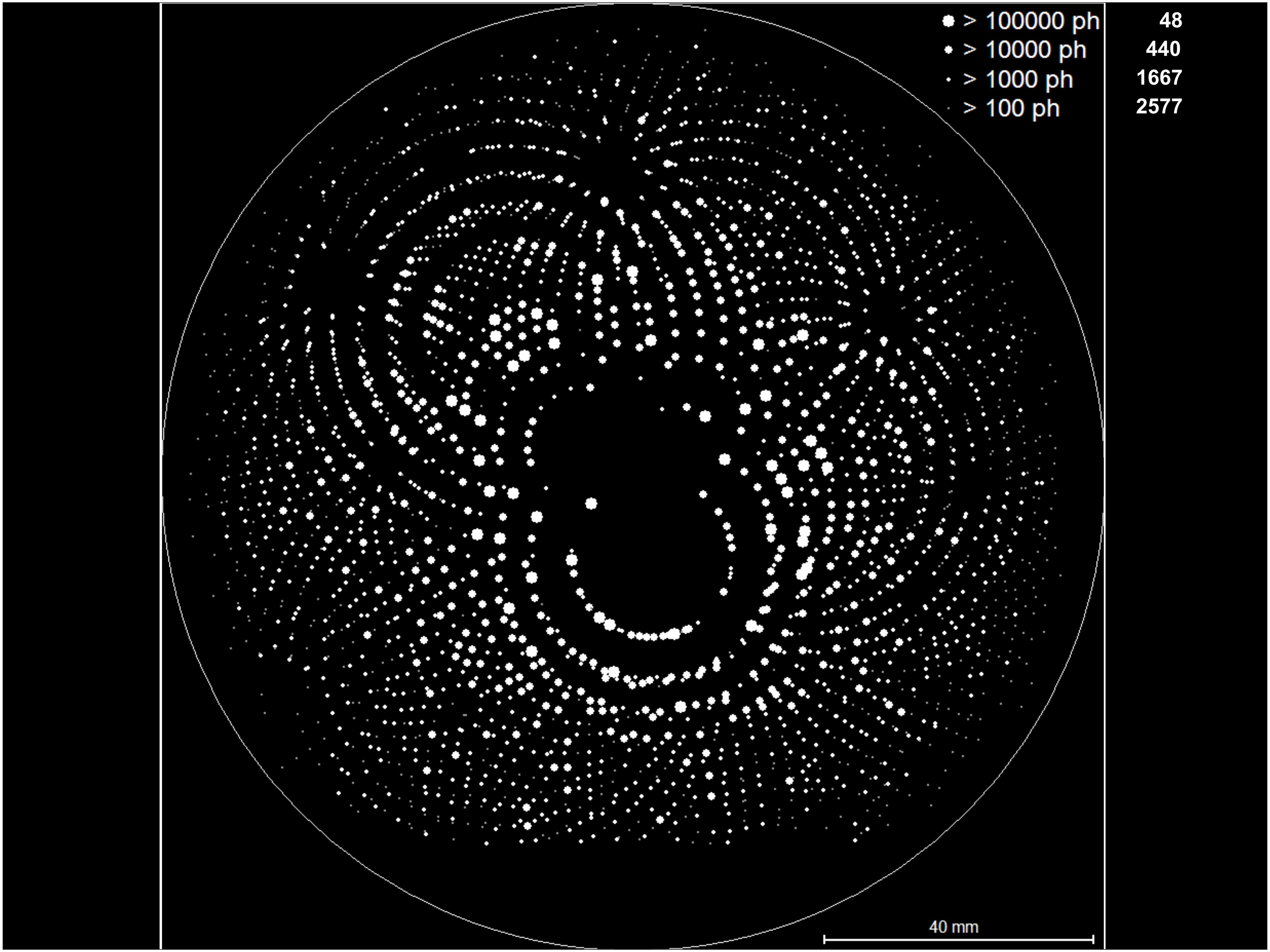


Calculated scattering pattern from lysozyme molecule

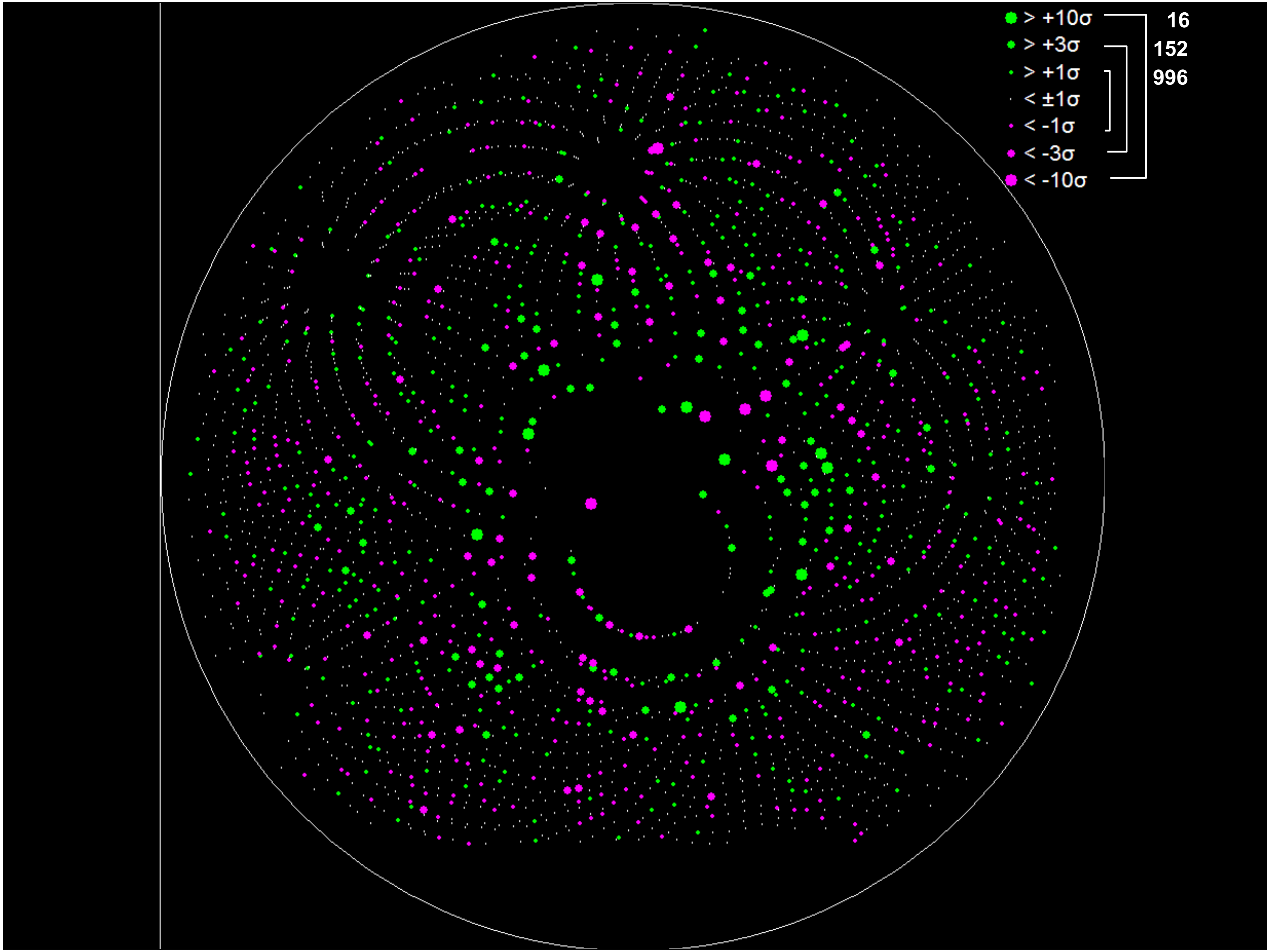
Implementation limited by radiation damage:

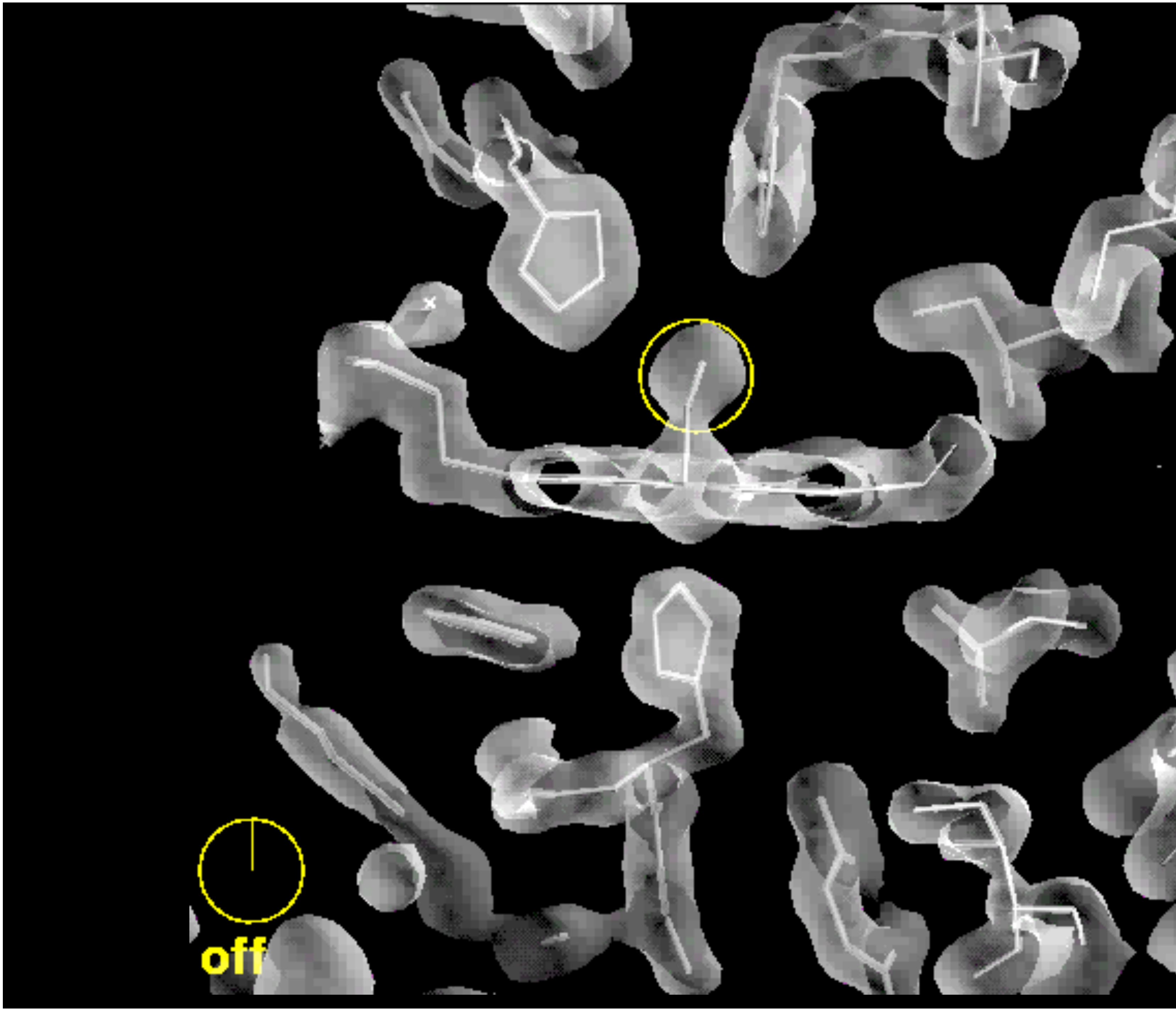
In **crystals** limit to damage tolerance is about **200 x-ray photons/Å^2**

For **single protein molecules** need about **10^{10} x-ray photons/Å^2** (for 2Å resolution)

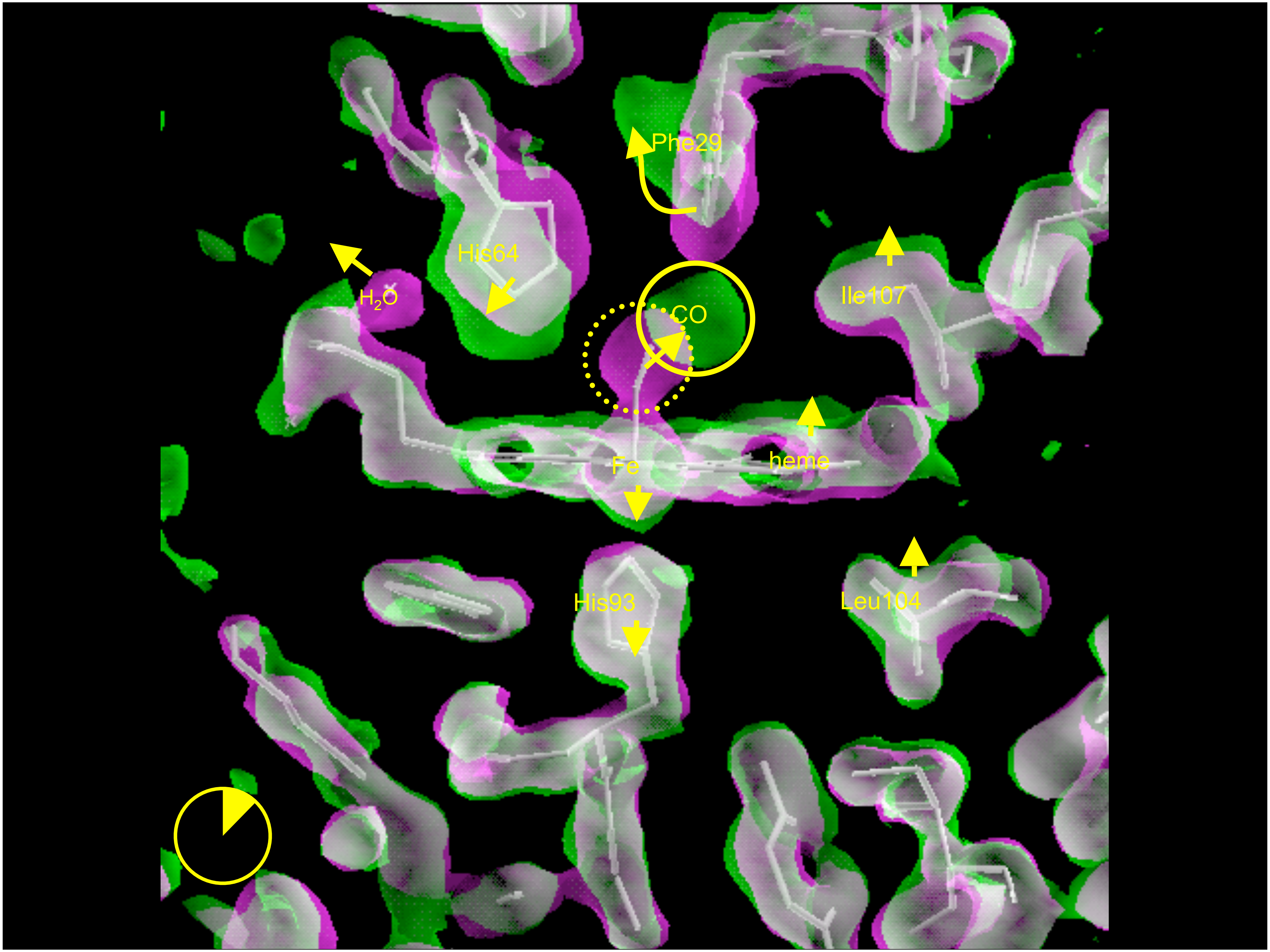


> 100000 ph 48
> 10000 ph 440
> 1000 ph 1667
> 100 ph 2577
40 mm


> +10σ
> +3σ
> +1σ
< ±1σ
< -1σ
< -3σ
< -10σ
16
152
996

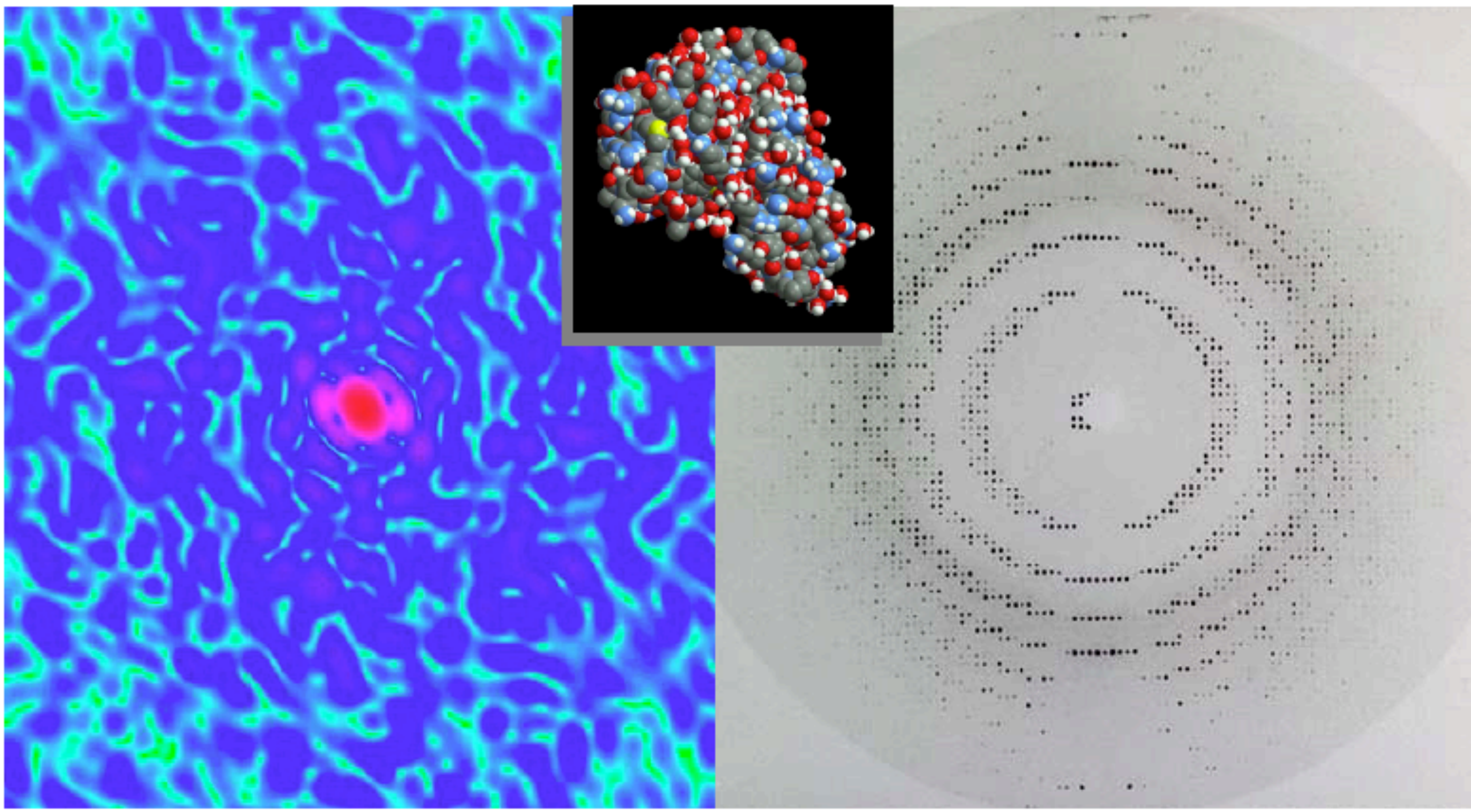


Science, 300, 194
(20 Jun 2003)



Phe29
His64
H_2O
CO
Ile107
Fe
heme
His93
Leu104

Scattering by a single molecule and by a crystal

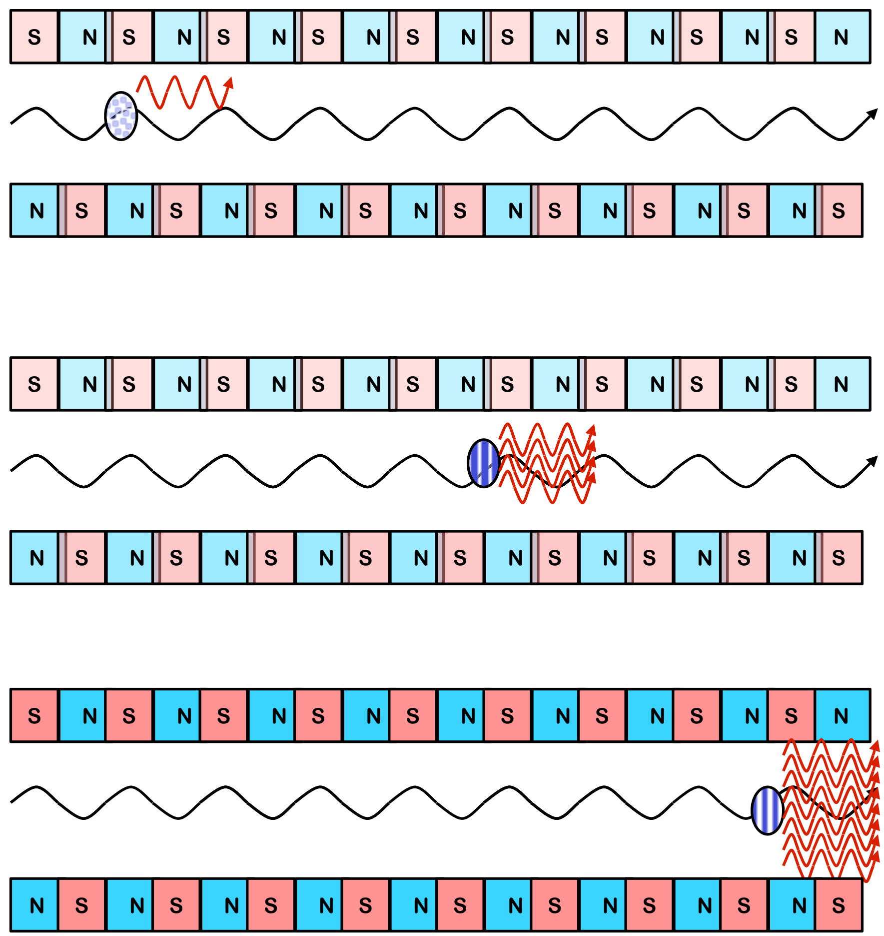


single molecule

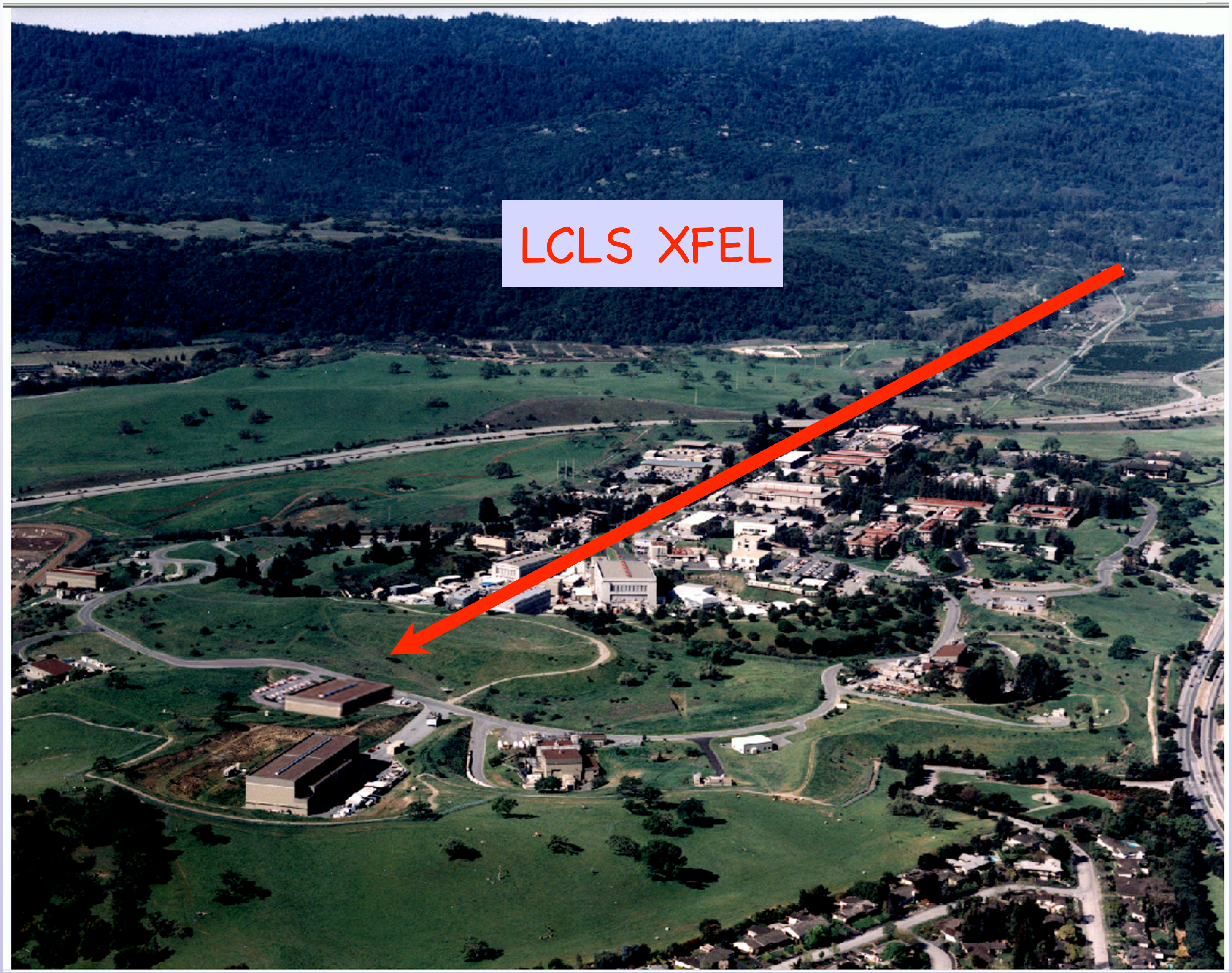
crystal

from Janos Hajdu

Self-Amplified Spontaneous Emission (SASE) produces intense and coherent x-ray pulses

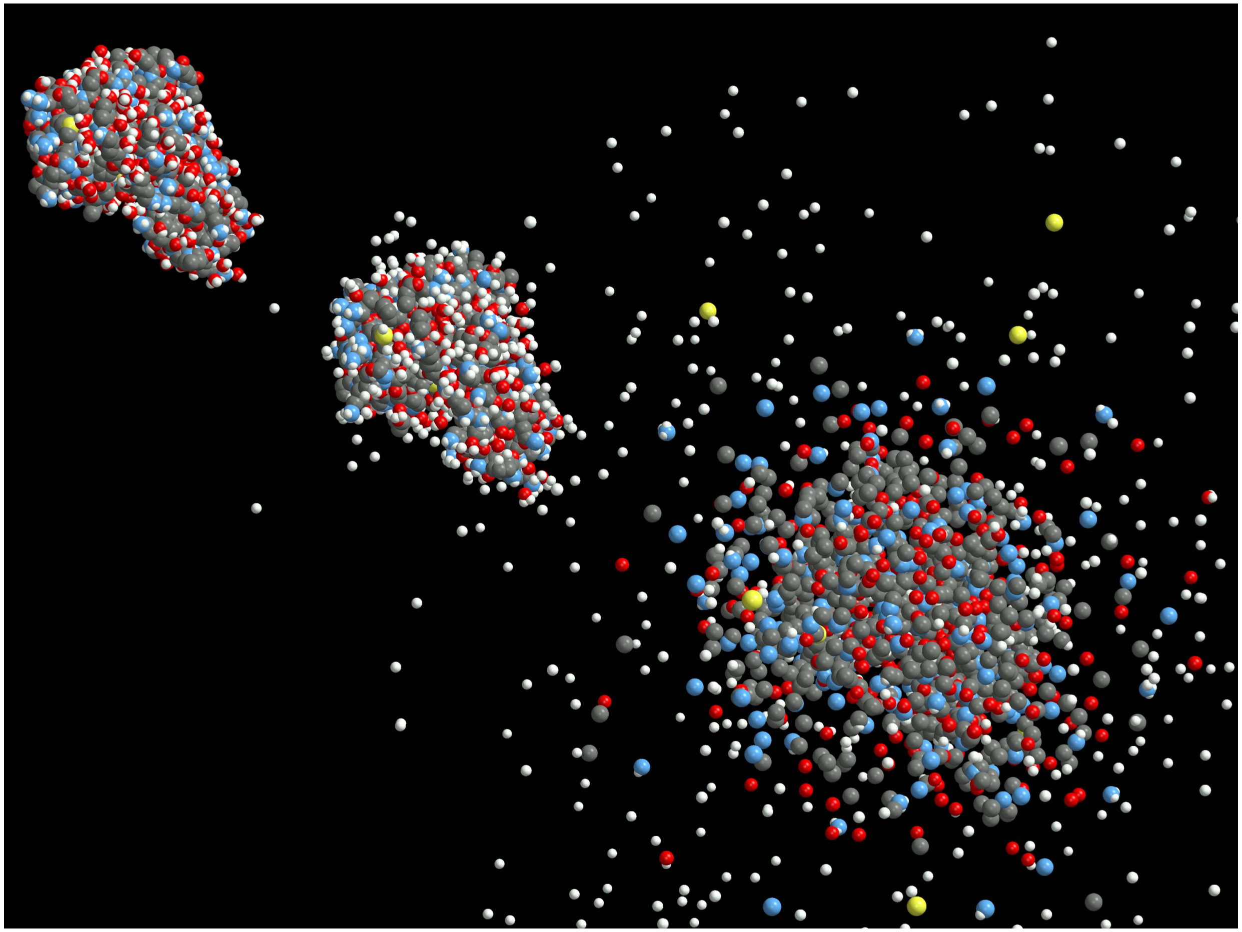


Stanford's SLAC LINAC is a source of fast x-ray pulses



Coulomb explosion of lysozyme

50 fs
3×10^{12} photons
100 nm spot
12 keV



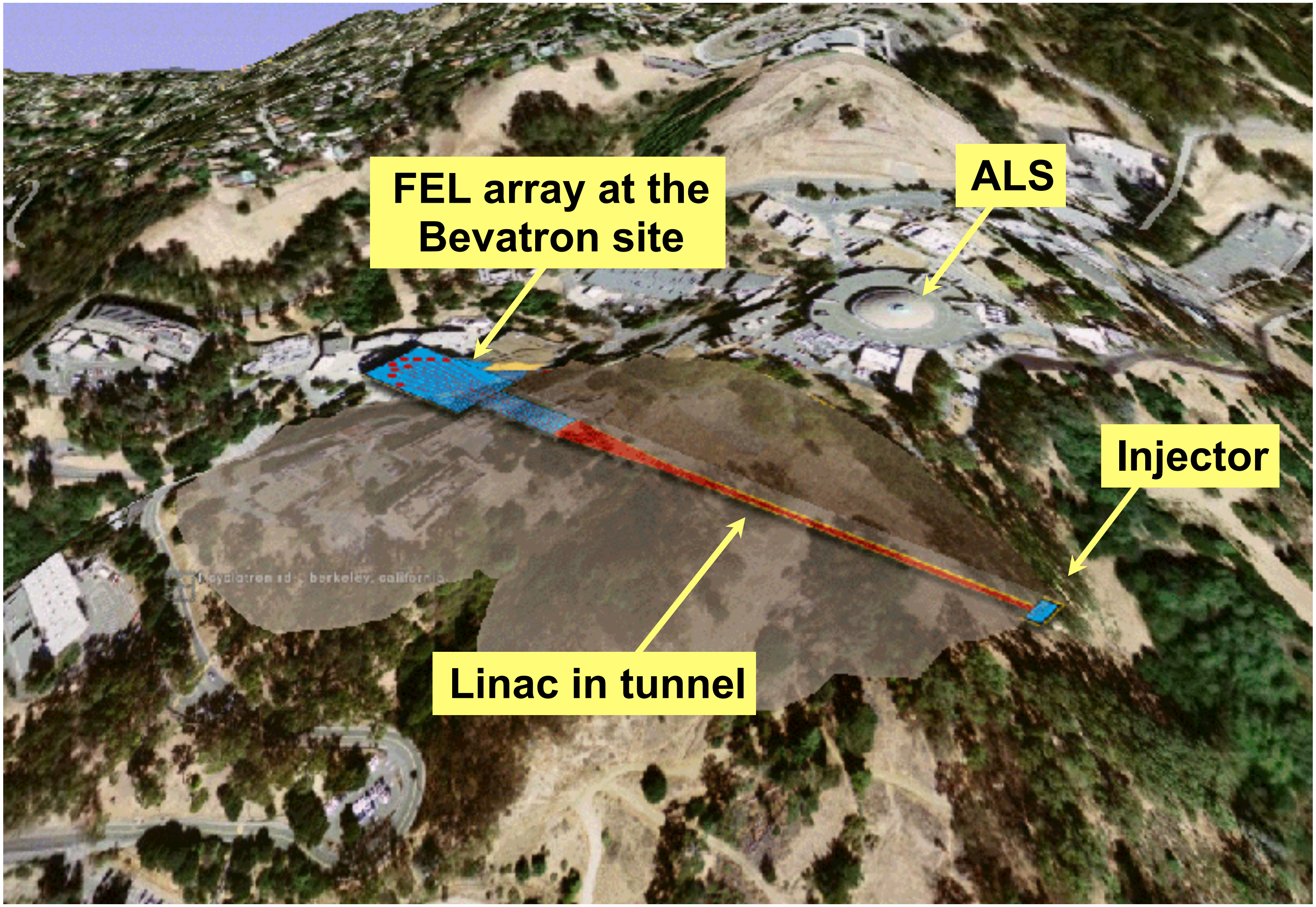
from Neutze, Wouts, van der Spoel, Weckert, & Hajdu, Nature **406**, 752 (2000)

- X-Rays reveal both where atoms are (structure) and how atoms are bonded

- Ultrafast timescales are used in nature to direct energy and information flow
  - beat the timescales for dissipation into unwanted modes
    - e.g., vision, photosynthesis - we need efficient photovoltaics
  - allow multimode excitation to dissipate energy and minimize damage
    - e.g., DNA, damage - we need materials that work in extreme conditions

- Beyond observation, control of matter and energy flow will utilize coherent radiation to drive atoms to new structures

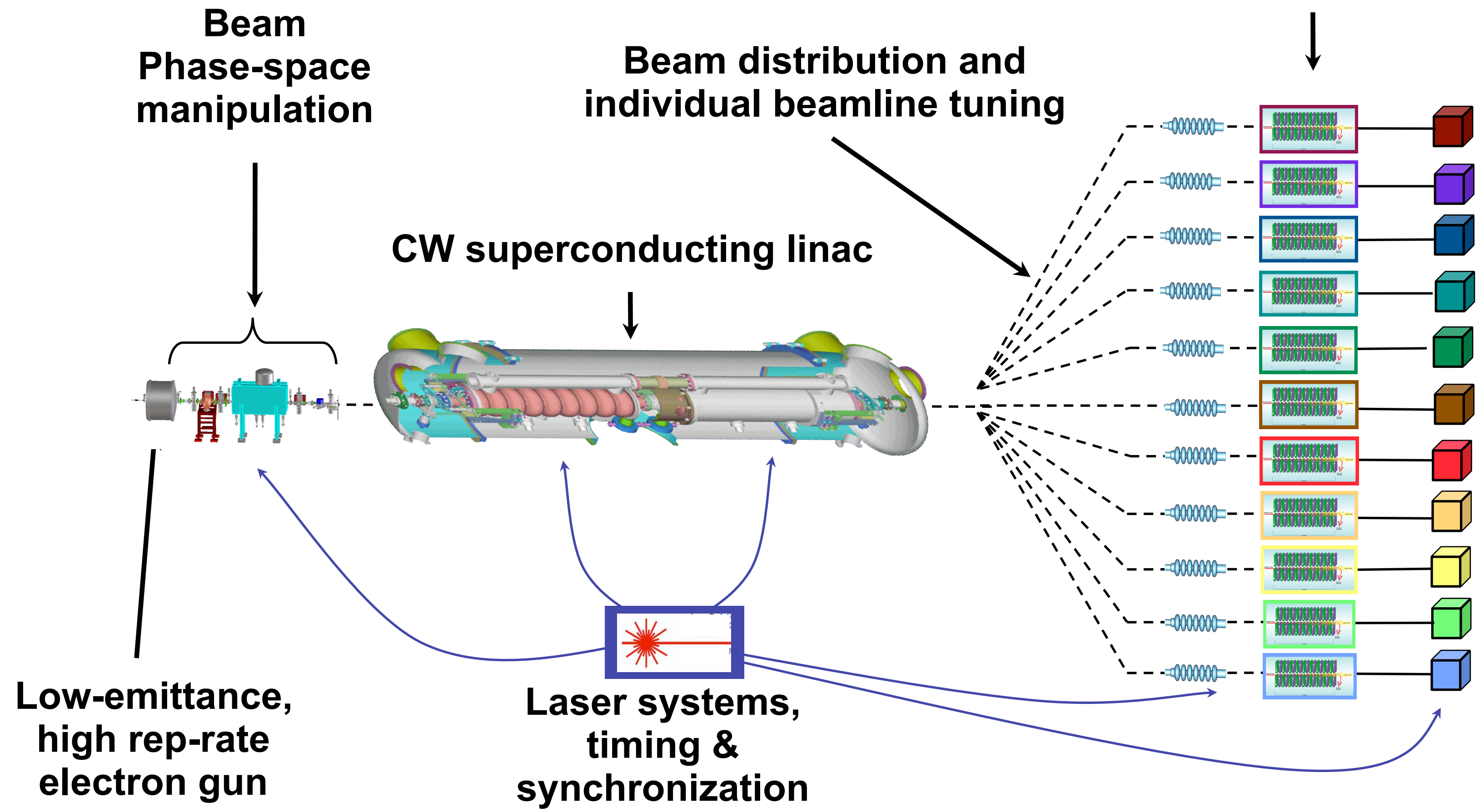
Vision for a future LBNL light source



LBNL vision for a future light source facility

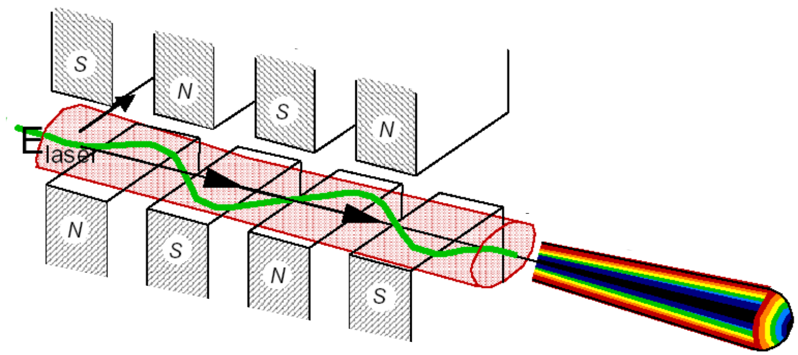
A HIGH REP-RATE, SEEDED, VUV — SOFT X-RAY FEL ARRAY

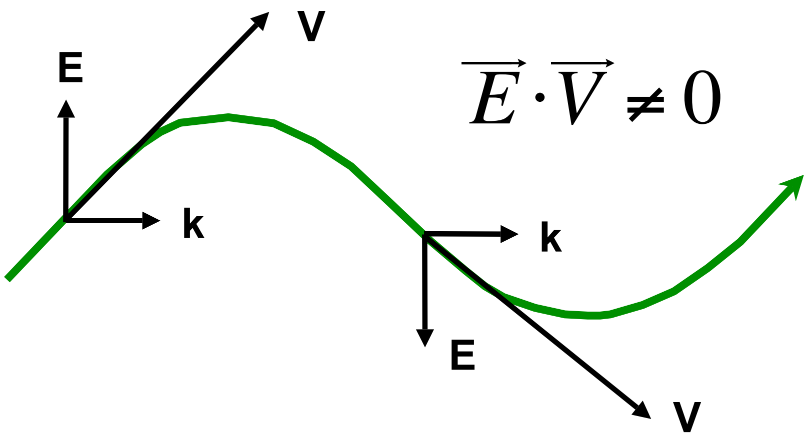
Array of configurable FELs
- Independent control of wavelength, pulse duration, polarization
- Each FEL configured for experimental requirements; seeded, attosecond, ESASE, etc



Optical manipulations

LASER PULSE USED TO MANIPULATE ELECTRON BEAM ENERGY





$$\vec{E} \cdot \vec{V} \neq 0$$

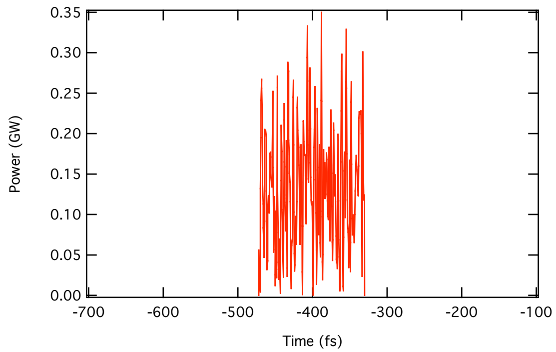
- **Electron beam couples to E-field of laser when co-propagating in an undulator**
- **Over one undulator period, the electron is delayed with respect to the light by one optical wavelength**

Seeded FEL

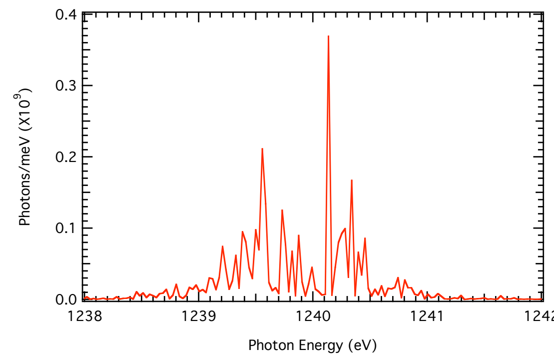
ENHANCED CAPABILITIES FOR CONTROL OF X-RAY PULSE

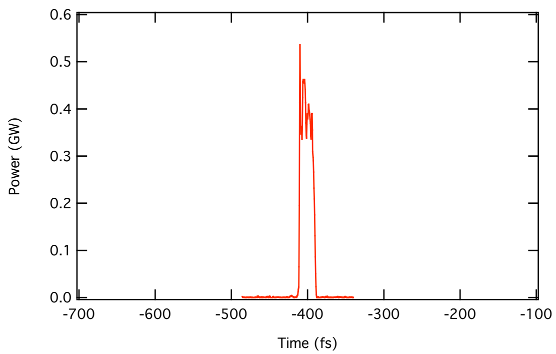
Pulse profile

Spectrum

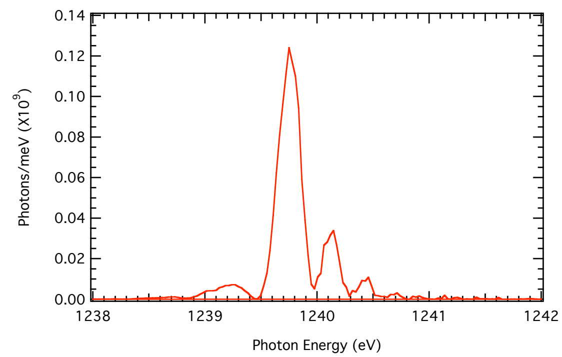


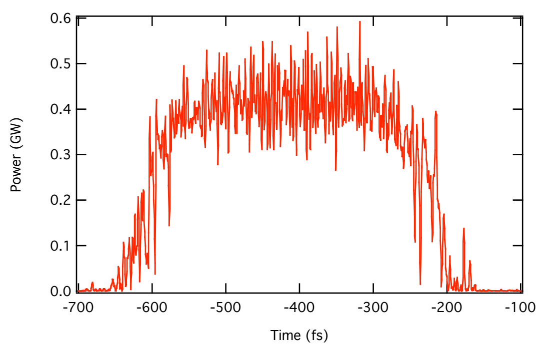
SASE



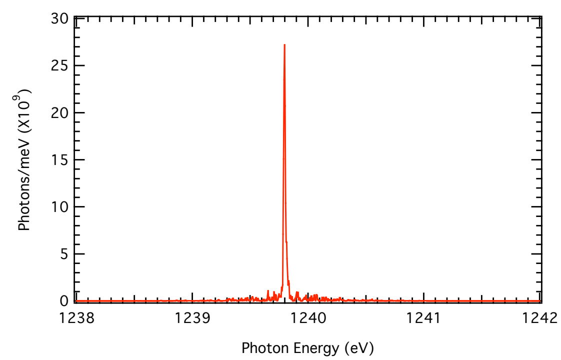


25 fs seed





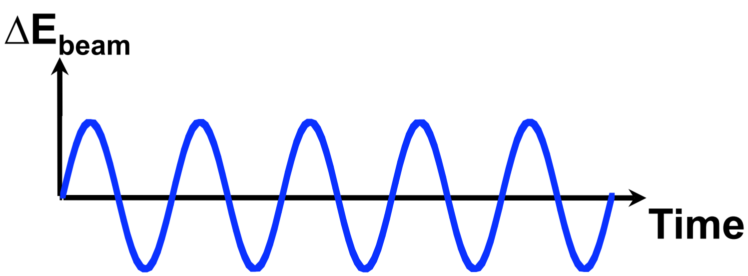
500 fs seed

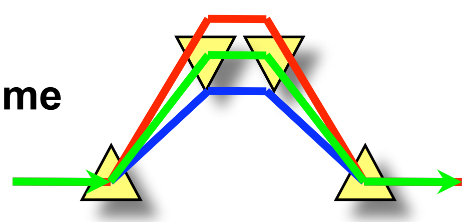


Electron beam is 1.5 GeV, energy spread 100 keV, 250 A current, 0.25 micron emittance; laser seed is 100 kW at 32 nm; undulator period 1 cm

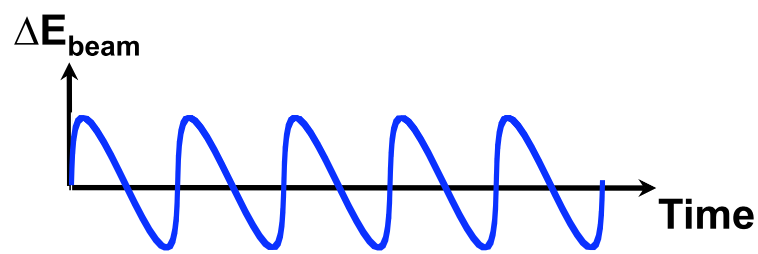
Bunching of the electron beam

ENERGY MODULATION FOLLOWED BY DISPERSIVE SECTION

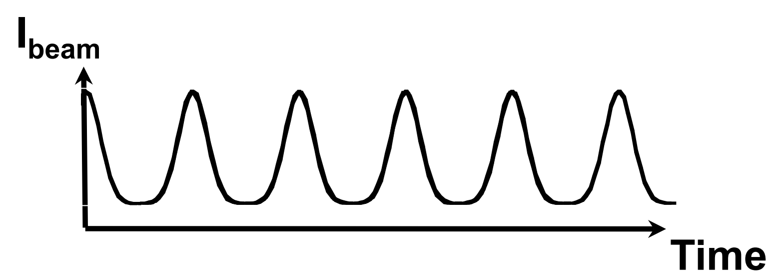




Energy-dependent
path length

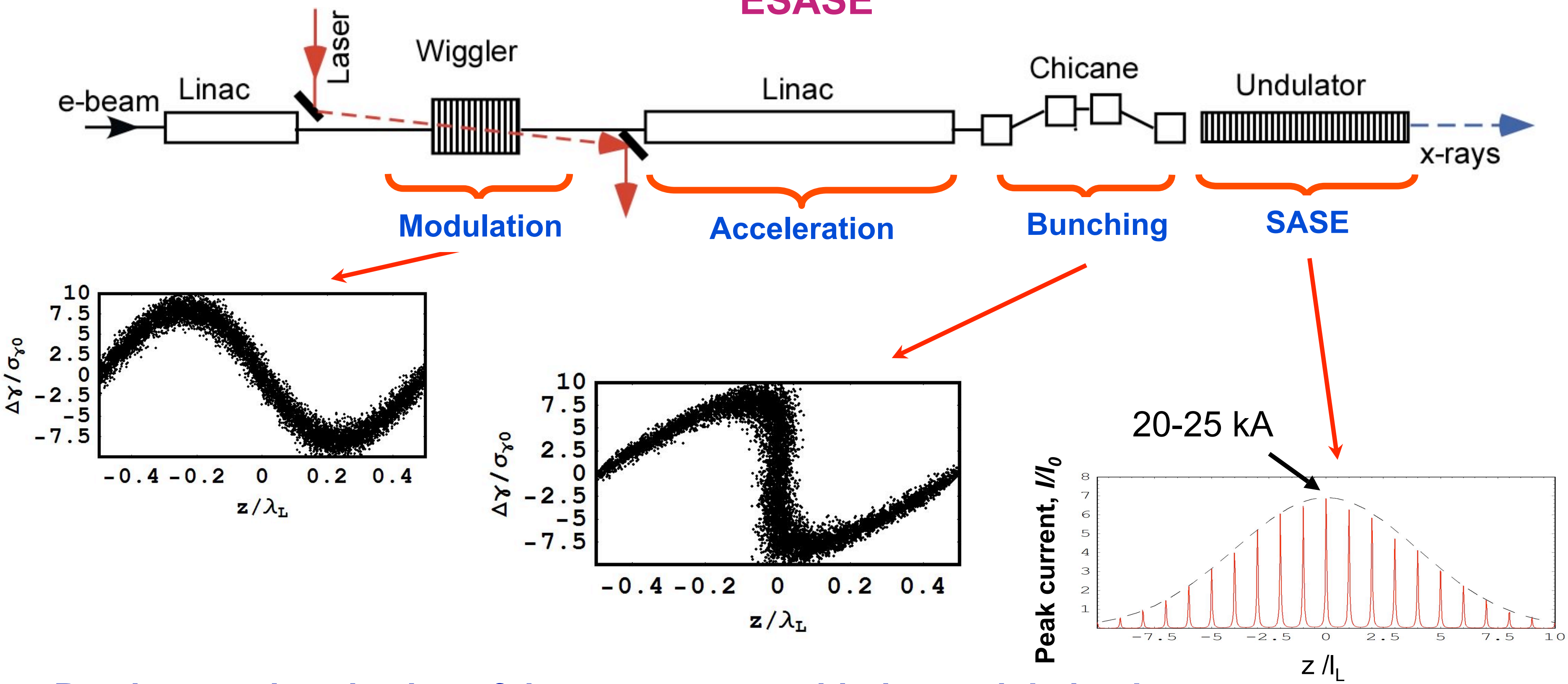


Induced current modulation in the electron beam

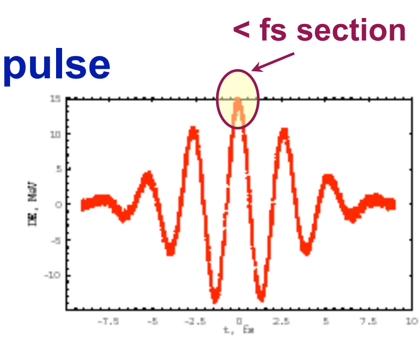


Optical manipulations techniques (1)

ESASE



- Precise synchronization of the x-ray output with the modulating laser
- Variable output pulse train duration by adjusting the modulating laser pulse
- Increased peak current
- Shorter x-ray undulator length to achieve saturation
- Capability to produce a solitary ~100-attosecond duration x-ray pulse
- Other techniques can be used to produce controlled x-ray pulses



A. Zholents, Phys. Rev. ST Accel. Beams 8, 040701 (2005)

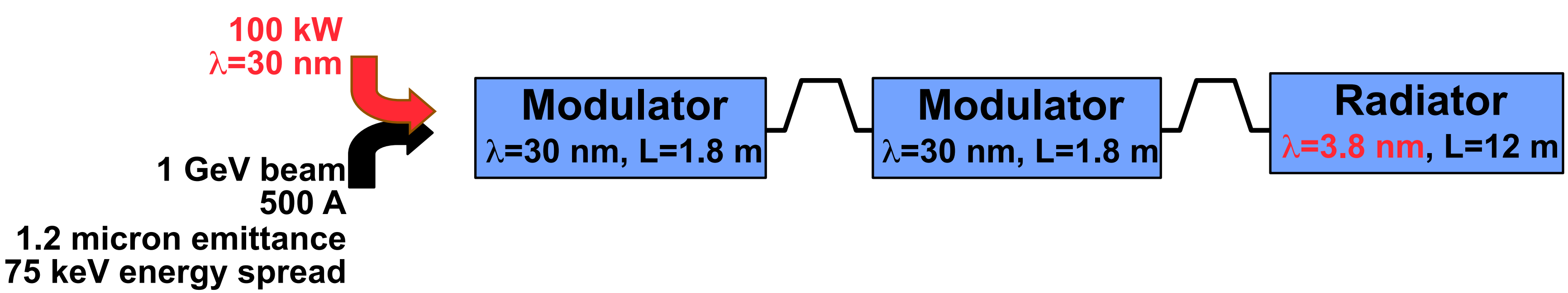
Optical manipulations techniques (2)

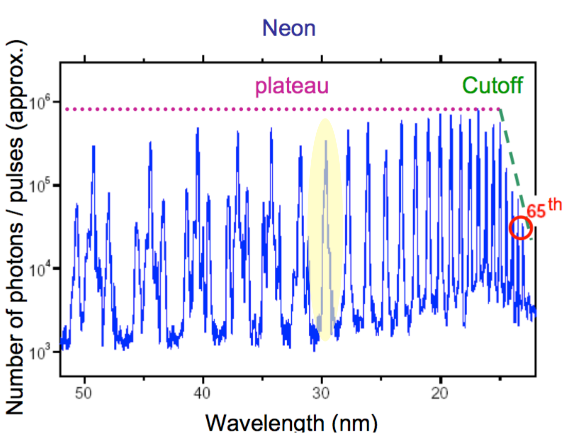
HHG LASER SEED

Example with seed at 30 nm, radiating in the water window

First stage amplifies low-power seed with “optical klystron”

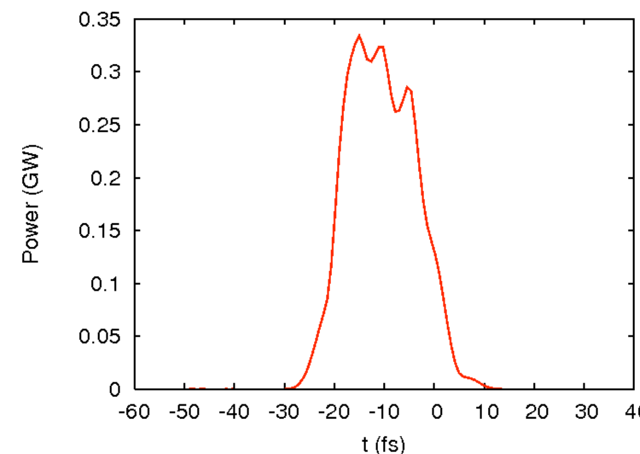
- **More initial bunching than could be practically achieved with a single modulator**
- **Output at 3.8 nm (8th harmonic)**





Lambert et al., FEL04

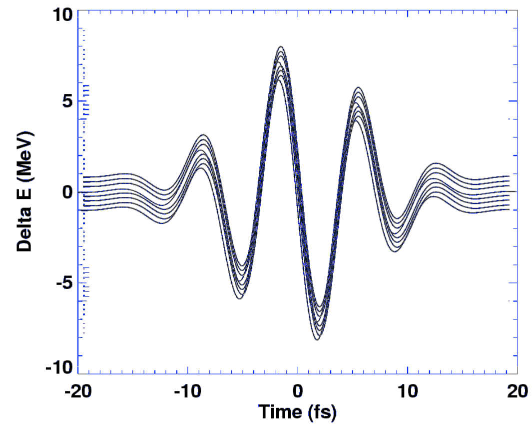
300 MW output at 3.8 nm (8th harmonic) from a 25 fs FWHM seed



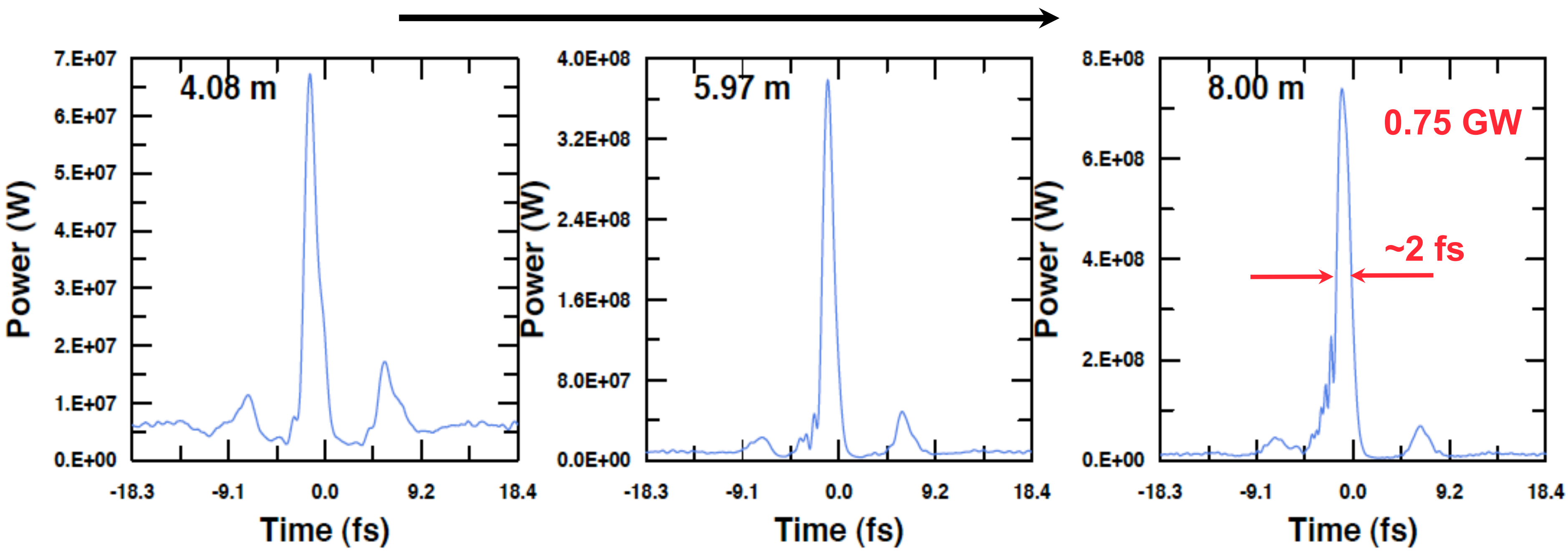
Optical manipulations techniques (3)

ULTRAFAST SASE PULSES IN VUV-SXR

- Again, a few-cycle optical pulse modulates electron beam
  - Modulating laser is possibly 1 - 2 μm wavelength
  - This time there is no compression following the modulation
  - Take advantage of the energy chirp in the bunch
  - Tapered FEL keeps the small section of appropriately chirped beam in resonance



Evolution of an 8 nm wavelength pulse along undulator



E.L. Saldin, E.A. Schneidmiller, and M.V. Yurkov, PRSTAB 9, 050702 (2006)

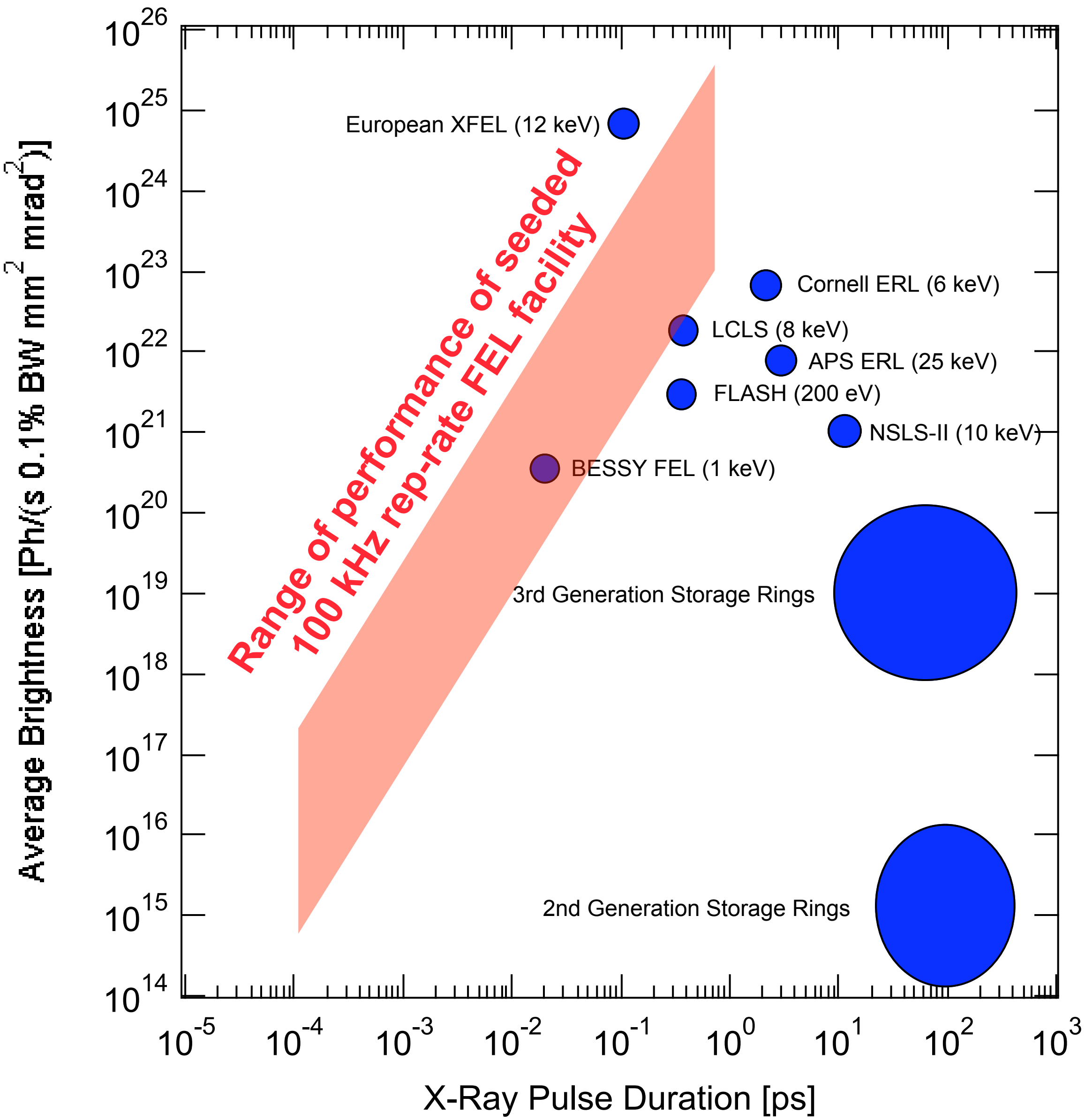
Performance goals

FELs WITH THREE MODES OF OPERATION

	Short-pulse beamlines	High-resolution beamlines	Sub-femtosecond beamlines
Wavelength range (nm)	~200 – 1	~200 – 1	~40 – 1
Photon energy (eV)	6 – 1240	6 – 1240	30 – 1240
Repetition rate (kHz)	100	100	1-100
Peak power (GW)	1	1	0.1 – 0.3
Photons/pulse (@1 nm)	5×10^{11} (in 100 fs)	2.5×10^{12} (in 500 fs)	1.5×10^{8} (in 100 as)
Timing stability (fs)	10	10	TBD
Pulse length (fs)	1 – 100	100 – 1000	0.1 - 1
Harmonics	≤ few%	≤ few%	≤ few%
Polarization	Variable, linear/circular	Variable, linear/circular	Variable, linear/circular

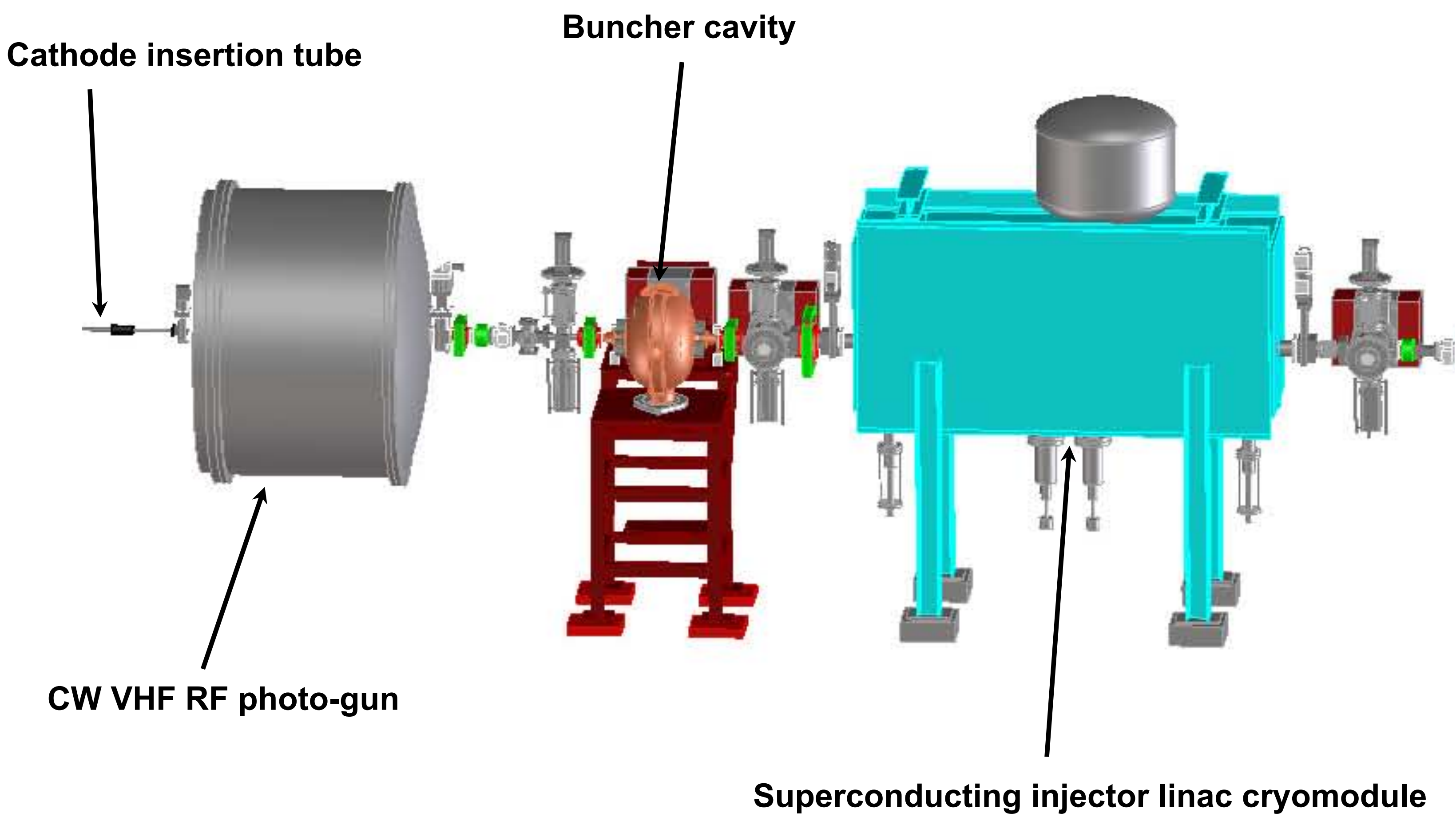
Performance comparison

TIME-DOMAIN RANGING FROM PICOSEC TO SUB-FEMTOSEC



Injector

CW VHF PHOTO-GUN, RF BUNCHING, SCRF INJECTOR LINAC



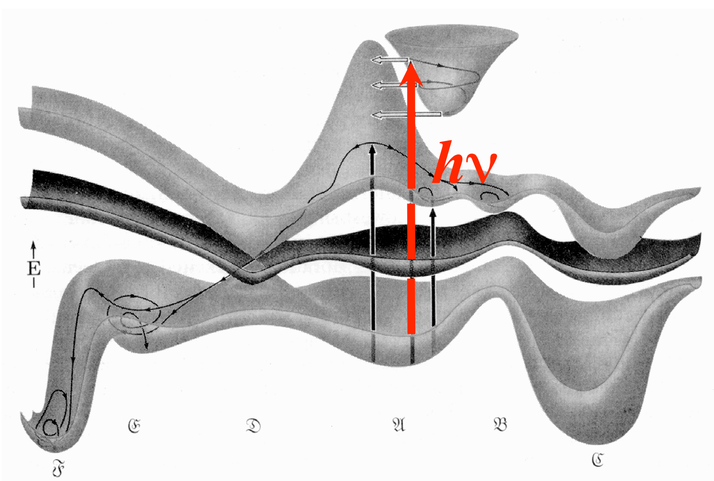
Injector linac in SBIR collaboration with Niowave

Scientific Challenges for the RLS (1)

Attosecond probe and control of electron dynamics in atoms and molecules -- X-ray pump and probe

- Understanding excited state chemistry that is not determined by simple adiabatic potential surfaces
  - Femtosecond probe and control of non-Born-Oppenheimer chemical dynamics
  - Conical intersections dominate photochemistry involved in energy applications (e.g., photosynthesis, inorganic and organic photochemistry)

For large (and many small) molecules there are multiple conical intersections (> 10 ?) that determine photochemistry



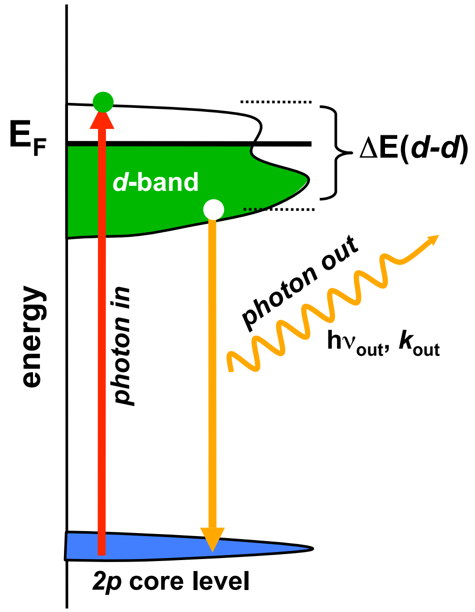
RLS will address the fundamental time scale for vibrational or reactive atomic motion vibrational period (T_{vib} = 10 -100 fs) with intensities and repetition rates sufficient to characterize non-Born-Oppenheimer dynamics

Scientific Challenges for the RLS (3)

Inelastic X-ray Scattering

(X-ray Raman, q>0)

Example - 3*d* metal



Energy conservation:

$\omega_{out} = \omega_{tin} - \Delta E(d\text{-}d)$

Momentum conservation:

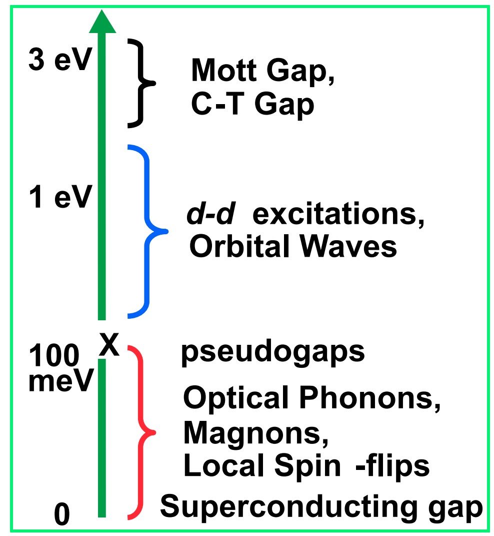
$k_{out} = k_{tin} - \Delta k(d\text{-}d)$

Electronic Structure:

Photoemission (ARPES)	$A(k,\omega)$ - single-particle spec.
Inelastic Neutron Scattering (INS)	$S(q, \omega)$ - spin fluctuation spec.
Inelastic x-ray scattering (IXS)	$S(q, \omega)$ - density-density correlation

Advantages:

- Bulk sensitive
- Insulating samples (organics, bio-materials ….)
- External fields (magnetic, electric) pressure, optical excitation
- Probe optically 'forbidden' transitions
- Resonant IXS
  - signal enhancement 10^2-10^3
  - element sensitivity (buried interfaces)
  - soft x-ray $2p \rightarrow 3d$ (spin, orbital ordering …)

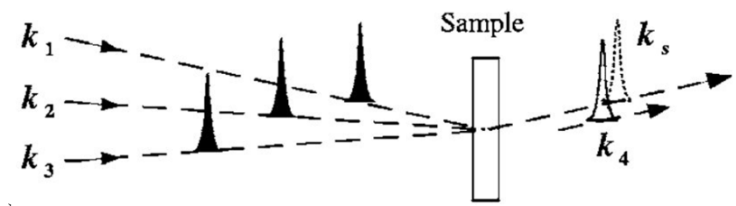


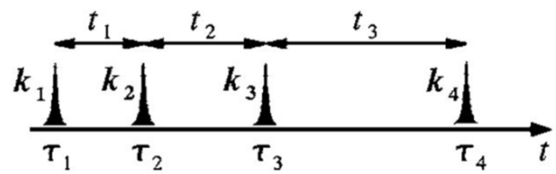
Average Flux – photons/sec/bandwidth

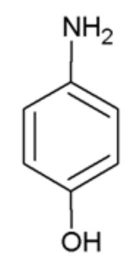
High Resolution - throughput

Scientific Challenges for the RLS (4)

- **2-dimensional X-ray Correlation Spectroscopy - Work in Progress**
- Correlation spectroscopy originated in NMR (1991 Nobel prize), very successful in IR and UV/Visible
- Spectra obtained by varying delays in a coherent time-resolved all-x-ray four-wave mixing signal + Fourier transform

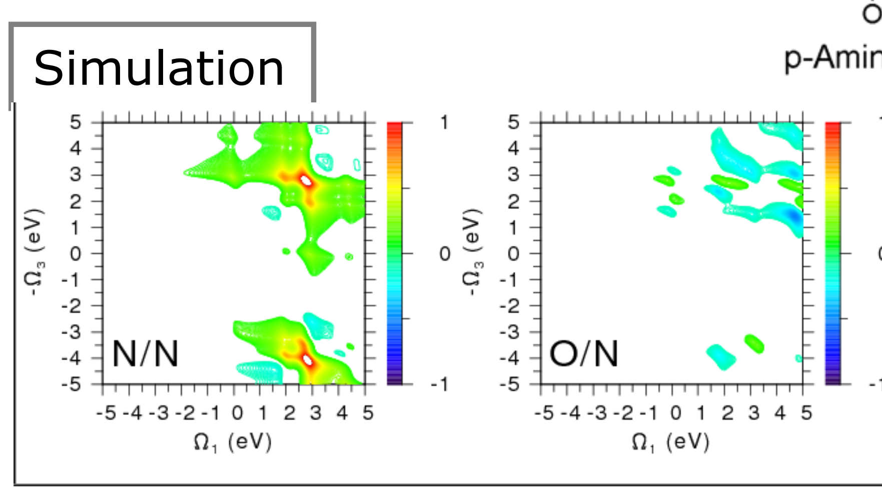






p-Aminophenol

Strong individual absorptions contribute to the diagonal part of 2D spectrum, and weak signatures of interactions emerge as "cross peaks"



ic/ALSaerial/11-96