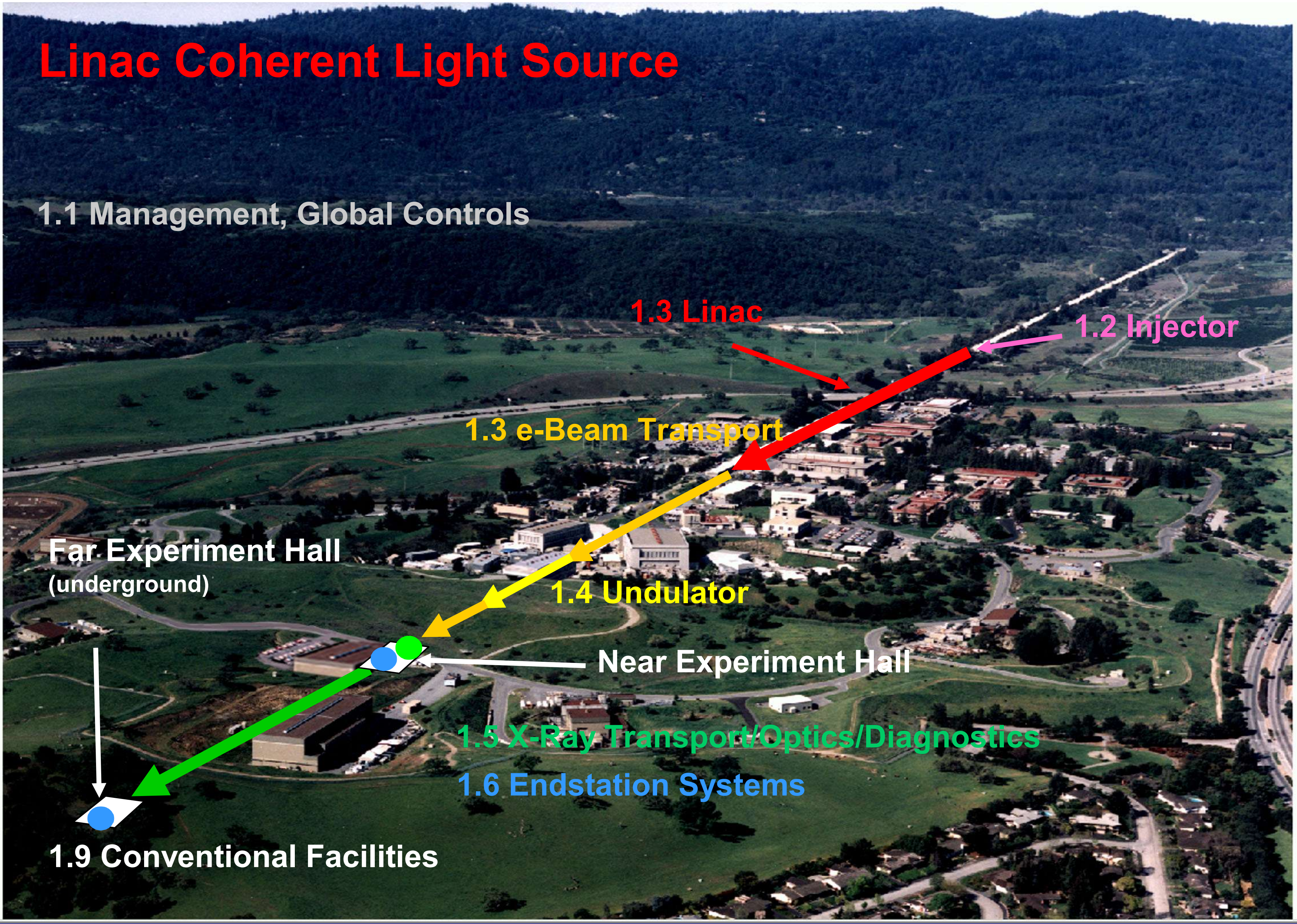
Linac Coherent Light Source



Stanford Linear Accelerator Center

SSRL

Performance Characteristics of the LCLS

SSRL

- Wavelength§ 1.5 Å (range 1.5-15 Å)
- Electron energy 14.35 GeV (range 14.35-4.54)
- Norm. emittance 1.5 π mm-mrad (rms)
- Peak current 3,400 A
- Bunch length 230 fs
- FEL parameter, ρ 4.7 $\times 10^{-4}$
- Gain length 11 m

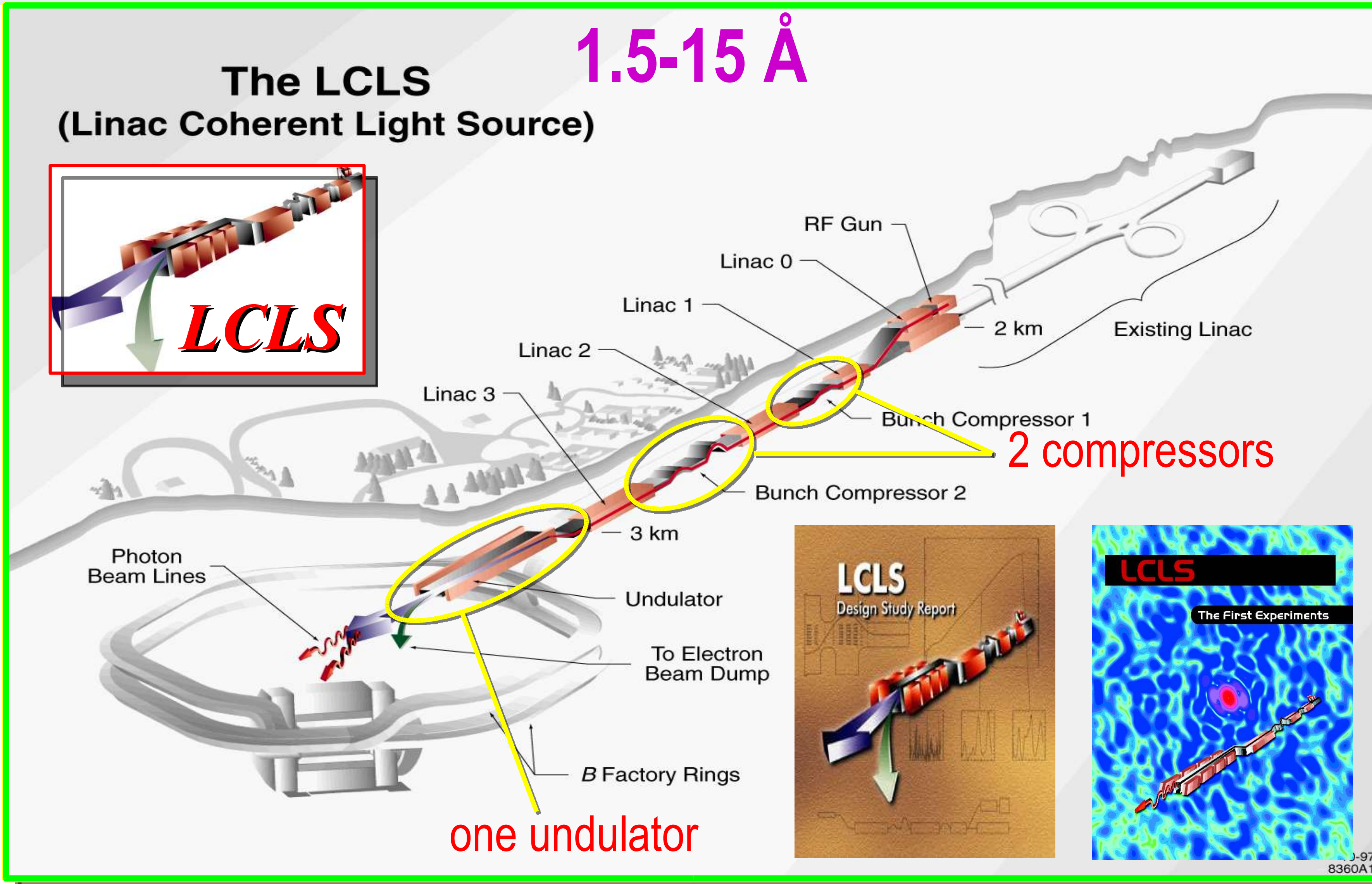
- Undulator length 112 m
- Undulator gap 6 mm
- Undulator par., K 3.7

- Saturation peak power 9 GW
- Peak brightness 1.2 $\times 10^{33}$
- Average brightness 4.2 $\times 10^{22}$

---

§ shorter wavelengths are possible using higher harmonics of a planar undulator. A superconducting helical undulator would give this possibility

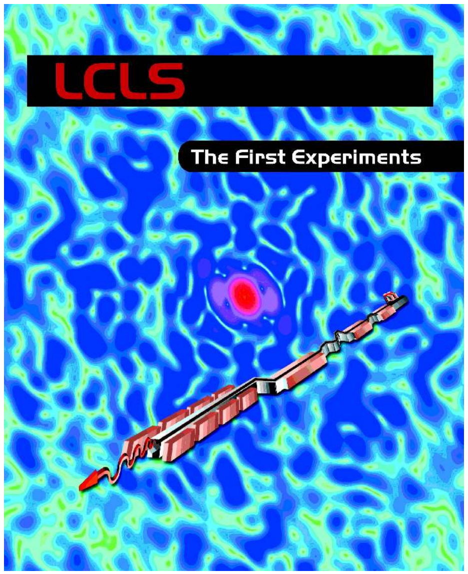
LCLS at *SLAC*



Stanford
Linear
Accelerator
Center
SSRL

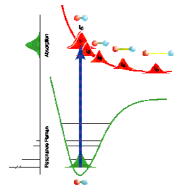
•Presented to BESAC 10-Oct-2000

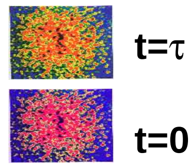
•Critical Decision 0 approved
13-June 2001

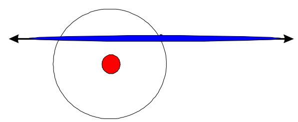


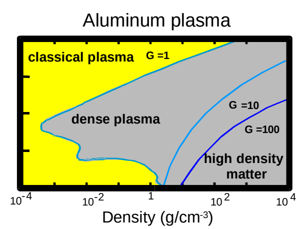
Program developed by international team of scientists working with accelerator and laser physics communities

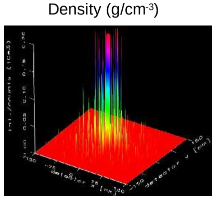
"the beginning.... not the end"

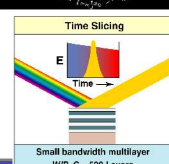












Femtochemistry

Nanoscale Dynamics in Condensed matter

Atomic Physics

Plasma and Warm Dense Matter

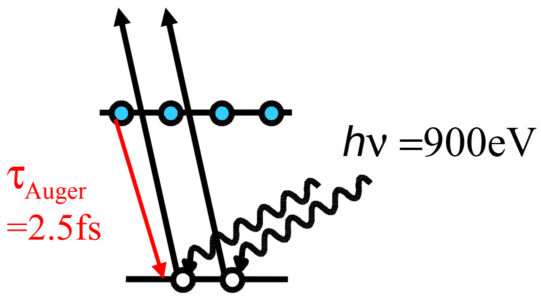
Structural Studies on Single Particles and Biomolecules

FEL Science/Technology

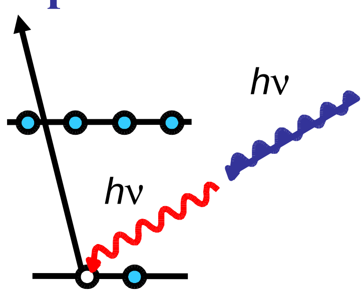
LCLS applications: *Atomic Physics*

Most basic LCLS experiments, aimed at understanding the physics of interaction of intense, ultra-fast pulse with atoms

Formation of Hollow Atoms:



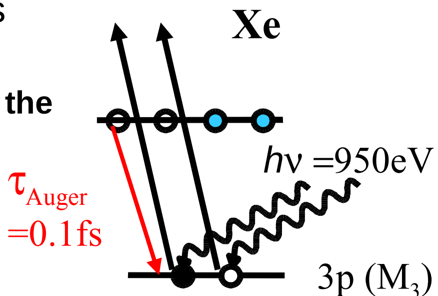
Multiphoton Ionization:



Giant Coulomb explosions of Xe clusters

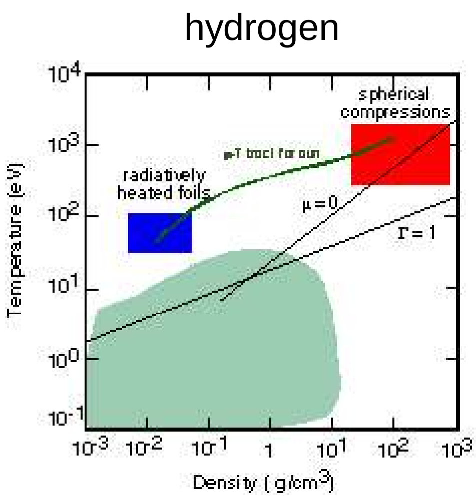
10^9 atoms

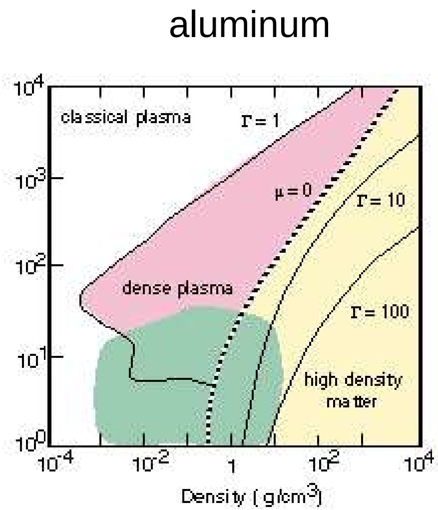
Understanding is central to the imaging of biomolecules



LCLS applications: *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

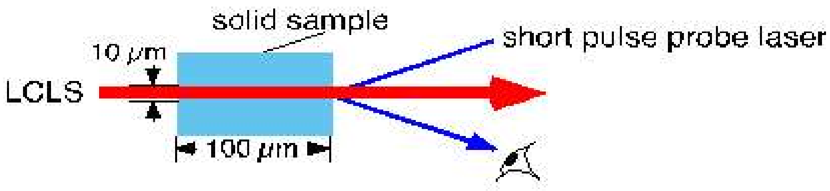
μ = chemical potential (atom interaction potential)

Astrophysical and weapons-related studies lie in the area of warm dense matter. Largest uncertainties in many applied research areas of chemistry and physics come in the warm dense regime

Studies of Warm Dense Matter

LCLS will be able, for the first time, to probe the warm dense matter regime. Use LCLS to create warm dense matter state and also (via delayed pulse) to probe it using x-ray scattering or imaging.

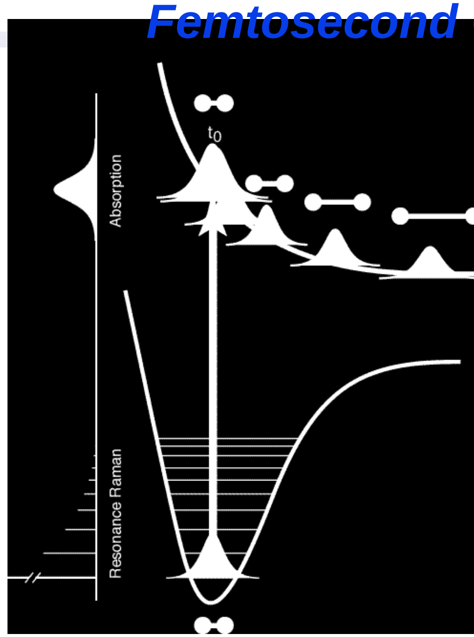
- **Creating Warm Dense Matter**
  - **Generate $\leq$10 eV solid density matter**
  - **Measure the fundamental nature of the matter via equation of state**



- **Probing resonances in HDM**
  - **Measure kinetics process, redistribution rates, kinetic models**
  - **All time scales**

LCLS applications: *Femtosecond Chemistry*

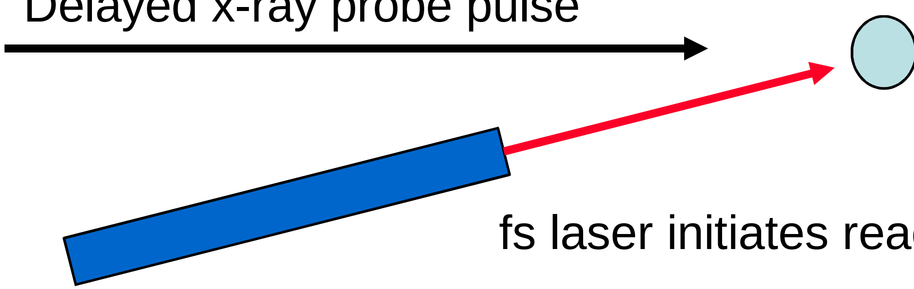
X-ray FEL offers the ability to follow the motions of atoms on a femtosecond time scale



udies of small system
actions can be compared
th theory

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

Delayed x-ray probe pulse

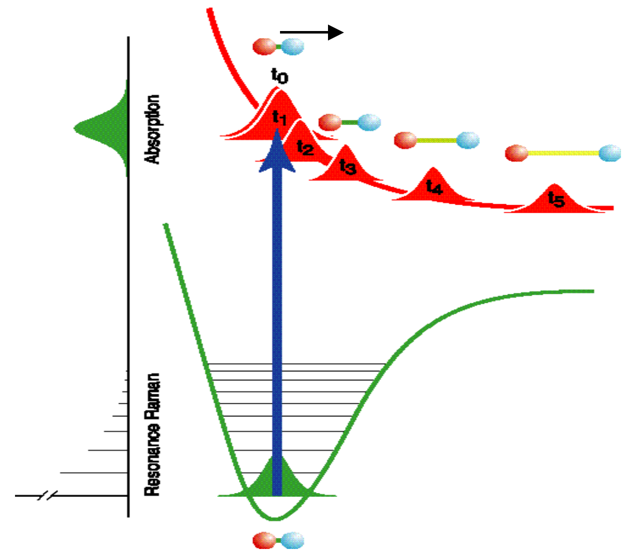


sample

fs laser initiates reaction

Femtosecond Chemistry

Lasers probe charge dynamics
Electron Diffraction limited to ps range
LCLS will probe 200 ⟶ 10 fs range
Chemical dynamics happens in fs - ps range



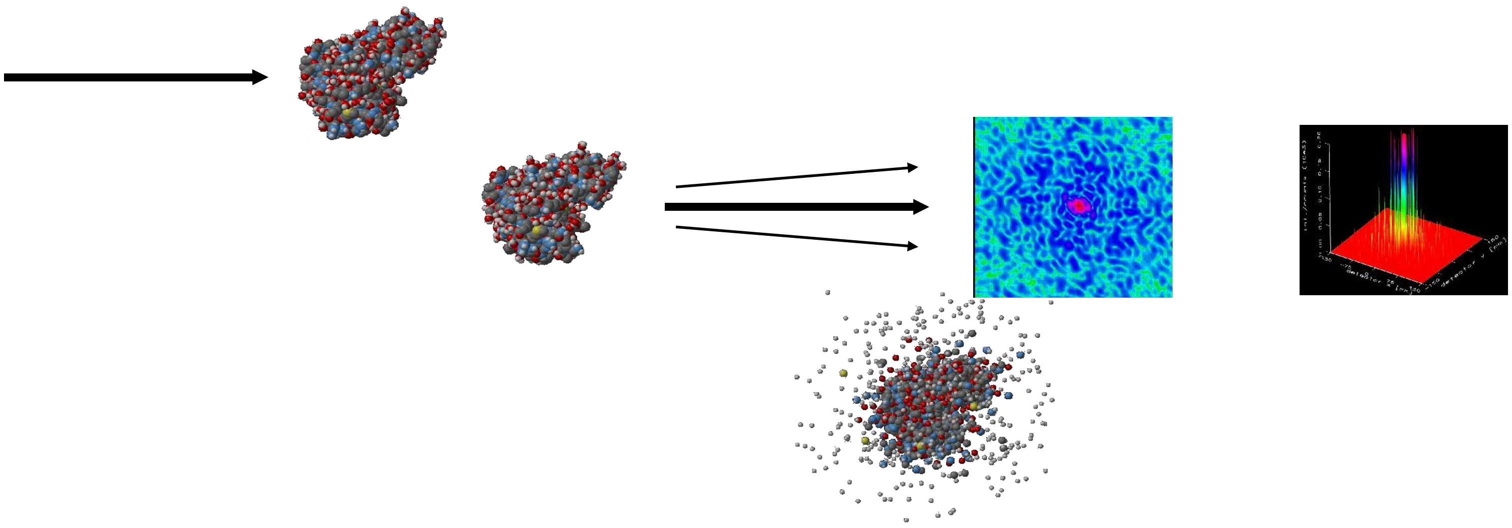
$H_2O \rightarrow OH + H$ — time depends on mass ⟶ — **$CH_2I_2 \rightarrow CH_2I + I$**

about 10 fs | **about 100 fs**

LCLS applications: *X-Ray Diffraction from a Single Protein Molecule*

Avoids radiation damage problem by taking diffraction data before damage occurs

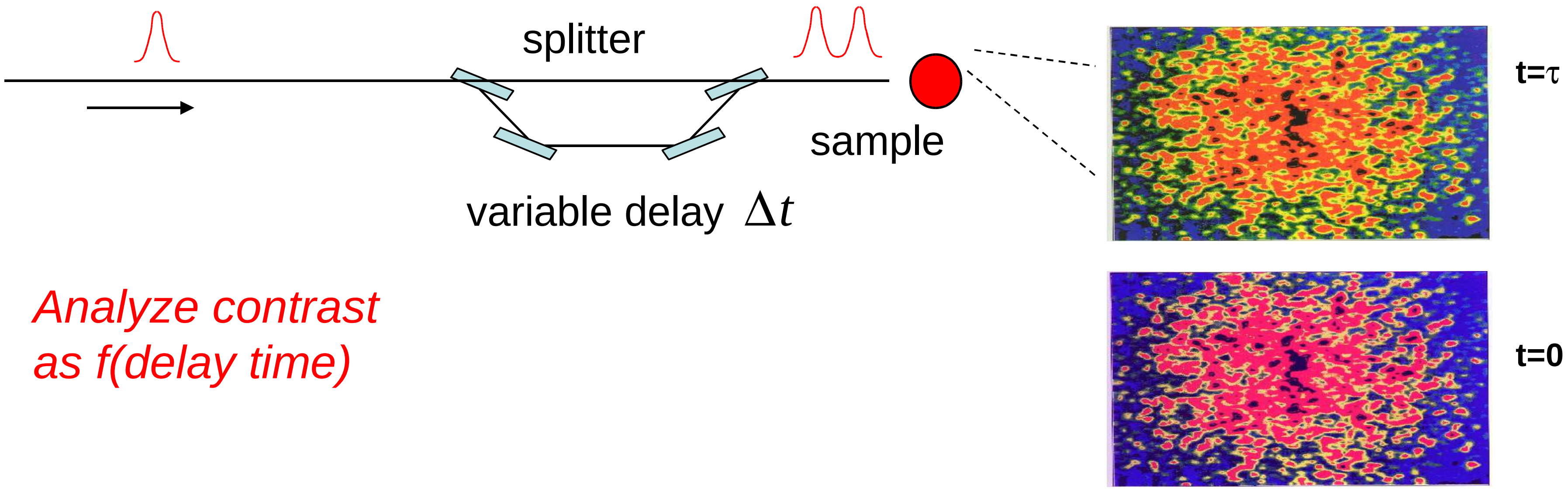
Would allow much broader range of biological structures to be determined



LCLS applications: *Nanoscale Dynamics in Condensed Matter*

Look at dynamics in solids and liquids on ps time scale

In **picoseconds - milliseconds** range



Analyze contrast as f(delay time)

Expected LCLS characteristics

Fundamental FEL Radiation Wavelength	**1.**	**15**	Å
Electron Beam Energy	14.3	4.5	GeV
Normalized RMS Slice Emittance	1.2	1.2	mm-mrad
Peak Current	3.4	3.4	kA
Bunch/Pulse Length (FWHM)	230	230	fs
Relative Slice Energy Spread @ Entranc	<0.01	0.025	%
Saturation Length	87	25	m
FEL Fundamental Saturation Power @ Exit	8	17	GW
FEL Photons per Pulse	1.1	29	10^{12}
Peak Brightness @ Undulator Exit	0.8	0.06	10^{33} *
Transverse Coherence	Full	Full	
RMS Slice X-Ray Bandwidth	0.06	0.24	%
RMS Projected X-Ray Bandwidth	0.13	0.47	%

*** photons/sec/mm^2/mrad^2/ 0.1%-BW**

Letters of Intent (as of Aug 04)

User Program Schedule

2004	15-Mar	Call for letters of intent to be distributed widely	✓
	21-Jun	Letters of Intent due	✓
	8-9 July	SAC: review LOIs, review proposal guidelines	✓
	1-Aug	LCLS/SSRL inform selected teams, move to proposal stage	✓
2005	1-Feb	Full proposals due to LCLS/SSRL	
	15-Feb	SAC review of full proposals	
	1-Mar	Proposals approved by LCLS/SAC	
	1-Apr	Proposals submitted to funding sources	
	1-Oct	Planned LCLS construction start	
2008	1 Oct	Planned LCLS operations start	

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Letters of Intent

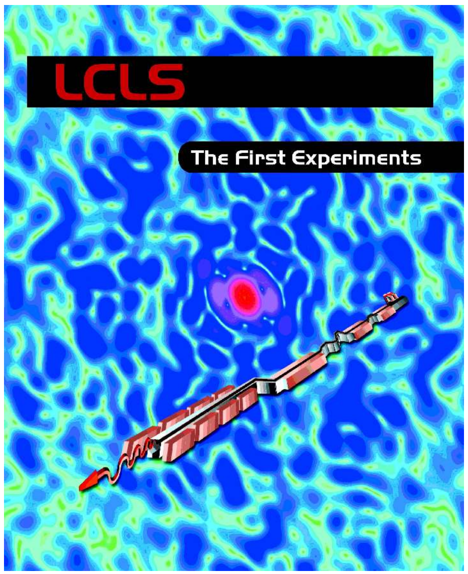
- Types
  - Category A: Complete Endstation
  - Category B: Specific Science Goals
  - Category C: Technical Innovations
- Response
  - Total of 32 received
  - 256 Independent investigators
  - 91 Institutions

LCLS SAC Response

- Identified 5 Thrust Areas
  - Atomic Molecular and Optical Physics
  - Pump/probe high-energy-density (HED) physics
  - Nano-particle and single molecule (non-periodic) imaging
  - Pump/probe diffraction dynamics
  - Coherent scattering at the nanoscale

First Experiments-SAC Response

SLAC Report 611



Program developed by international team of scientists working with accelerator and laser physics communities

First Experiments	SAC Response
Femtochemistry	*Pump/probe diffraction dynamics*
Nanoscale Dynamics in Condensed matter	*Coherent scattering at the nanoscale*
Atomic Physics	*Atomic Molecular and Optical Physics*
Plasma and Warm Dense Matter	*Pump/probe high-energy-density (HED) physics*
Structural Studies on Single Particles and Biomolecules	*Nano-particle and single molecule (non-periodic) imaging*
FEL Science/Technology	

LCLS SAC Response (cont'd)

- All LoI's were reviewed and fit into thrust areas
- Supported Short pulse (beyond baseline) R&D
  - Will enable new science
- LCLS efforts in AMO and detector development (endstation systems) important for early turn on

User workshop held in Fall 2004

Stanford Linear Accelerator Center SSRL

Thrust areas:		SSRL/LCLS Contact
(1) Coherent scattering at the nanoscale	G.B. Stephenson* K. Ludwig	S. Brennan
(2) Pump/probe diffraction dynamics	K. Gaffney* D. Reis J. Larsson	A. Lindenberg
(3) High energy density (HED) physics	R. Lee* P. Heimann	J. B. Hastings
(4) Nano-particle/single molecule(non-periodic) imaging	J. Hajdu* J. Miao H. Chapman	J. Arthur
(5) Atomic, molecular, and optical science	L. DiMauro* N. Berrah	J. B. Hastings

* Team leader

Stanford Linear Accelerator Center

SSRL

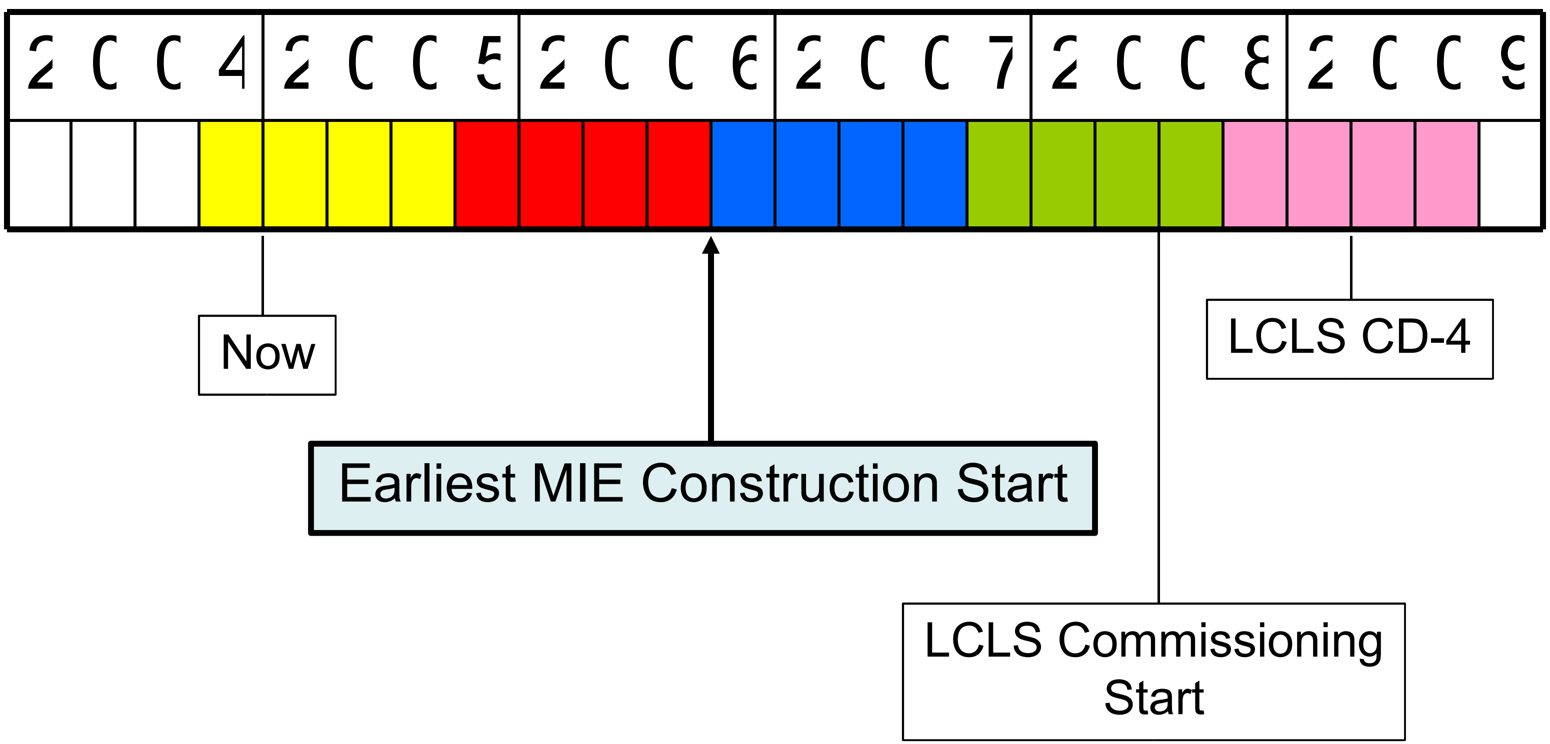
The way forward:
Major Item of Equipment

- Funded thru BES
- Science community develops the science case
- The project engineering and management is the responsibility of SLAC/SSRL
- Full rigor of DoE review is in place
- Insures compatibility, common design, ease of maintenance

MIE Cont'd
Team Responsibilities

- Thrust area teams responsible for the science
- Thrust area teams provide the specifications for the instruments
- Collaborate on the conceptual design
- As appropriate given responsibility for construction of specific components

Schedule



2004
2005
2006
2007
2008
2009
Now
Earliest MIE Construction Start
LCLS CD-4
LCLS Commissioning Start

LCLS Science Thrust Areas

- Atomic, Molecular, and Optical (AMO) science
- High-energy-density (HED) science
- Diffraction studies of stimulated dynamics
- Coherent-scattering studies of nanoscale fluctuations
- Nano-particle and single-molecule (non-periodic) imaging

BES approach to the Thrust Areas

- AMO science will be included in LCLS construction project
- HED science deemed to be outside the mission of BES

LUSI Scope

- Build instruments for hard x-rays that address 3 Thrust Areas: X-ray pump-probe, XPCS, Coherent x-ray imaging
- Include one additional instrument, to address the soft-x-ray portions of pump-probe and coherent imaging Thrust Areas
- Detector development

Detector Development

- LCLS experiments need new detector technology
- Dual development strategy for fast 2-d detectors
  - Several technologies look promising, no clear leader
  - LCLS will pursue one strategy
  - LUSI will try a different technology
  - Both prototypes should be ready by 2009

LUSI Phased Approach

- First LCLS light may come in mid-2008
- Budget will not support building 4 instruments by 2008

- Phased approach
  - 2 instruments in phase 1
    - *sufficient functionality by mid-2008 to begin experiments*
    - *phase 1 instruments can support early work in all four areas*
    - *complete phase 1 while phase 2 is ramping up*
  - remaining instruments in phase 2
    - *begin phase 2 after 2008*
  - complete all work in 2012

Role of the LCLS Science Teams

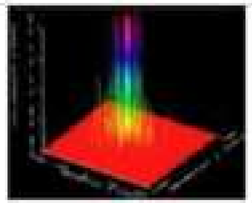
- Teams are responsible for preparing physics requirements for instruments
- Teams have designated leaders
- Quarterly meetings at SLAC with leaders
- Start weekly teleconferences soon
- Yearly general meeting
- Web site is up: <http://www-ssrl.slac.stanford.edu/lcls/lusi/>

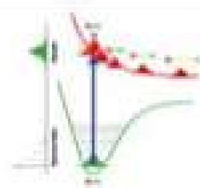
LUSI web site

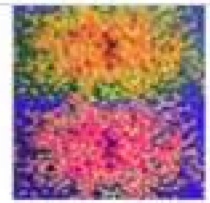
http://www-ssrl.slac.stanford.edu/lcls/lusi/

LCLS Ultrafast Science Instruments

LUSI







search

Go

- Home
- Project Pages
- LUSI Instruments
- Uniqueness of FEL X-rays
- X-ray FEL Science
- About LCLS
- Science with LCLS
- Calendar & Meetings
- Contact Us

A suite of x-ray instruments for exploiting the unique scientific capability of the Linac Coherent Light Source will be produced by the LUSI project. LUSI hopes to receive major funding starting in 2007, and to build four instruments over a period of about five years. Two of these instruments will be optimized for hard x-ray studies of ultrafast dynamics at the atomic level, addressing basic problems in chemistry and materials science. A third instrument will concentrate on hard x-ray coherent imaging of nano-particles and large biomolecules. The fourth instrument will give LCLS the capability of using soft x-rays to study magnetic structures and surface chemistry. These instruments will complement other instruments at LCLS, which are directed towards atomic physics and plasma physics. A summary of LCLS scientific applications can be found here.

Current News:

Job Openings

Meetings:

LUSI Science Group Leaders Meeting October 18-19

SSRL User Meeting - Soft X-ray Workshop Oct 18-19

SSRL User Meeting Oct 15-19, 2005

LCLS FAC Meeting Oct 27 -28, 2005

Office of Science/ U.S. D.O.E.

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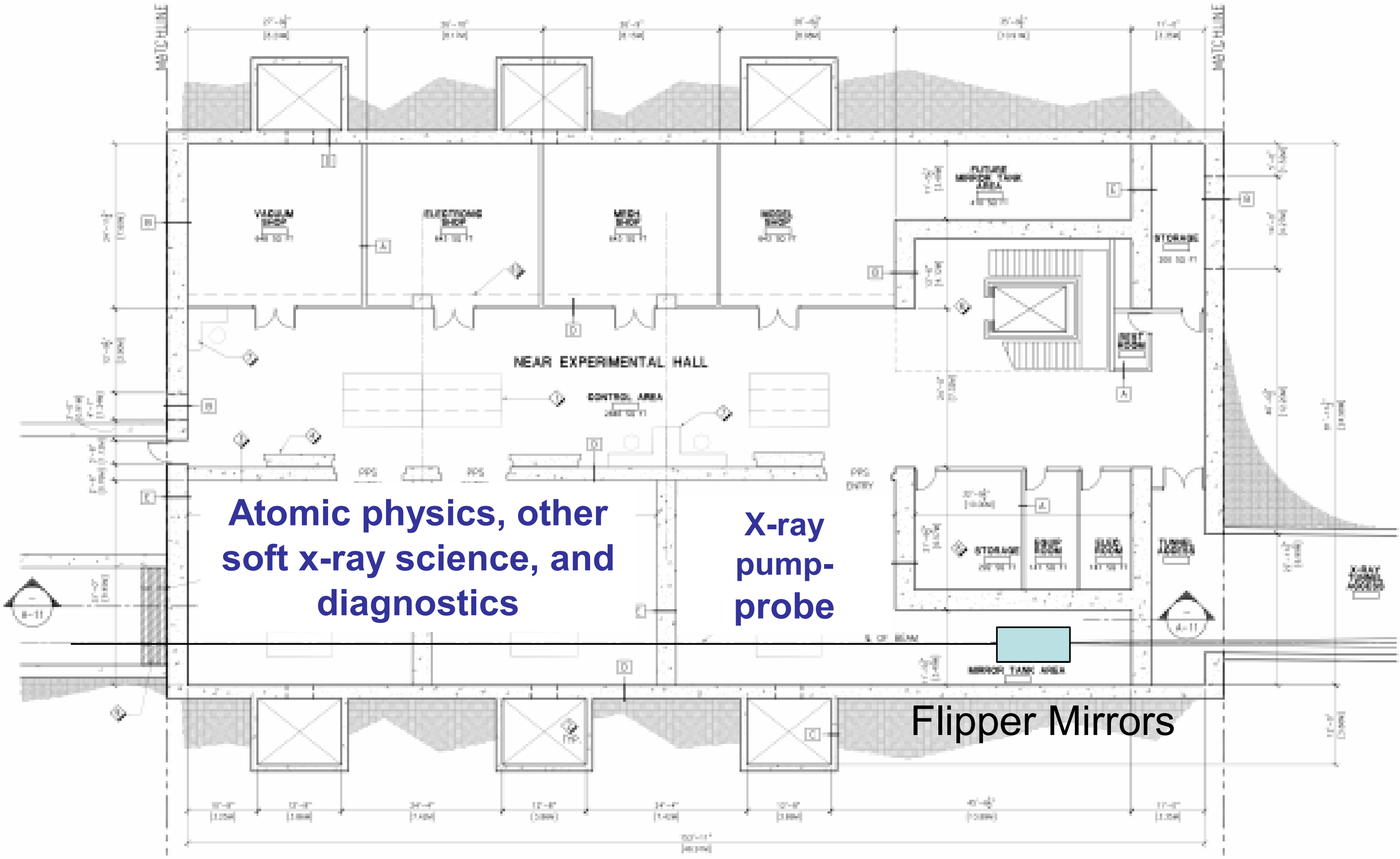
Steps to achieve CDR

- Instrument concept
  - optics, sample, detector, controls
- First level design
  - ray trace, signal rates
- Design review — Oct-Nov 2005
- Second level design — Jan 1, 2006
  - component choice, layout, costing
- CDR first draft — Feb 1, 2006
- Lehman review — June 2006

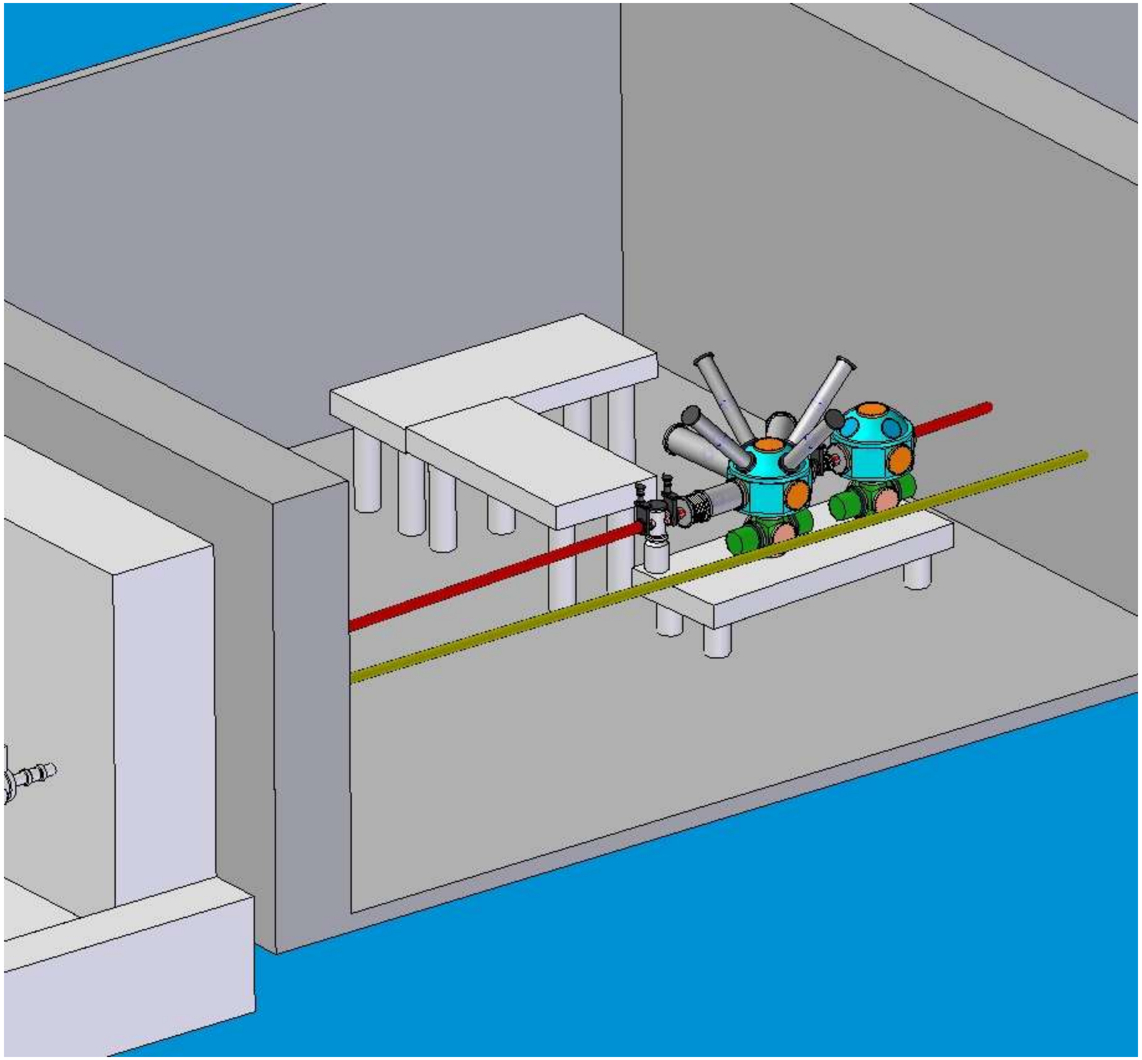
Latest LUSI Progress

- CD0 signed in August, project is official
- Initial hiring taking place
- Input from potential users is helping to define instruments
- Working closely with XES and XTOD groups to develop an optimal layout for experiments

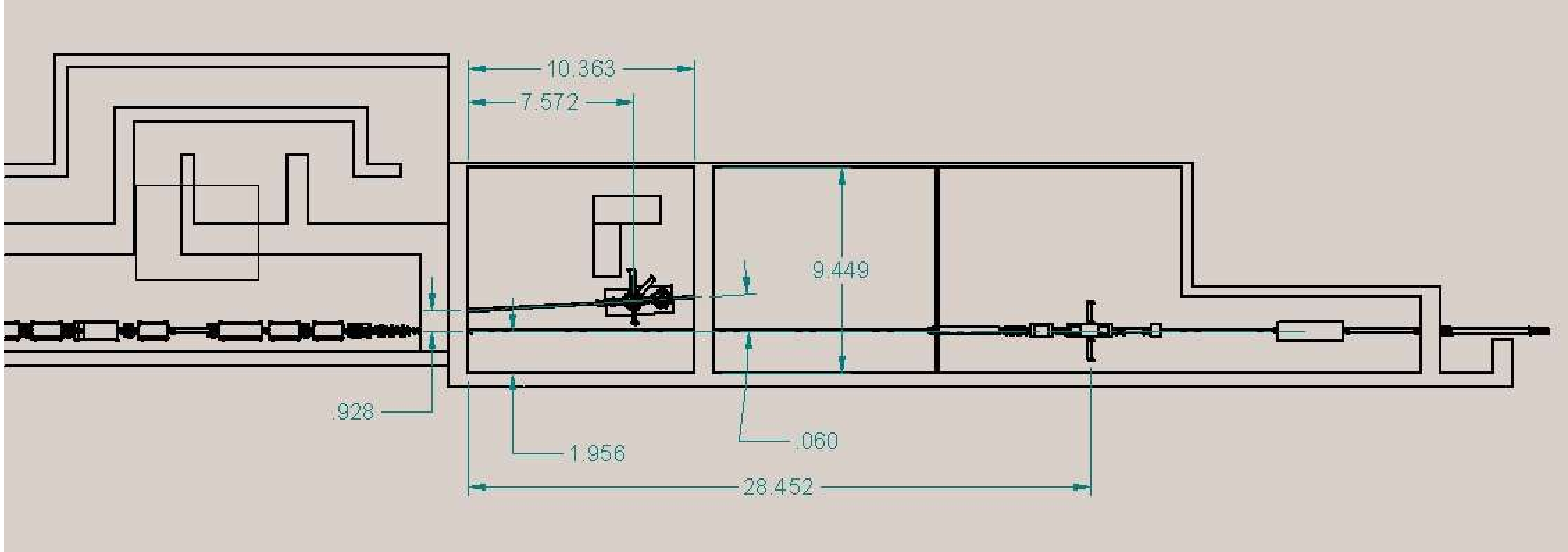
NEH


NEAR EXPERIMENTAL HALL
CONTROL AREA
STORAGE
MIRROR TANK AREA
Atomic physics, other soft x-ray science, and diagnostics
X-ray pump-probe
Flipper Mirrors

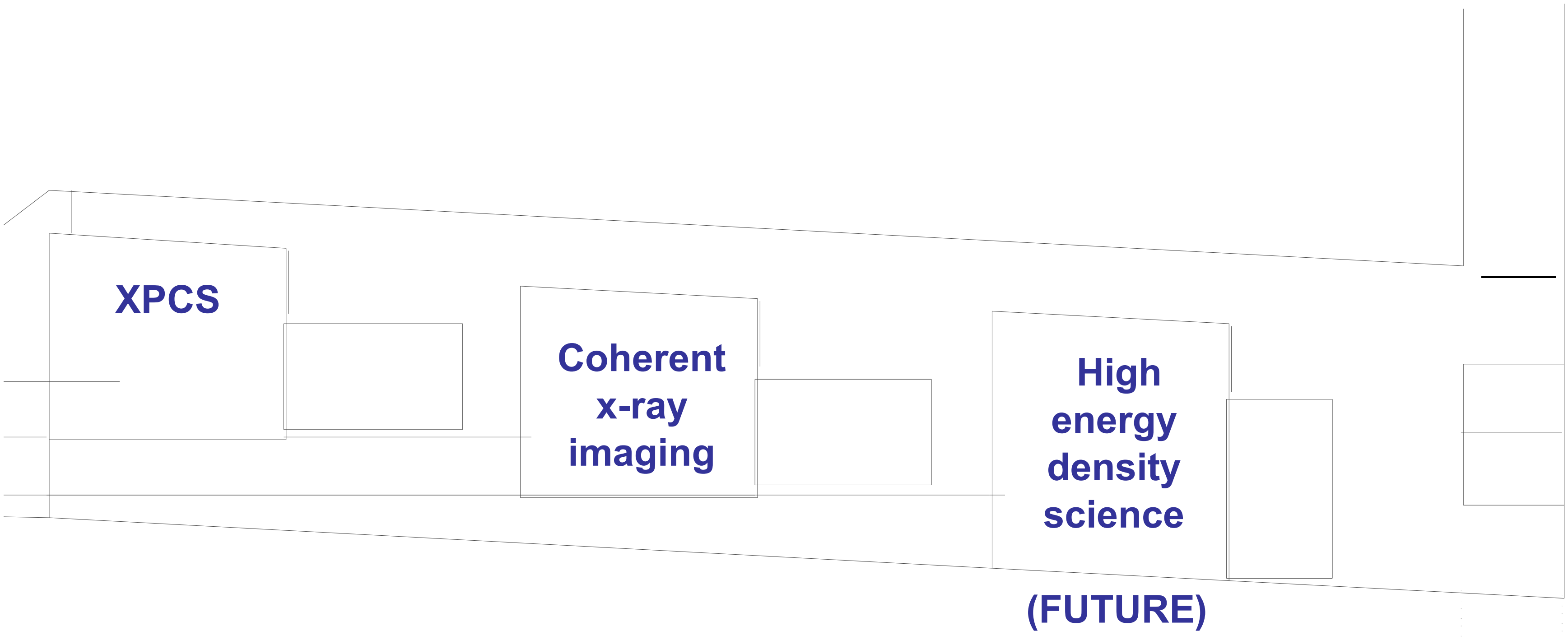
CAD layouts are used to see how instrumentation fits in hutches



A soft x-ray pick-off mirror in the FEE could provide a 'soft x-ray beamline' for Hutch 1 (and maybe Hutch 2), allowing easy switching between experiments

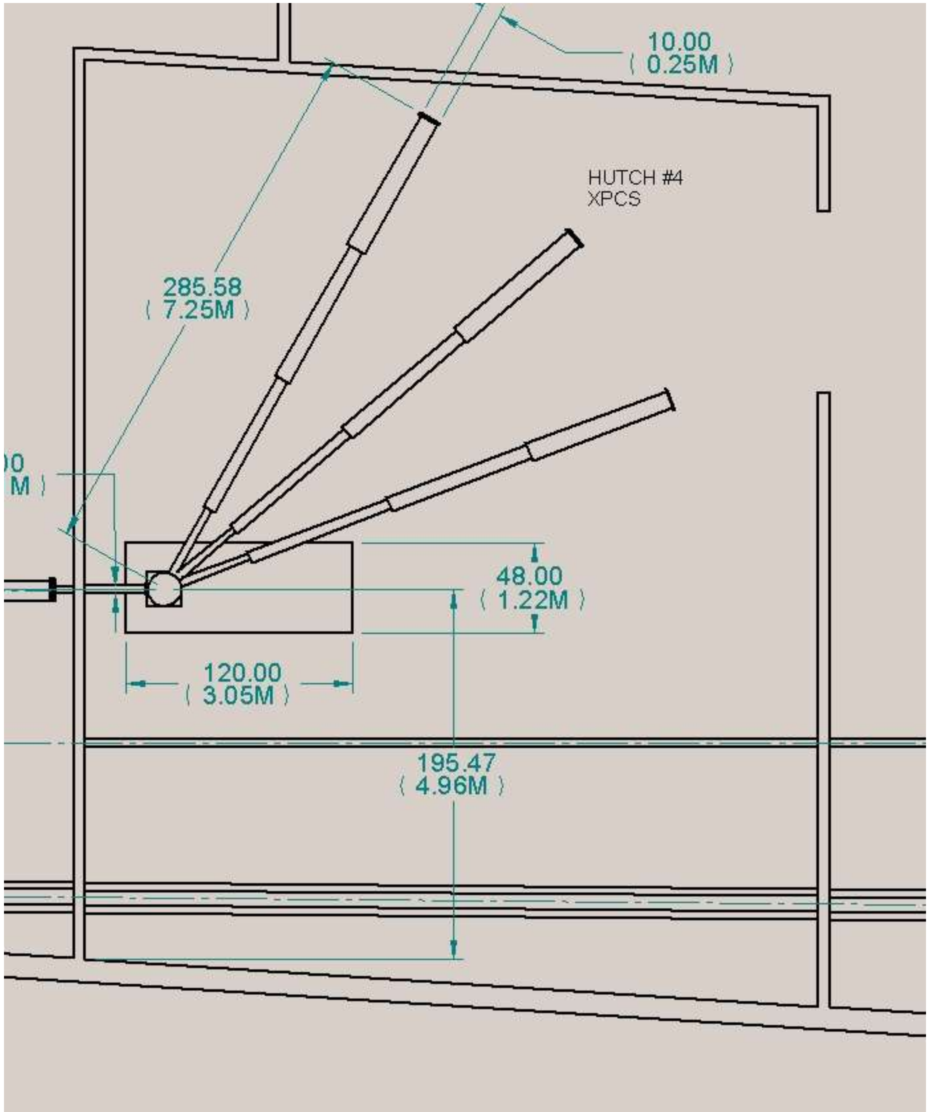


FEH


XPCS
Coherent x-ray imaging
High energy density science
(FUTURE)

Very large hutches can accommodate large instruments

(XPCS concept with vacuum flight path longer than 5 m)



Plans for FY2006

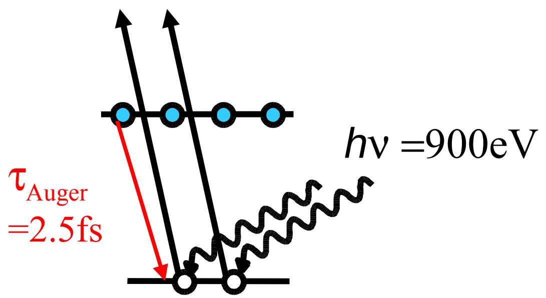
- Initial funding has been provided ($1.9M)
- Staff up, including 3 Instrument Scientists
- Prepare CDR
- Lehman review in ~June
- Continue design
- Another Lehman review in ~October

LUSI Summary

- LUSI is on schedule now but needs to pick up the pace
- Will build 4 unique instruments, plus detector R&D
- The next year will be very interesting

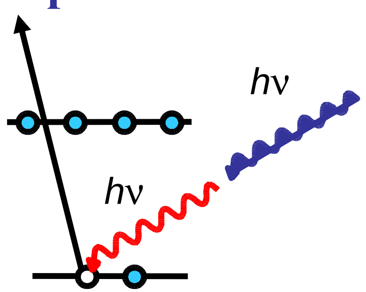
Atomic Physics

Formation of Hollow Atoms:



Most basic LCLS experiments, aimed at understanding the physics of interaction of intense, ultra-fast pulse with atoms

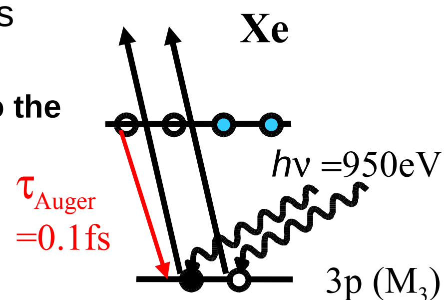
Multiphoton Ionization:



Giant Coulomb explosions of Xe clusters

10^9 atoms

Understanding is central to the imaging of biomolecules



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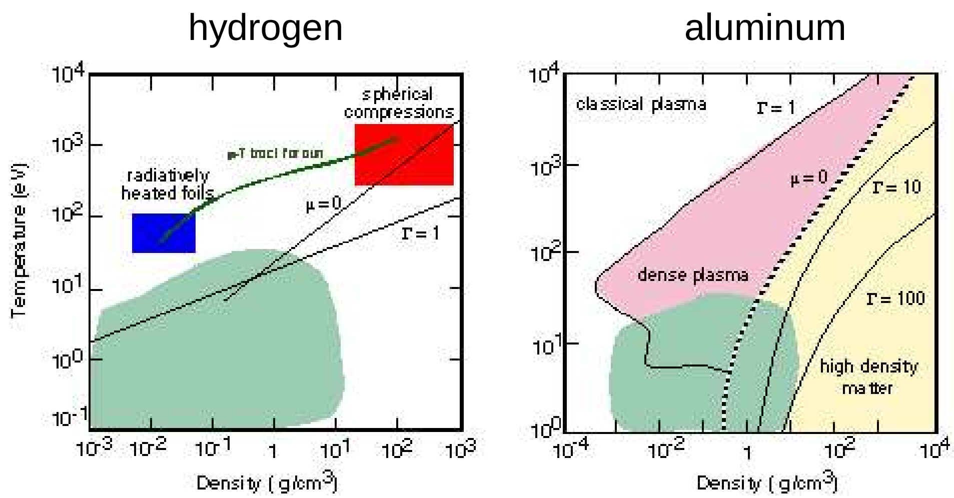
Studies of Warm Dense Matter

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

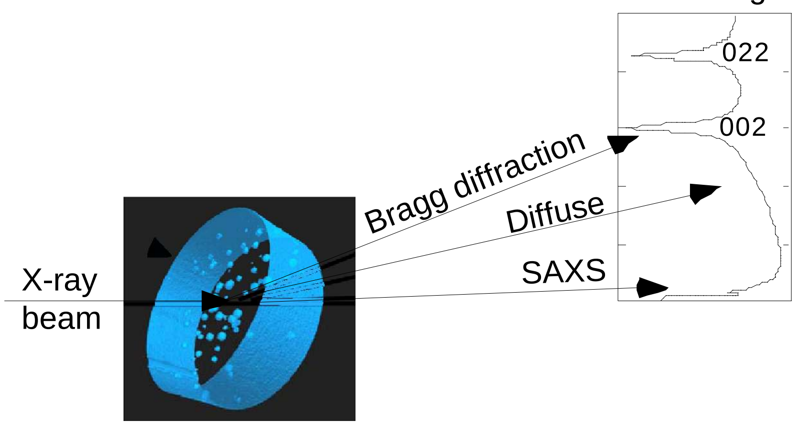


Γ = ratio between electric and thermal potential energy
μ = chemical potential (atom interaction potential)

Astrophysical studies lie in the area of warm dense matter. Largest uncertainties in many applied research areas of chemistry and physics come in the warm dense regime

Intense x-ray probes can characterize the states of heated and compressed matter

Classic X-ray Scattering provides structure data

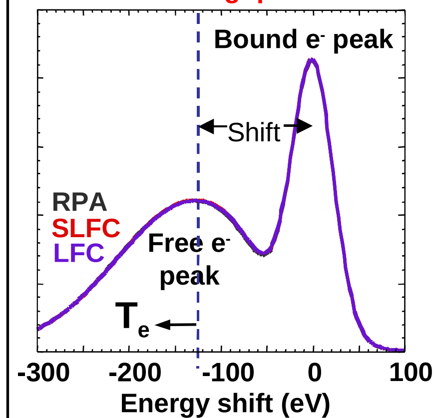


- **Currently we only have capability to study recovered samples**

- ***Diffraction → lattice compression and phase change***
- ***Diffuse → dislocation content and lattice disorder***
- ***SAXS → sub-micron defect scattering***

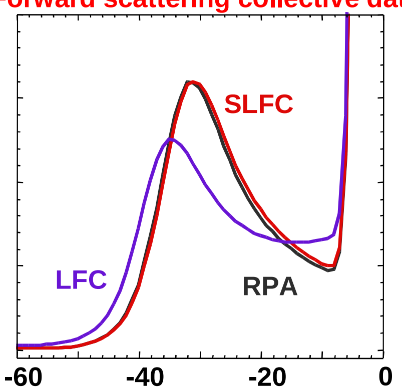
Current Status:
Thomson scattering

Back scattering: particle data



- provide direct measure of T_e

Forward scattering collective data



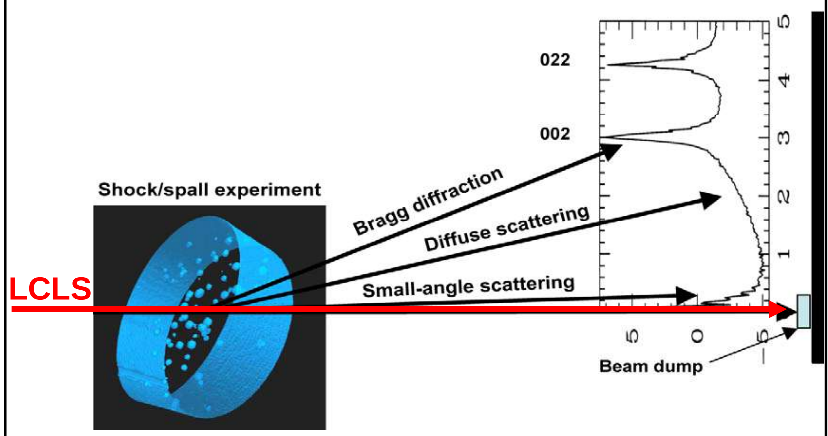
- Models disagree and no data

- ***Forward → large size scale → collective modes***
- ***Back → small size scale → bound e⁻, free e⁻, f(v)***

Challenge is to match experimental and theoretical capabilities for HED studies

Future:

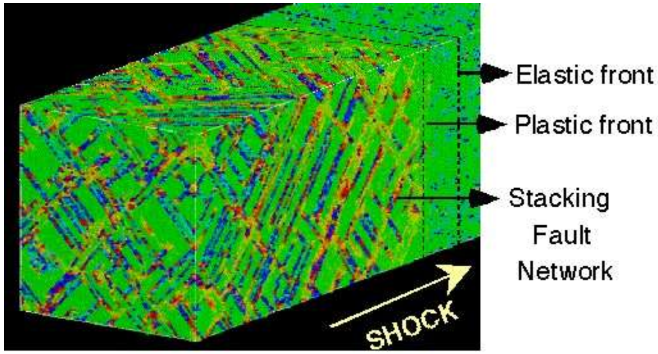
Same measurements during shock



- **LCLS will provide unprecedented fidelity to measure dynamics of the microstate with sub-picosecond resolution**

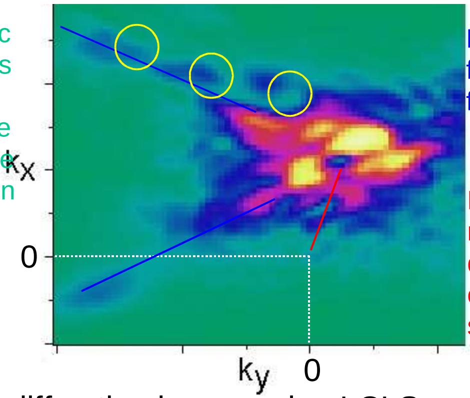
Current Status

Elastic Scattering



- MD simulation of FCC Cu taking 400,00 CPU hours

Periodic features => average distance between faults



Diffuse scattering from stacking fault

Peak diffraction moves from 0,0 due to relaxation of lattice under shock

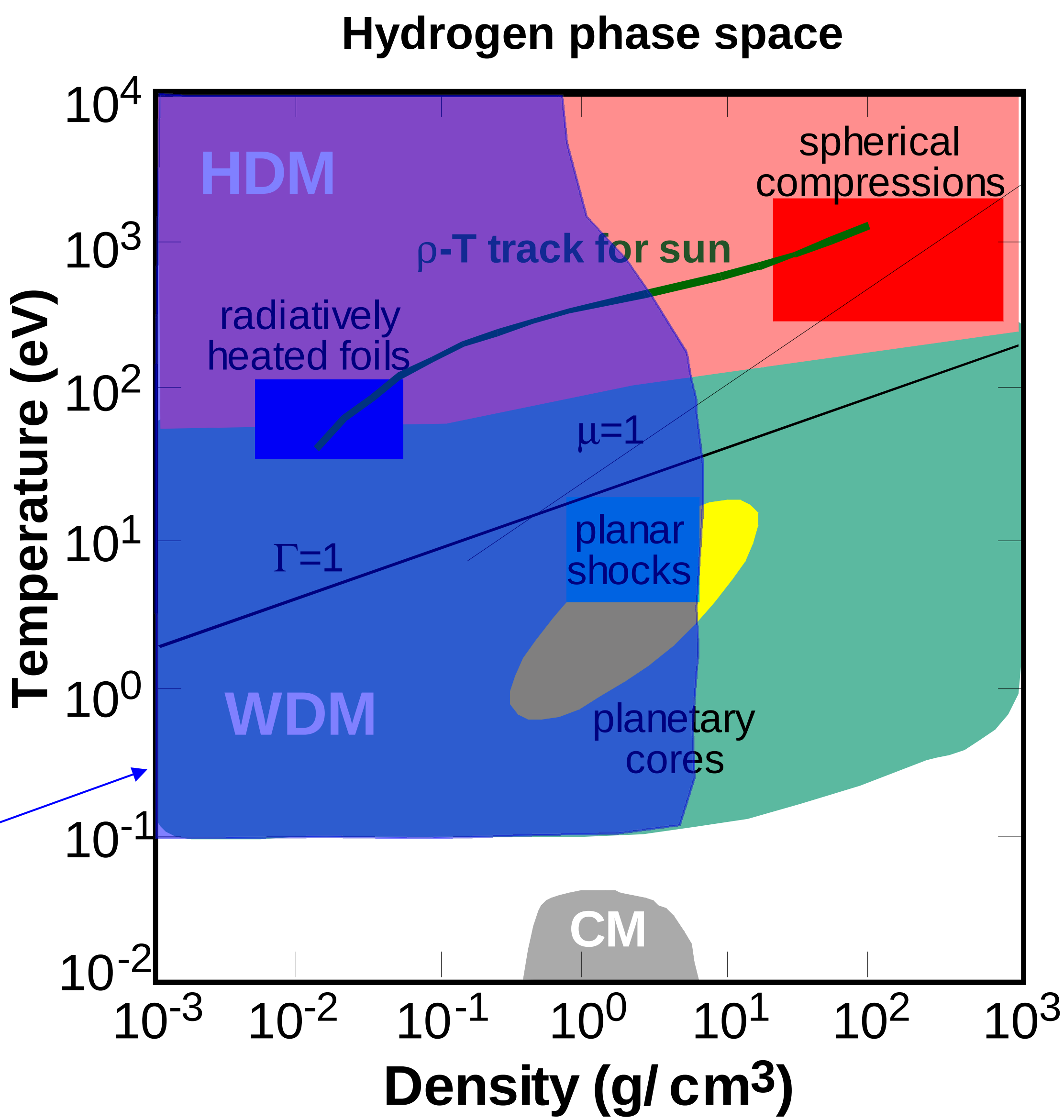
- X-ray diffraction image using LCLS probe of the (002) shows *in situ* stacking fault information

Hot Dense Matter (HDM)

- Supernova, stellar interiors, accretion disks
- Plasma devices: laser produced plasmas, Z-pinches
- Directly and indirectly driven inertial fusion experiments

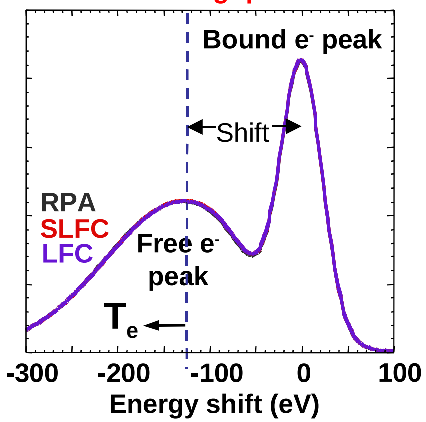
•Access large parts of the HED phase space with:

- End station with high energy long pulse laser and intense short pulse laser



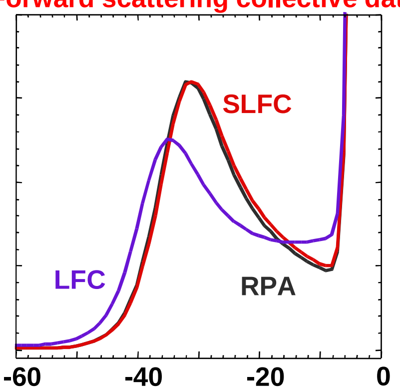
Current Status: Thomson scattering

Back scattering: particle data



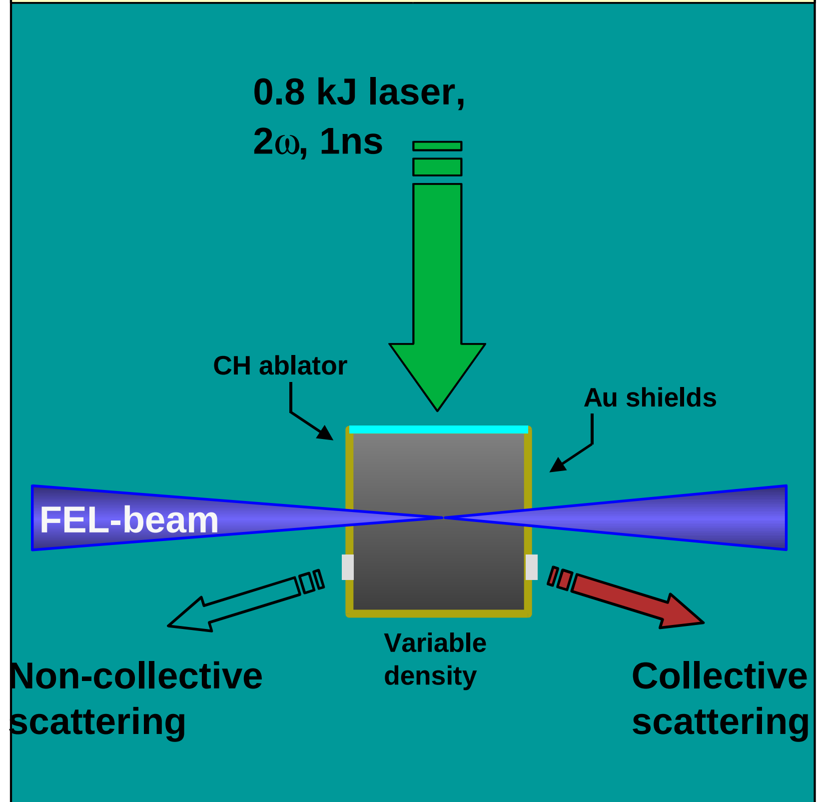
• provide direct measure of T_e

Forward scattering collective data



• Models disagree and no data

Future



All current measurements maintained.
Add direct, *in situ*, measurement of
temperature and densities.

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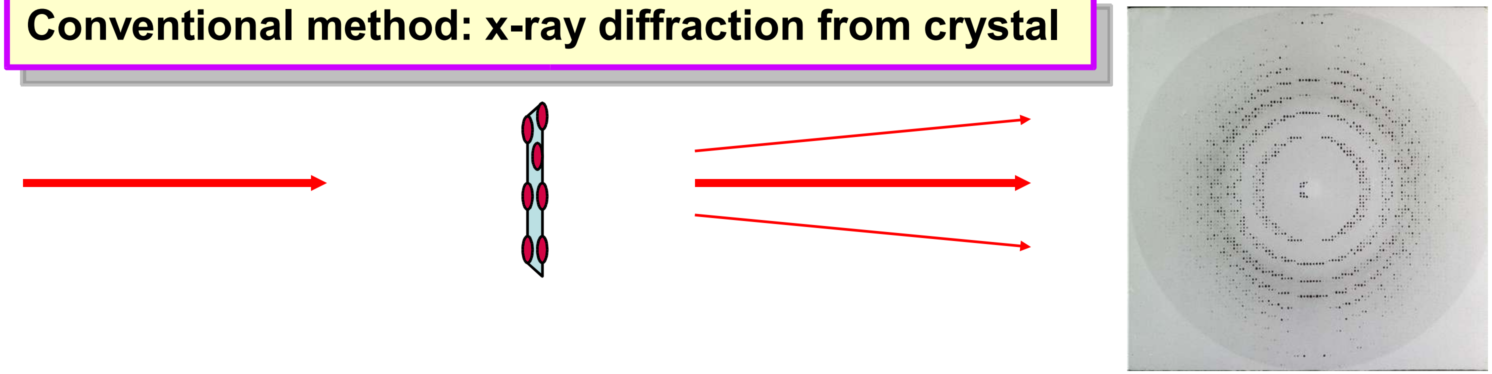
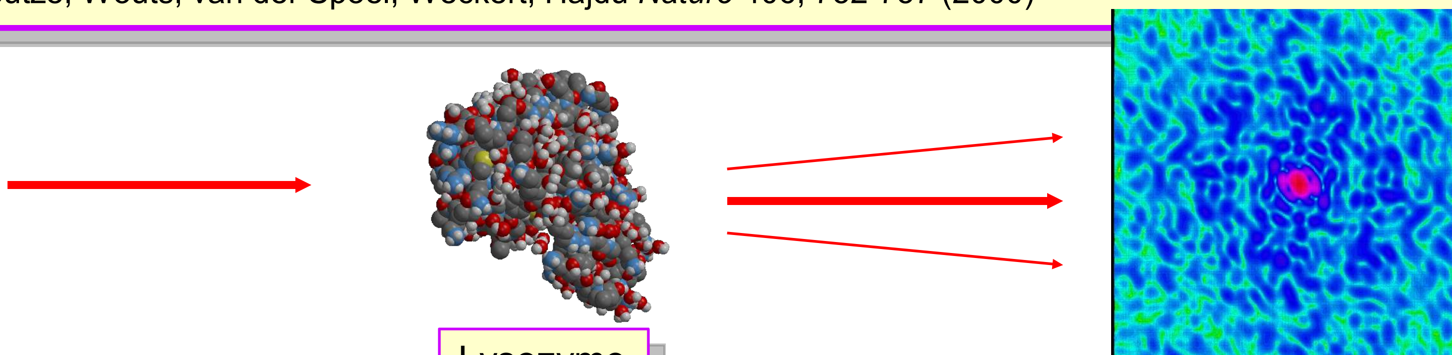
Structural Studies on Single Particles and Biomolecules

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)



Lysozyme

Calculated scattering pattern from lysozyme molecule

Implementation limited by radiation damage:

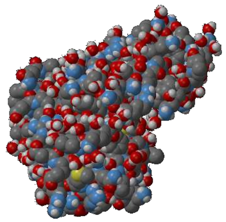
In **crystals** limit to damage tolerance is about **200 x-ray photons/Å^2**

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

X-Ray Diffraction from a Single Molecules

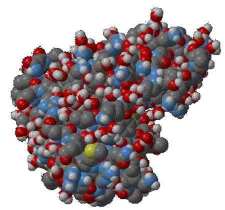
A bright idea:

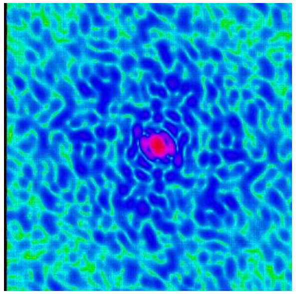
Use ultra-short, intense x-ray pulse to produce scattering pattern before molecule explodes



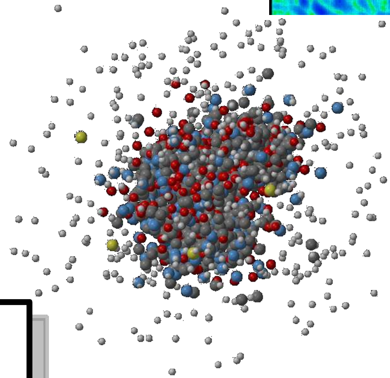
Just before LCLS pulse

Just after pulse





Long after pulse



The million dollar question: Can we produce an x-ray pulse that is

short enough?

intense enough?

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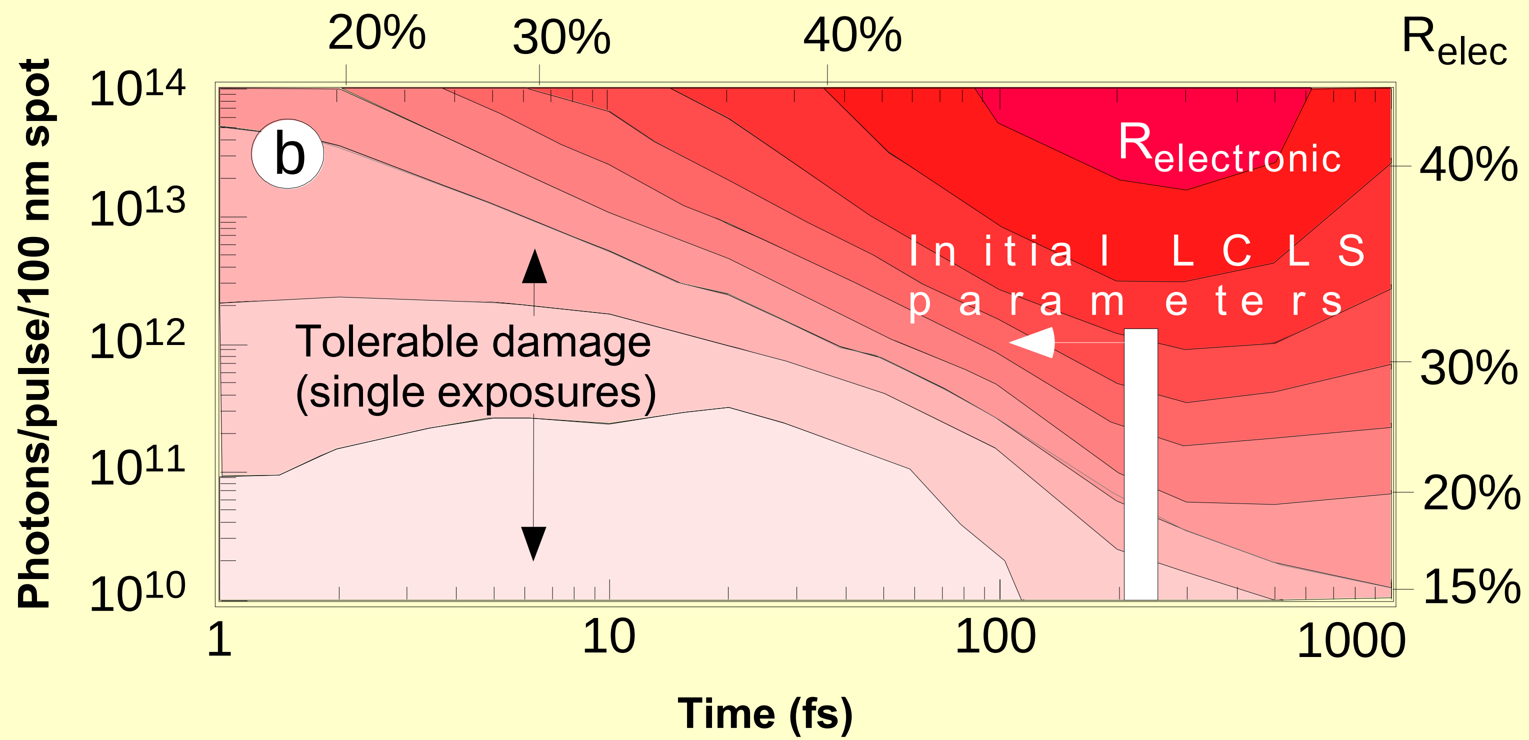
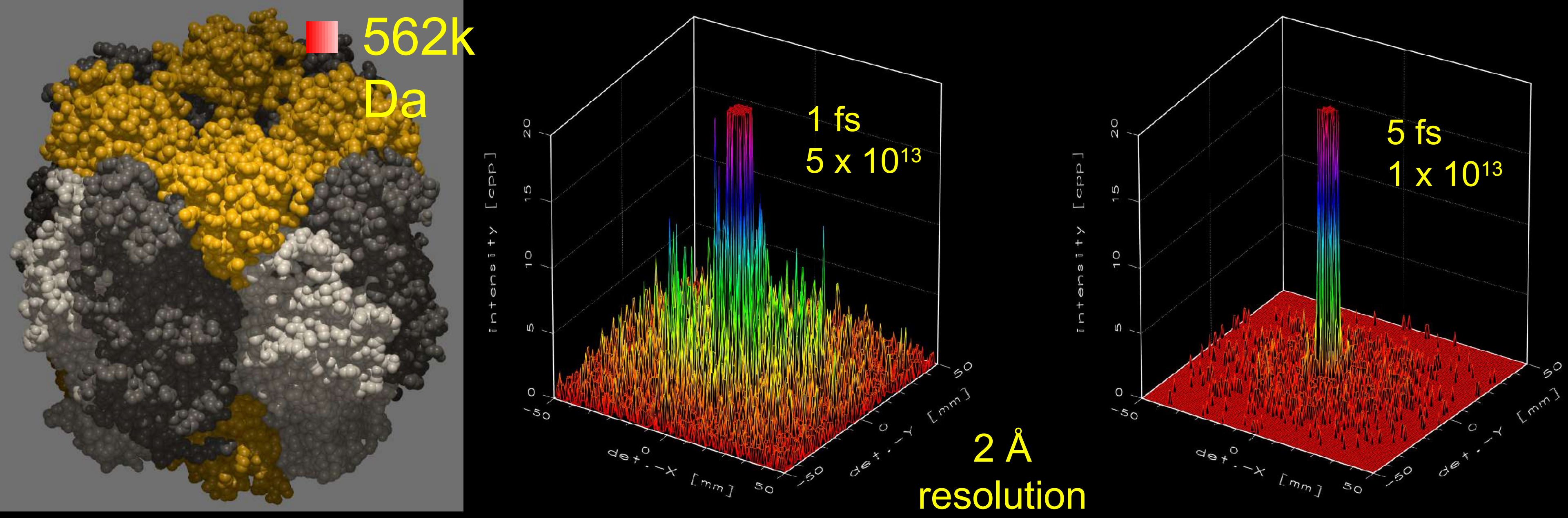
Landscape of Damage Tolerance

Ionisation and subsequent sample explosion causes diffraction intensities to change

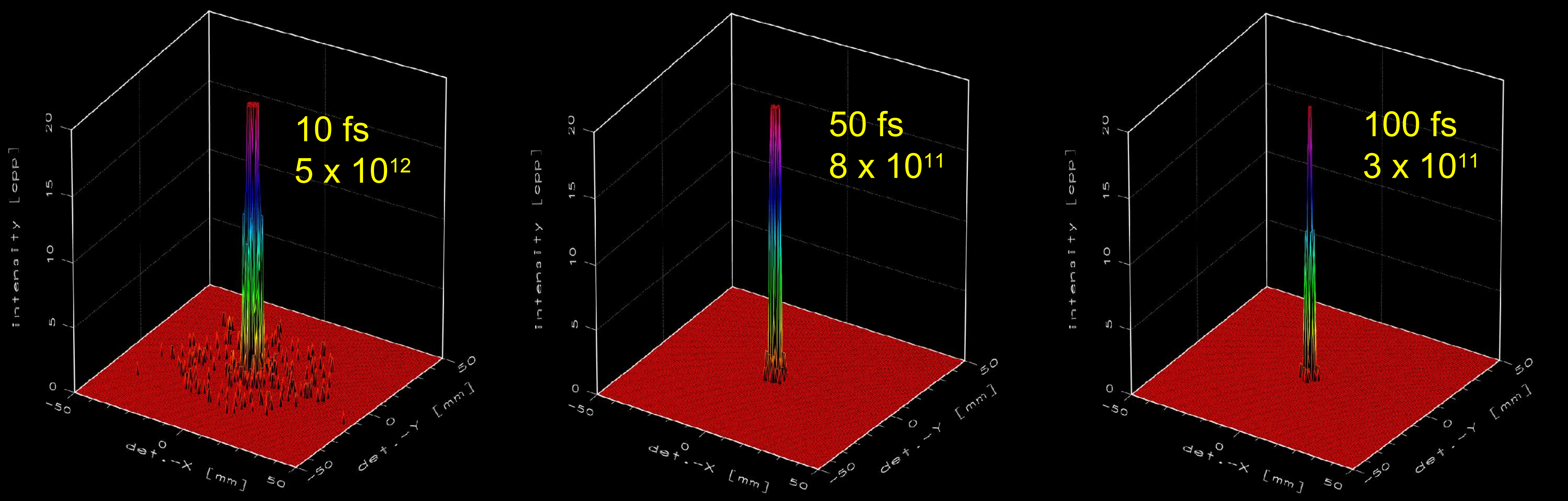
Agreement factor:

$$R = \frac{\left| \sqrt{I(t)} - \sqrt{I_o} \right|}{\sqrt{I_o}}$$





Predicted scattering from a single RUBISCO molecule ($R_{electronic}$ = 15%)



Nanocrystal of lysozyme