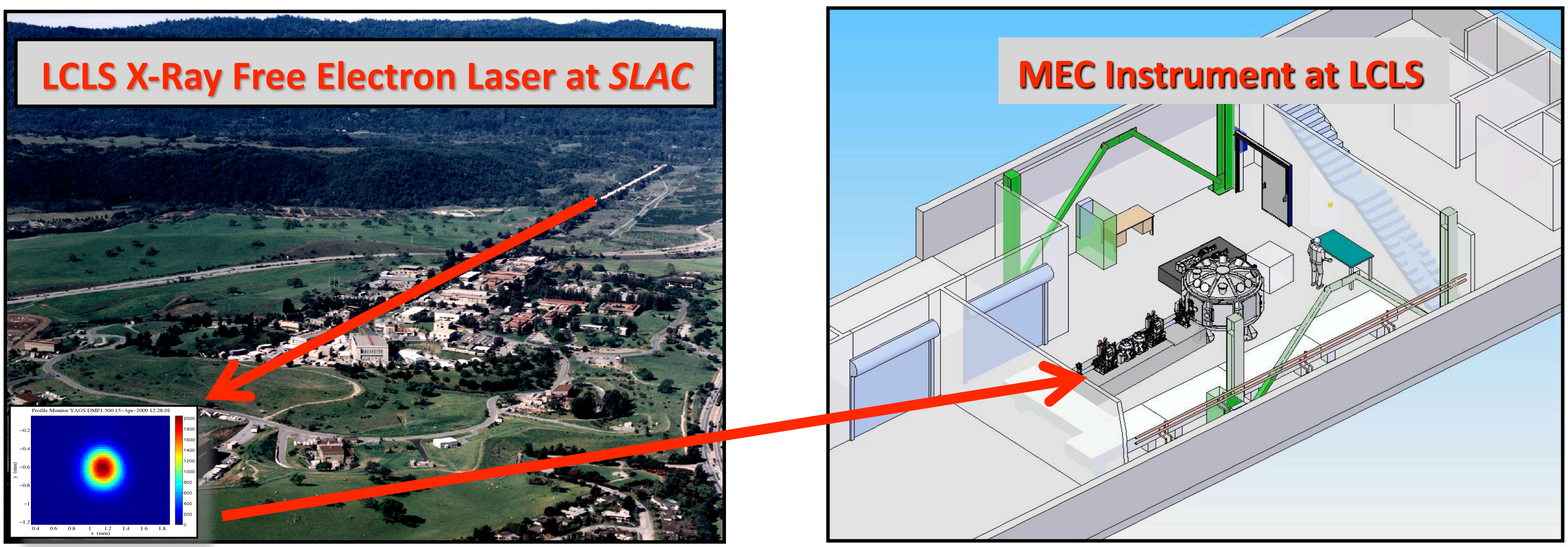
New FES-Funded Activity
at the SLAC National Accelerator Laboratory

- **High Energy Density Science**
- **At the LCLS X-Ray Free Electron Laser**
- **Using the Matter in Extreme Conditions (MEC) Instrument**

Roger Falcone
UC Berkeley and LBNL



FESAC 3/10/08

MEC at LCLS: The Context

- LCLS project in commissioning stage with early experiments
  - 6 beamlines have received funding
    - AMO = atomic and molecular science, under LCLS project
    - SXR = soft x-ray materials science, international consortium
    - XPP = hard x-ray pump and probe
    - PCS = photon speckle correlation spectroscopy
    - CXI = coherent x-ray imaging of nano-scale object
    - MEC = matter in extreme conditions
    - (XPP, PCS, CXI: LUSI MIE)
  - x-ray laser works well; early experiments successful
  - BES indicates possible funding for LCLS II - extends spectral range & capacity

- Key properties of LCLS x-ray laser beam for MEC science
  - tunability = spectroscopy and optimal Thomson scattering
  - coherence = diffractive imaging
  - intensity = heating matter
  - ultrafast = imaging of dynamics

- FES - ARRA funding of MEC instrument

- BES plans funding of MEC operations, as for other 5 LCLS instruments

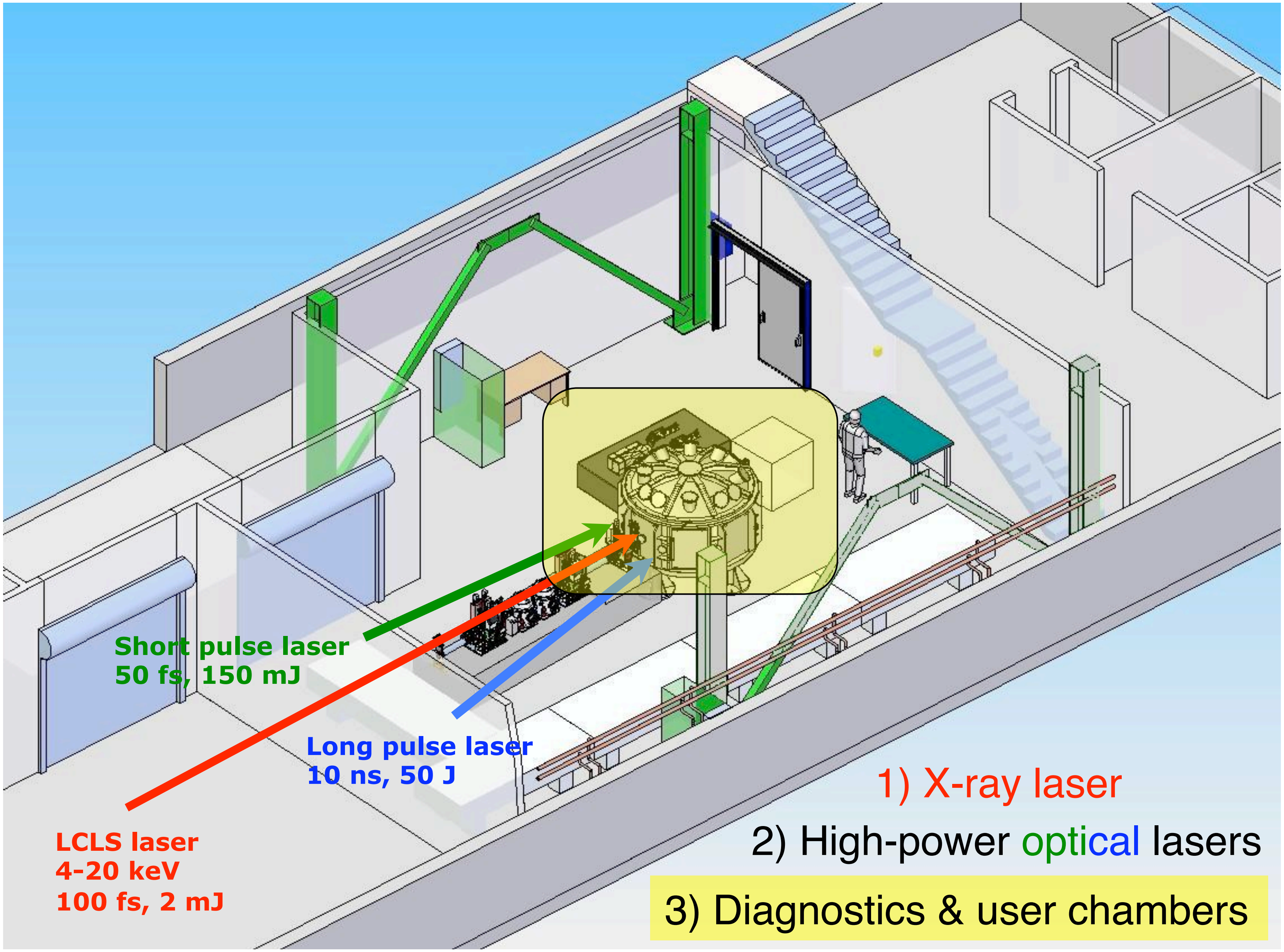
- Interest at SLAC for development of locally led program by leading PI

- Need for a national program in HED science summarized by ReNeW (Rosner)

MEC at LCLS: The Context

- Open access general user facility funded by DoE Basic Energy Sciences focused on *Best Science*
- Keys to success
  - Fully instrumented endstation permitting ‘single investigator’ research. *MEC funded by FES ARRA*
  - Fully funded endstation operations, including staff and consumables to support ‘single investigator’ research. *Funded by BES*
  - Strong in-house research program to interact with the user community *To be funded by FES*
  - Funding for proposal driven peer reviewed research. *To be funded by FES*

Layout of the MEC Instrument



Parameters of the MEC instrument

1. LCLS Parameters at MEC: Intense x-ray source, short pulse, coherent, and tunable

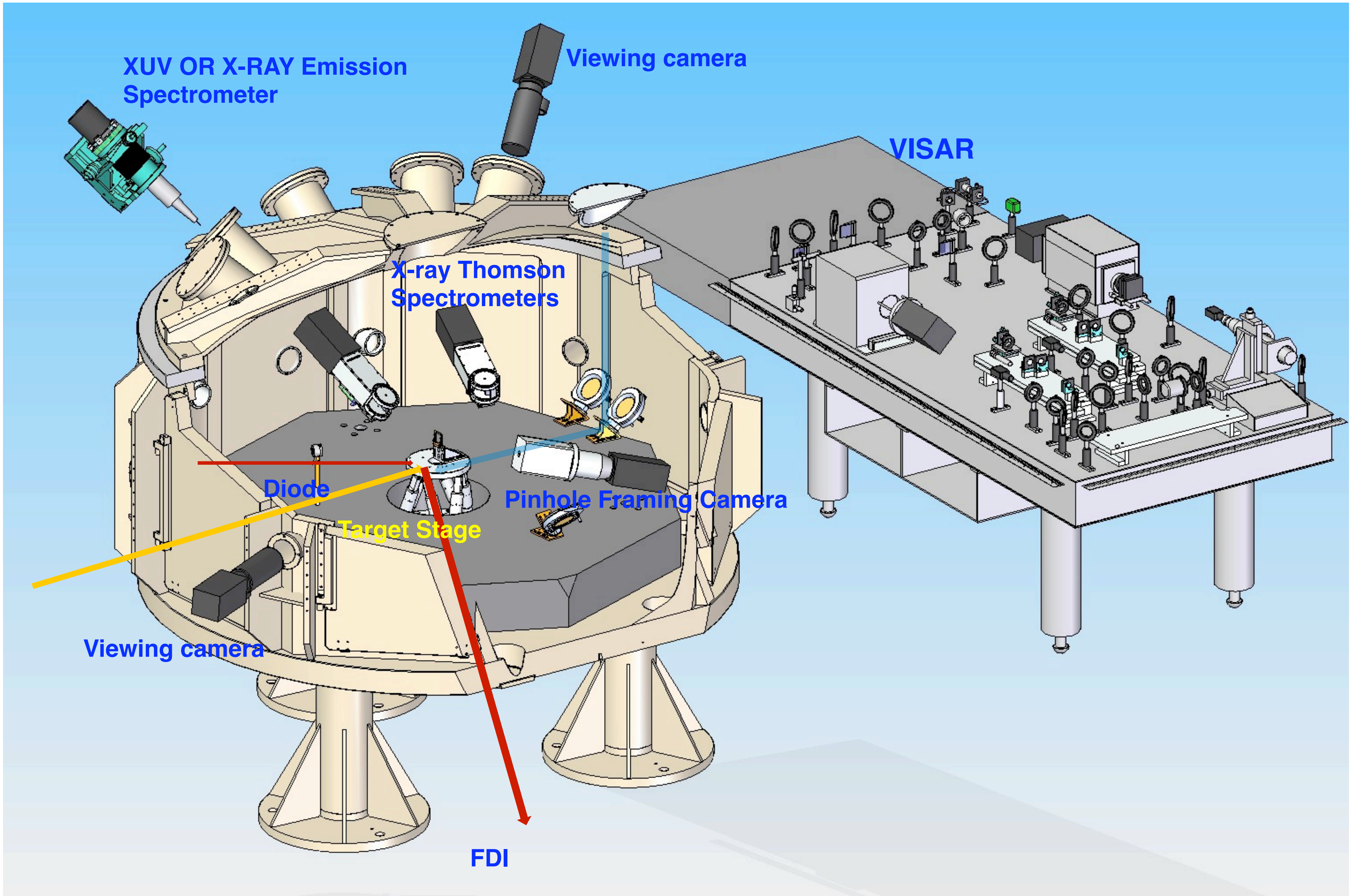
Parameter	Value	Units	Notes
Photon energy range	4.0-20	keV	optics transmission limited
Pulse energy	1.0-1.5	mJ	harmonics at reduced energy
Pulse duration	2-300	fs	ultrafast limit to be confirmed
Spot size	0.5-50	micron	optics limited
Repetition rate	one pulse to 120 Hz		pulse picker

2. MEC LASER systems:

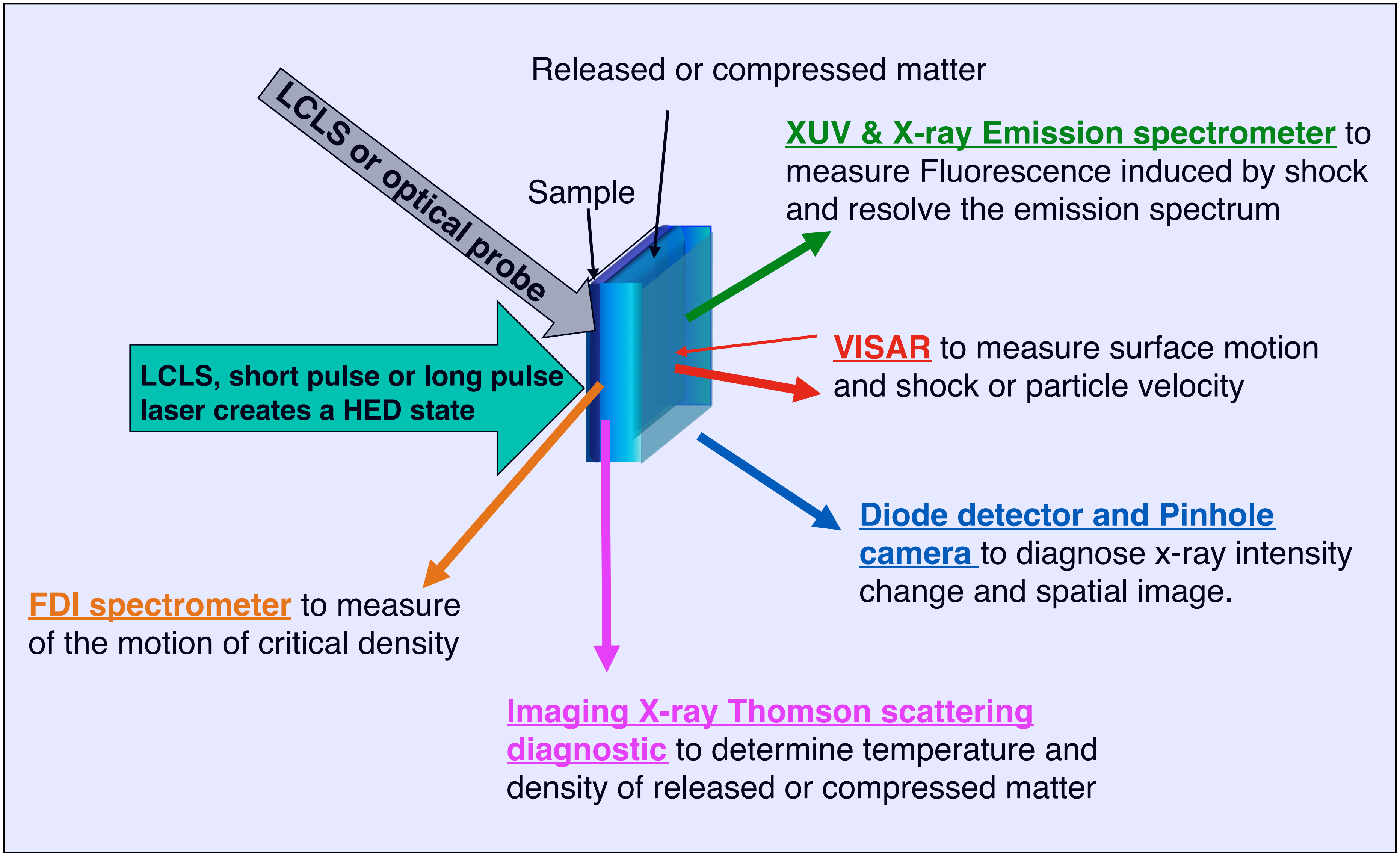
	Short Pulse Laser		Long Pulse Laser	
Parameters	Value	Units	Values	Units
Wavelength	800	nm	527	nm
Pulse width	35	fs	2-200	ns
Repetition rate	10, 30, 120	Hz	1 shot	10 min
Pulse energy	150	mJ	50	J

3. Suite of Target Diagnostics: measure the physical properties of matter in extreme conditions

MEC Instrument: Target Chamber and Diagnostics



Schematic of typical experiment and diagnostics



Now, the science: Interest in HEDS is growing within the scientific community

- *Joint Research Needs Workshop on High Energy Density Laboratory Plasmas*, November 2009 (Rosner presentation)

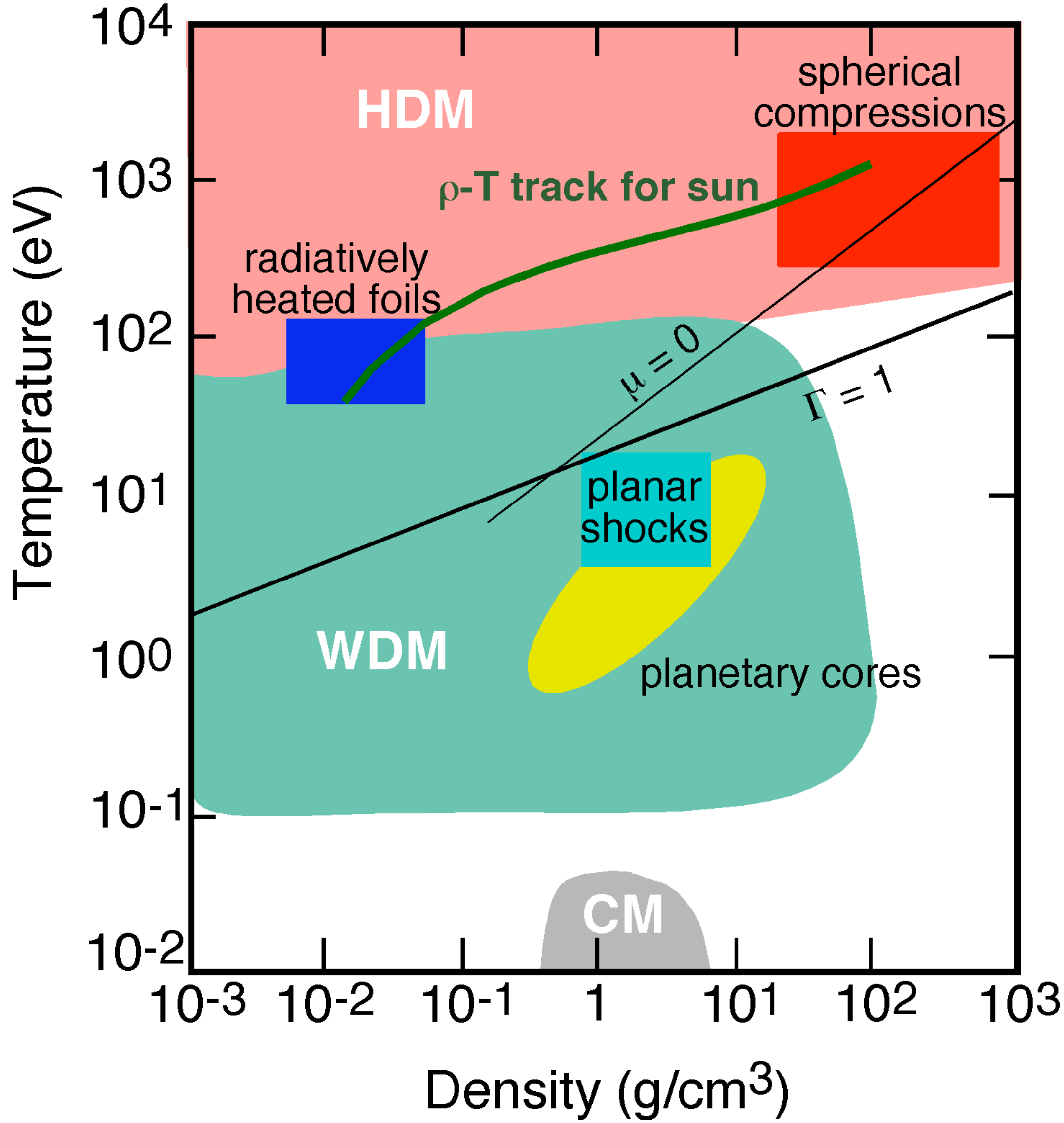
- *Advancing the Science of High Energy Density Laboratory Plasmas*, prepared by FESAC Panel on High Energy Density Laboratory Plasmas (Betti, Chair)

- Facilities are now available that will enable the study of matter under extreme conditions of temperature and pressure

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
  - Systems that start solid and end as a plasma
  - X-ray driven inertial fusion experiments

Hydrogen phase diagram



A HEDS experimental program at LCLS will cover broad range of applications

Experiment	Description
Warm Dense Matter Creation	Using the XFEL to uniformly warm solid density samples
Equation of State	Heat / probe solids with XFEL to obtain material properties
Absorption Spectroscopy	Heat solids with optical laser or XFEL / use XFEL to probe
High Pressure Phenomena	Create high pressure with high-energy laser, probe with the XFEL
Surface Studies	Probe ablation/damage processes
XFEL / Gas Interaction	Create exotic, long-lived highly perturbed electron distribution functions in dense plasmas
XFEL / Solid Interaction	XFEL directly creates extreme states of matter
Plasma Spectroscopy	XFEL pump/probe for atomic state
Diagnostic Development	Develop Thomson scattering, SAXS, interferometry, and radiography

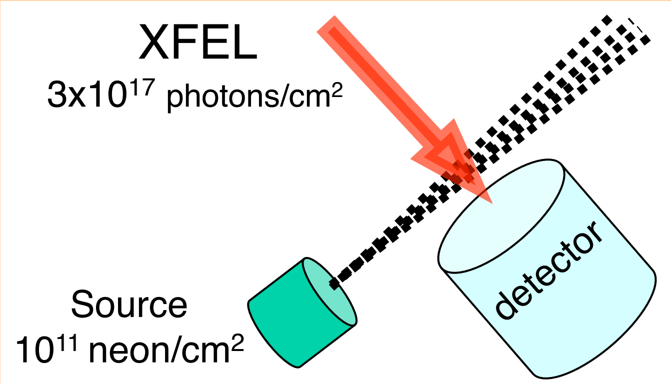
Hot Dense Matter

For Hot Dense Matter (HDM) the short-pulse, intense x-ray source creates a unique initial state

- Population kinetics is complex for realistic cases
  - The model construct requires vast amounts of atomic data
    - Atomic data: Energy levels, oscillator strengths, autoionization rates
    - Collisional cross-sections for excitation (BB) and ionization (BF) processes
  - Due to the vast number of states and the effects of the plasma environment, additional model assumptions are required
    - Ionization potential depression
    - Rydberg states
    - Level details
- Comparisons with benchmark data would be a key to make progress
  - However, there are very, very few cases where the plasma temperature, density, charges state distribution and spectrum have been measured.

LCLS provides an opportunity for HED plasma spectroscopy – synergy with AMO science

- AMO atomic physics case:
  - Source for hollow ion experiment prepared as an atomic beam

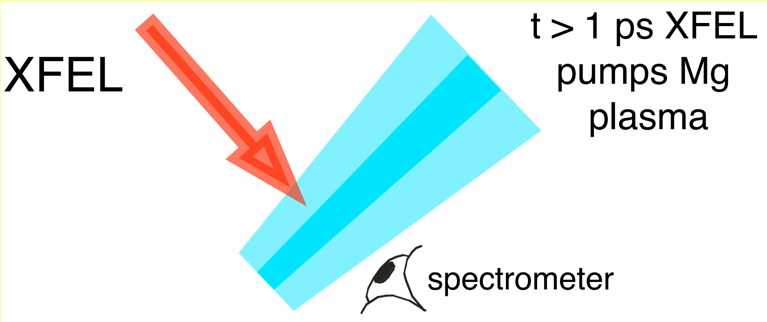


- **Photoionization**:
  $Ne+h\nu_{>870eV} \rightarrow Ne^{+*}(K)+e$
- **Auger Decay:**
  $Ne+h\nu_{>870eV} \rightarrow Ne^{+*}(K)+e \rightarrow Ne^{2+*}(LL)+e \rightarrow Ne^{3+*}+e$

XFEL only

- **Sequential multiphoton ionization:**
  $Ne+h\nu_{>870eV} \rightarrow Ne^{+*}(K)+e+h\nu_{>993eV} \rightarrow Ne^{2+*}(KK)+e \rightarrow Ne^{3+}+e \rightarrow Ne^{4+}+e \rightarrow \ldots$
  $Ne+h\nu_{>870eV} \rightarrow Ne^{+*}(K)+e+h\nu_{>993eV} \rightarrow Ne^{3+*}(KLL)+e$
- **Direct multiphoton ionization:**
  $Ne+2h\nu_{>932eV} \rightarrow Ne^{2+*}(KK)+2e$

- HED 'atomic physics' case:
  - Source for hollow ion experiment prepared by high energy laser



- Study the $K^0L^yM^z \rightarrow K^1L^{y-1}M^z+h\nu_{emitted}$

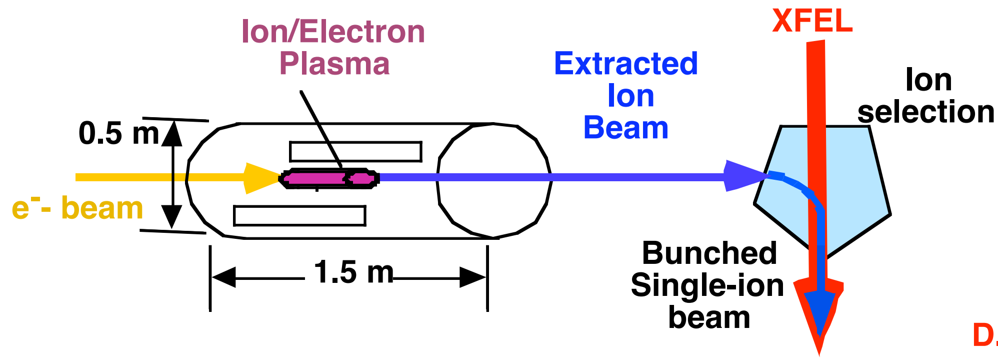
- **Photoionization of multiple ion species**:
  $K^xL^yM^z+h\nu_{XFEL} \rightarrow K^{x-1}L^yM^z+e$ (x=1,2; y=1-8; z=1,2)
- **Auger Decay of multiple ion species:**
  $K^xL^yM^z+h\nu_{XFEL} \rightarrow K^{x-1}L^yM^z+e \rightarrow K^xL^{y-2}M^z+e$
- **Sequential multiphoton ionization:**
  $K^xL^yM^z+h\nu_{XFEL} \rightarrow K^{x-1}L^yM^z+e+h\nu_{XFEL} \rightarrow K^0L^yM^z+e+h\nu_{XFEL} \rightarrow K^0L^{y-1}M^z+e+h\nu_{XFEL} \rightarrow \ldots$
  $K^xL^yM^z+h\nu_{XFEL} \rightarrow K^{x-1}L^yM^z+e+h\nu_{XFEL} \rightarrow K^{x-1}L^{y-2}M^z+2e$
- **Direct multiphoton ionization:**
  $K^xL^yM^z+2h\nu_{XFEL} \rightarrow K^0L^yM^z+2e$

Non-LTE kinetics simulations require *basic* atomic data, previously inaccessible

- For example, hollow ion studies generate much needed data
  - Require a setup similar to that planned for the AMO initial experiments
  - Controllable source of moderately charged ion is necessary

- Use of a modern EBIT will provide ideal capability
  - EBIT specifications
    - Extracted beam of ions, e.g., Mg, $>10^8/cm^3$/pulse
    - In $1mm^2$ x 10cm can have $> 10^7/cm^3$
    - Size: 1.5 m x 0.5 m x 0.5 m plus stand
    - Tests at GSI on the PHELIX laser coupled to the EBIT have been performed

  - An EBIT exists and could be available for the AMO XFEL experiments
  - Collaboration: Harvard-Smithsonian, NIST, U. of Stockholm, GSI, LLNL



D. Schneider and E. Silver

High Peak Brightness of 4th generation x-ray light sources are well matched to HEDS

- For Hot Dense Matter the plasma collision rates and spontaneous decay rates are large

- To effectively move population, pump rate, R_{photo}, must be greater than radiative decay rate, A_{value}

$$\Rightarrow R_{photo} > A_{value}$$

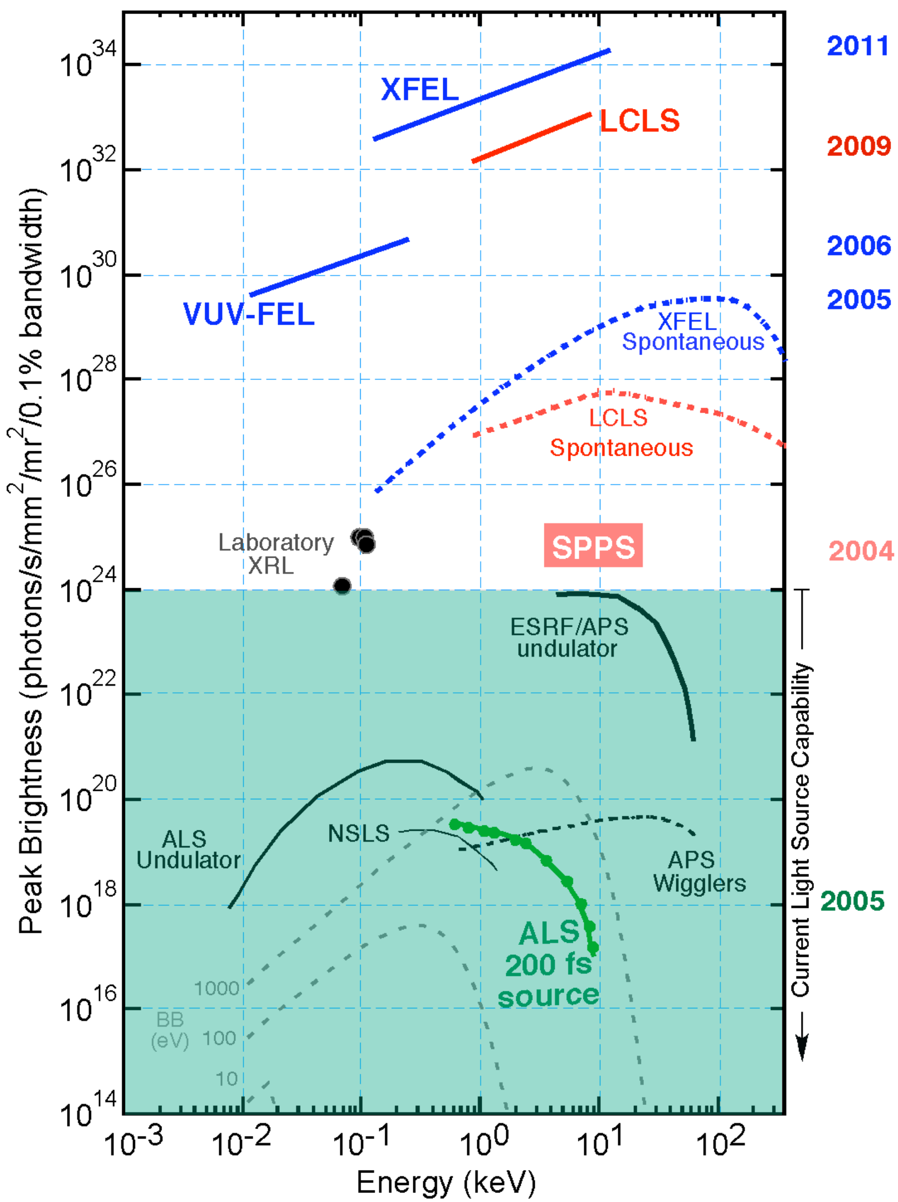
- For $\mathrm{I} = 10^{14}$ W/cm^2

$$R_{photo}/A_{value} \sim 10^{-4}\, g_U/g_L\, \lambda^4$$

- FELs attains needed excitation strength

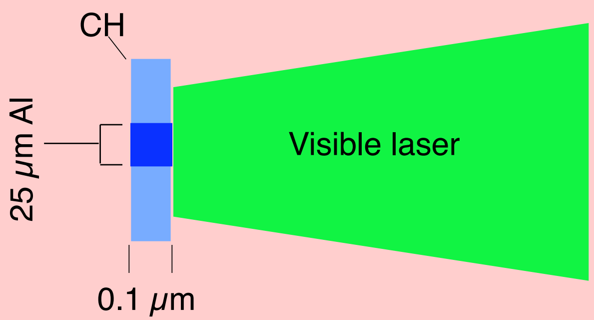
$$\lambda \sim 10\ \text{Å} \Rightarrow R_{photo}/A_{value} > 1$$

- To obtain brightnesses ~ 10^{31} the effective blackbody radiation temperature at 2.5 Å would be ~ 63 MeV

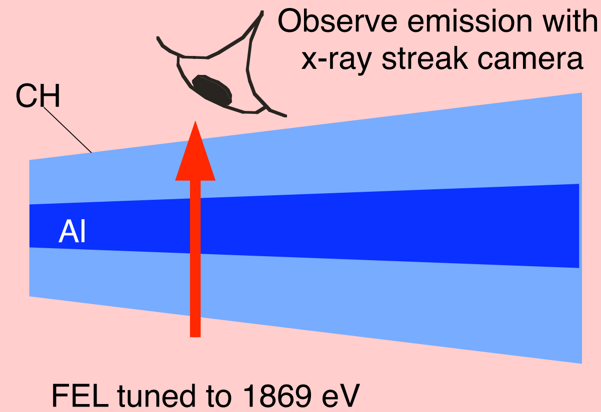


To provide NLTE benchmarks pumping K-shell emitters provides critical data

- **Schematic experiment**

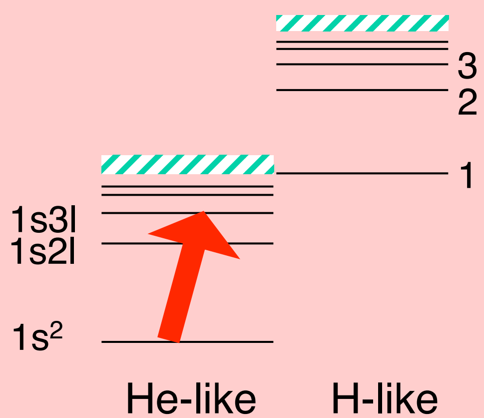


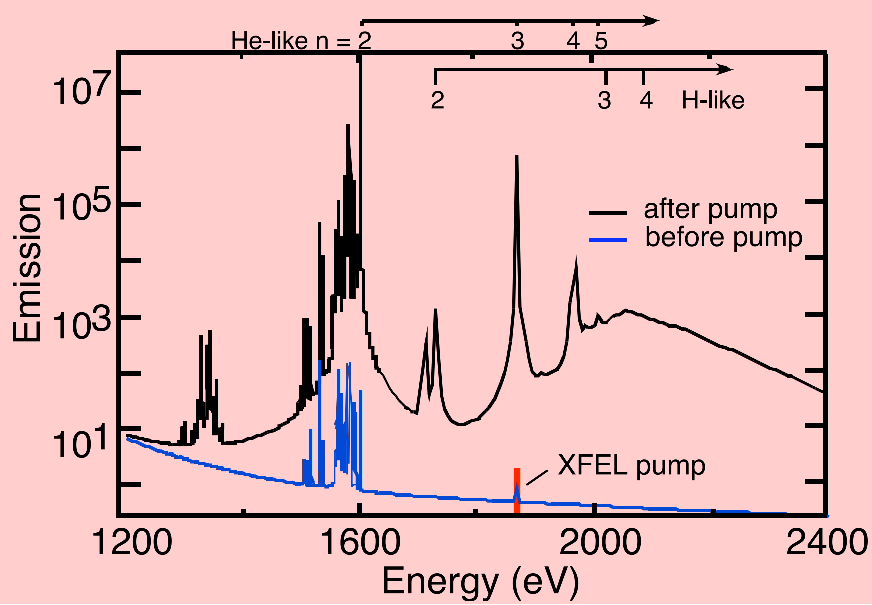
- **t = 0 laser irradiates Al dot**



- **t = 100 ps FEL irradiates plasma**

- **Simulation**





Warm Dense Matter

Broadly speaking, there are two paths to producing WDM

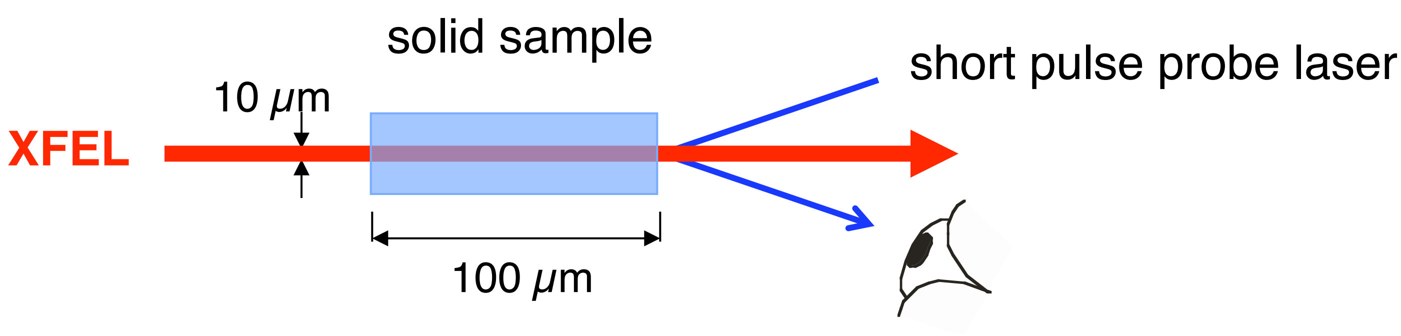
- As the issue with WDM is not to just create it
  - Because it occurs widely and is easily realized

- Need to create it so that it can be studied in well defined conditions

- One: Use a great deal of energy to make a large enough volume of WDM so that gradient at the boundaries are a small part of the sample

- Two: Use an intense fast x-ray source to heat the matter uniformly and rapidly. Then make measurement before hydrodynamic expansion

Intense short-pulse x-ray sources can create WDM



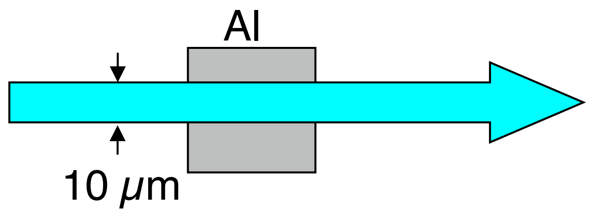
- For a 10x10x100 μm thick sample of Al
  - Ensure sample uniformity by using only 66% of beam energy
  - Equating absorbed energy to total kinetic and ionization energy

$$\frac{E}{V} = \frac{3}{2} n_e T_e + \sum_i n_i I_p^i \quad \text{where } I_p^i = \text{ ionization potential of stage } i-1$$

  - Find 10 eV at solid density with $n_e = 2 \times 10^{22}\ cm^{-3}$ and $\langle Z \rangle \sim 0.3$
- State of material on release can be measured with a short pulse laser
- Material, rapidly and uniformly heated, releases isentropically

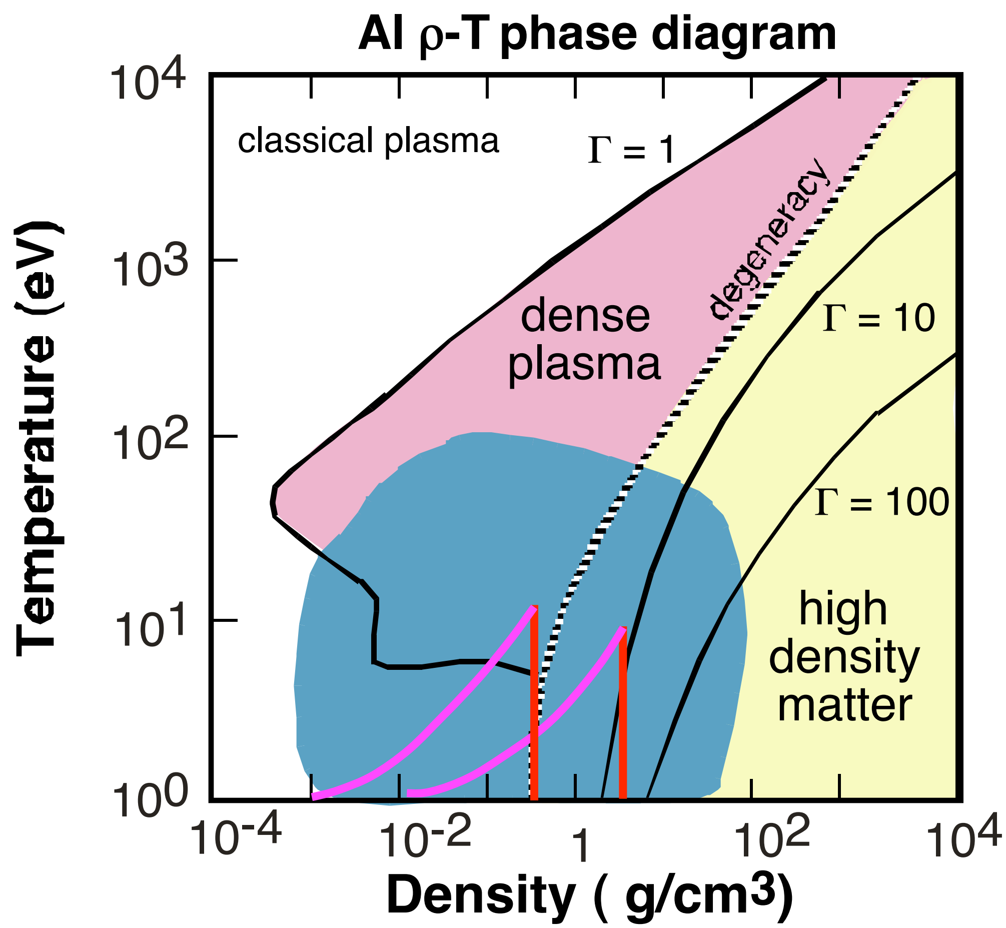
WDM created by isochoric heating will isentropically expand sampling phase space

- Concept is straightforward



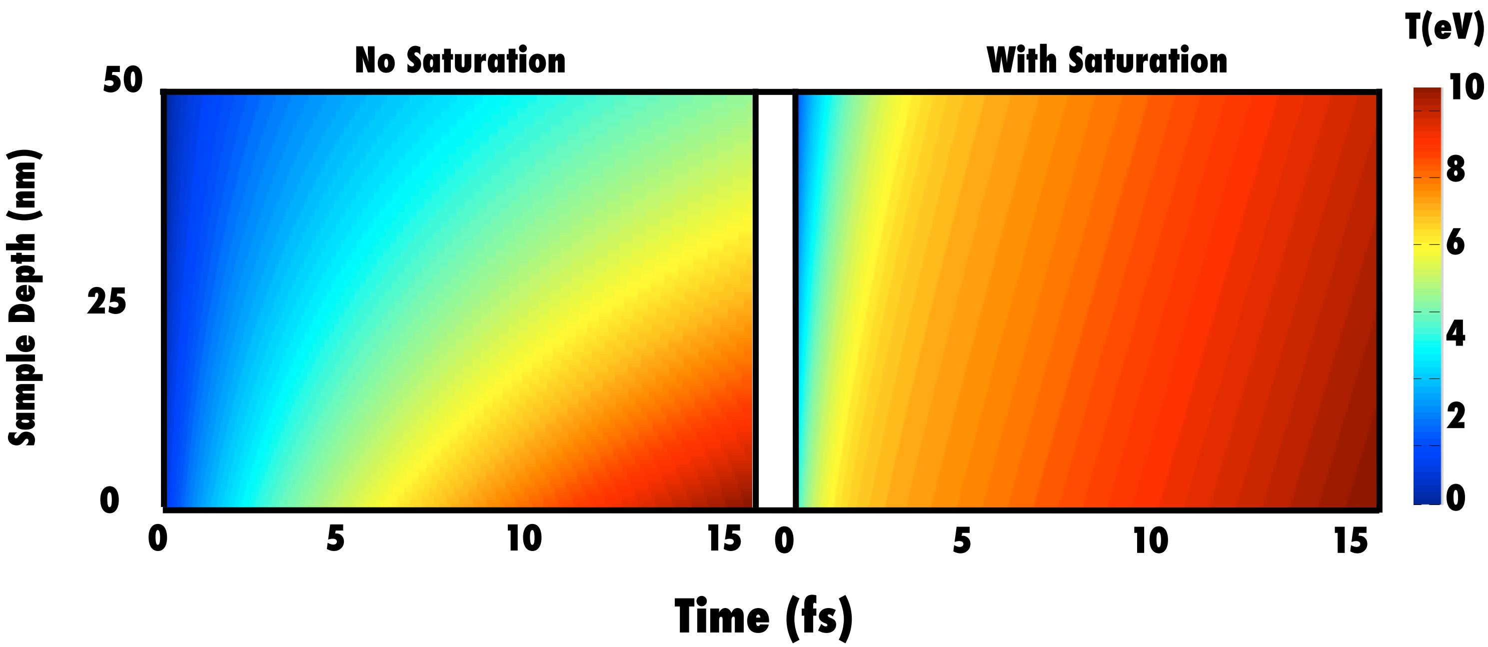
- XFEL can heat matter rapidly and uniformly to create:
  - Isochores (constant ρ)
  - Isentropes (constant entropy)

- Using underdense foams allows more complete sampling
  - Isochores (constant ρ)
  - Isentropes (constant entropy)



An important consequence of intense x-ray illumination: Saturation creates homogeneously heated WDM sample

- Essential to create WDM in a well-defined state (LTE)
  - fast & homogeneous heating imperative to obtain near constant (T,ρ)
- Saturation provides an order-of-magnitude more efficient production of homogeneity



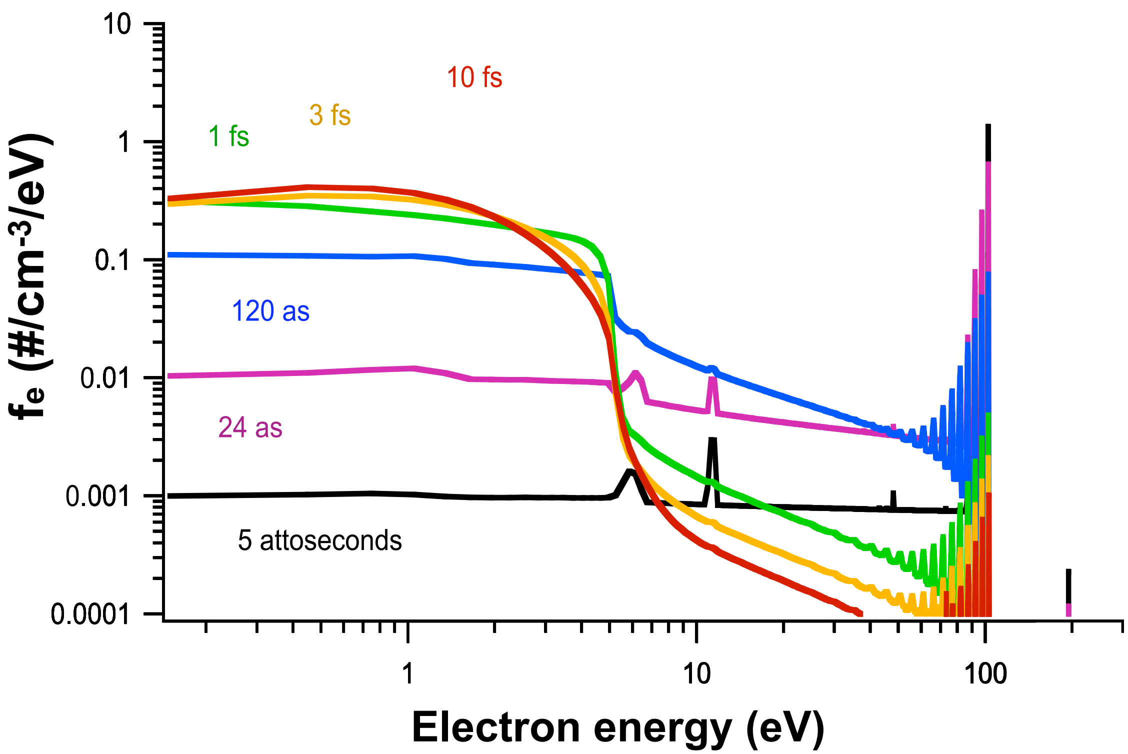
Plasma Physics

Plasma physics of photoionized gases

- Important to understand heating of gases and clusters
- Photoionization (PI) of gas jets provided a mechanism to produce unique engineered plasmas with densities ~10^{19}
- PI with high energy photons and long collisional relaxation => NLTE
  - Self Thomson scattering as function of angle provides a probe of the velocity distribution.
- Depending on the plasma and the photon energy, both photoelectron Weibel (PEW) and two stream (PETS) instabilities can occur
- Characteristic times scales:
  - $T_{Thermalization} \sim 1ps\ (10^{19}/n_e)$
  - $T_{growth\ PEW} \sim 2\ ps\ (10^{19}/n_e)^{1/2}$
  - $T_{growth\ PETS} \sim 100\ fs\ (10^{19}/n_e)^{1/2}$
- Signatures vary with gas density and observation angle

FEL-solid interaction creates unique photoelectron generated plasmas

- Case study for λ ~ 200 eV (FLASH)
- Primary innershell photoelectrons produced at 105 eV
- e^- thermalize due to *inelastic* electron-ion collisions
- Average e^- energy sharply decreases then rises



- At 5 attoseconds:
  - T_e ~65 eV
  - N_e ~10^{16} cm^{-3}
  - N_i ~$6x10^{22}$ cm^{-3}
- e^--e^- elastic ν_{ee} :
  - Coulomb ~$1.4x10^9$ s^{-1}
- e^--ion inelastic ν_{ei} :
  - excitation ~$5x10^{16}$ s^{-1}
  - ionization ~$2x10^{16}$ s^{-1}

H.-K. Chung

High Pressure States

Two areas of interest for studies of dynamics of materials under high pressure

- For studies of material strength one requires both high pressure and high strain rates.
  - *In situ* studies of dislocation dynamics can be performed at LCLS
  - Phenomenology and MD simulation predict dislocation densities orders of magnitude larger than measured post-shock
    - Creation and destruction of dislocation is dynamic => need short duration high intensity x-ray pulse as an *in situ* probe

- For phase transformations the LCLS HEDS capability will provide information on sub-ps timescales
  - Phase transformations can occur on times scales <100 ps
  - MD simulations indicate, e.g., Fe goes through a ~1ps phase transformation

High pressure studies illustrate a unique feature of the intense short pulse x-rays

- Hydrodynamic times are usually considered slow (> 1ps)

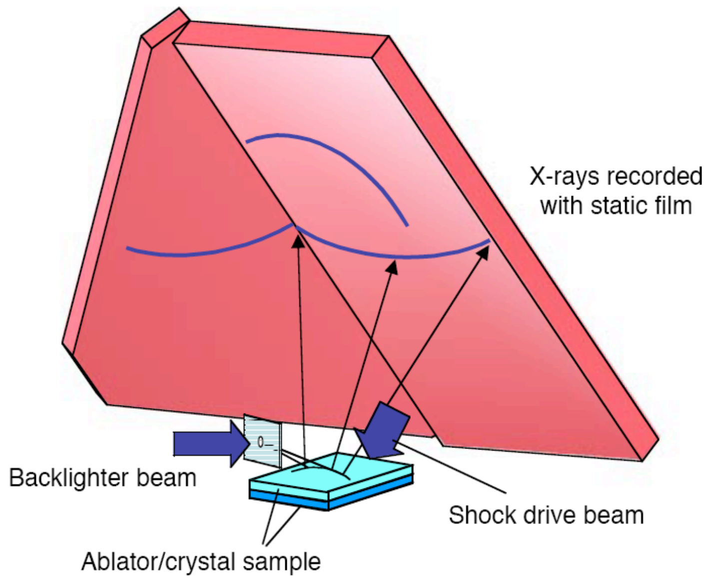
- In cases where phase changes occur two aspects of diffraction require sub-ps pulses

  - First, when one wants to look at a sample the undergoes bulk solidification the smearing of the signal due to locally rapid modification will compromise the data (Ta study by Steitz)

  - Second, there are currently indication that some, i.e.,diffusionless or Martensitic, transitions *may* undergo phase changes very rapidly (Fe study by Kadau)

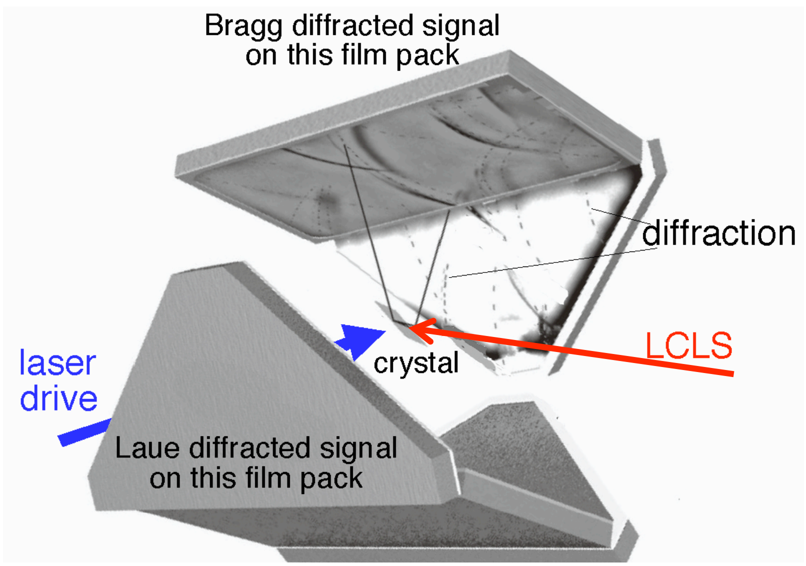
Lasers provide shocks *and* high divergence probe - LCLS provides low divergence probe

- **Schematic of High Energy Laser shock experiment**



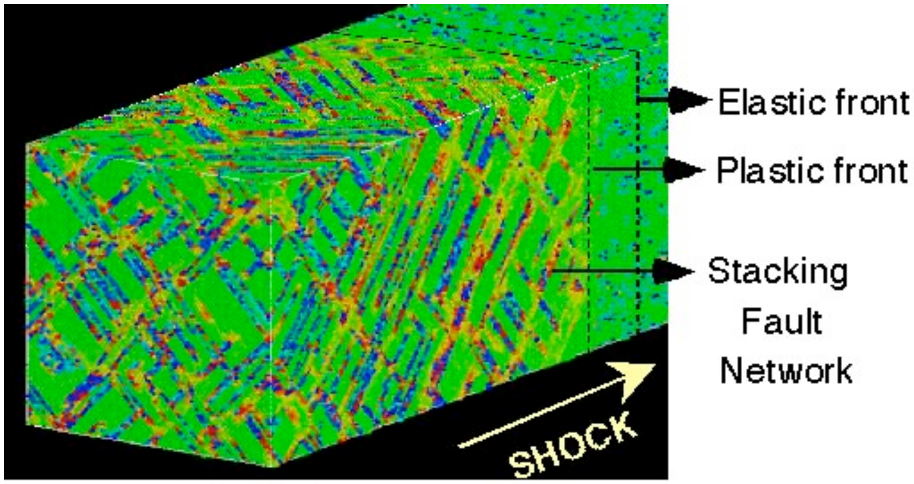
- Laser creates a shock in a single-crystal sample
- Delayed beams create ns-scale highly divergent x-ray source
- Angular spread of the x-ray source samples many crystal planes
- **Technique provides critical data on dynamics at high pressure**

- **Schematic of LCLS XFEL shock experiment**

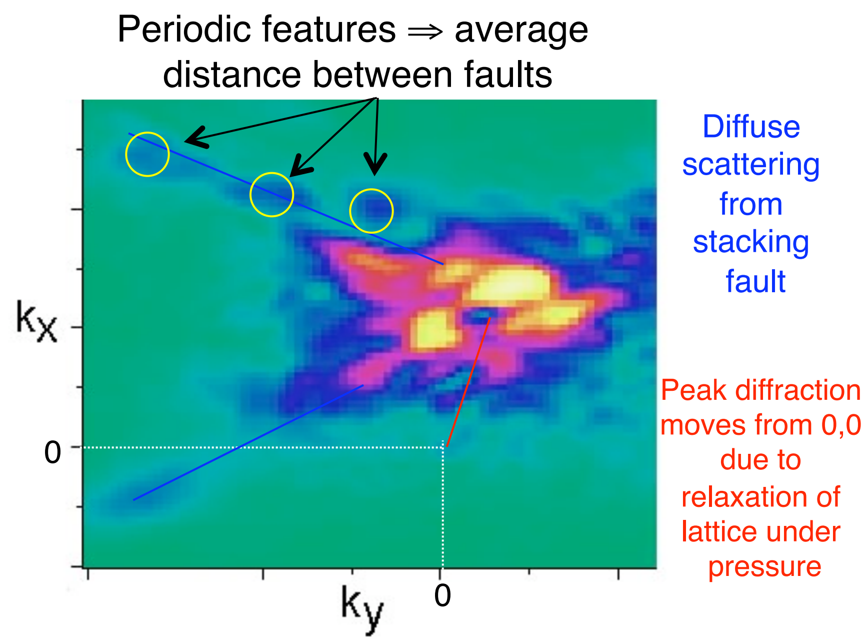


- Laser creates a shock in a polycrystalline sample
- XFEL creates fs-scale non-divergent monochromatic source
- Grains in the polycrystal diffract the beam
- **Low Divergence ⇒ *nm-scale fs diffraction of real solids***

LCLS enables real-time, *in situ* study of deformation at high pressure and strain rate



- **MD simulation of FCC copper**



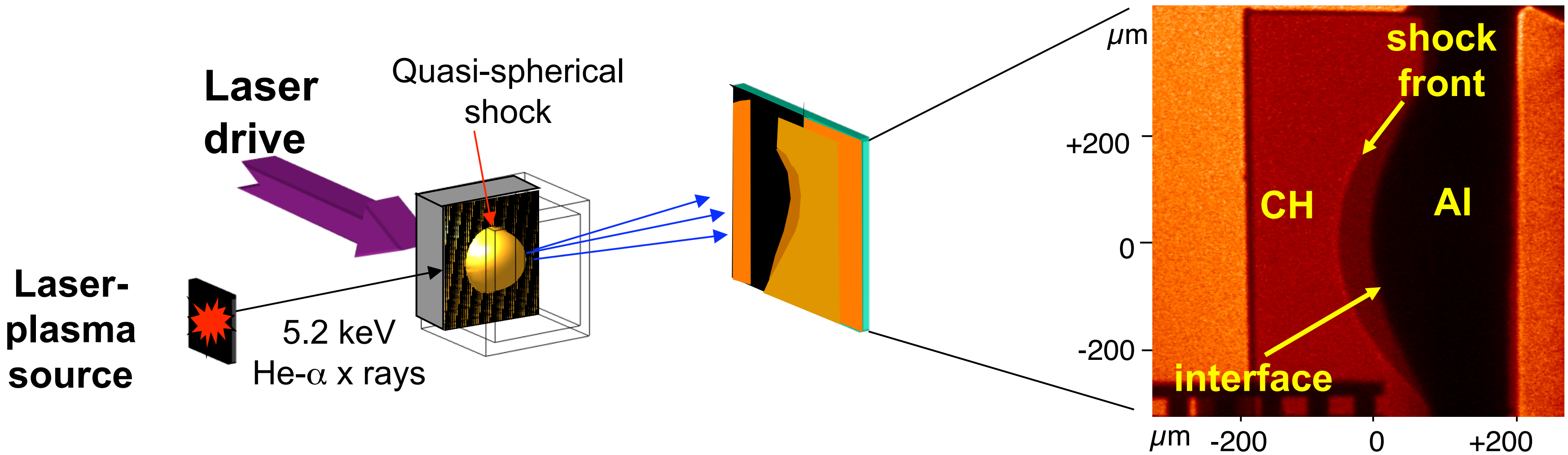
- X-ray diffraction image using LCLS probe of the (002) shows *in situ* stacking fault data

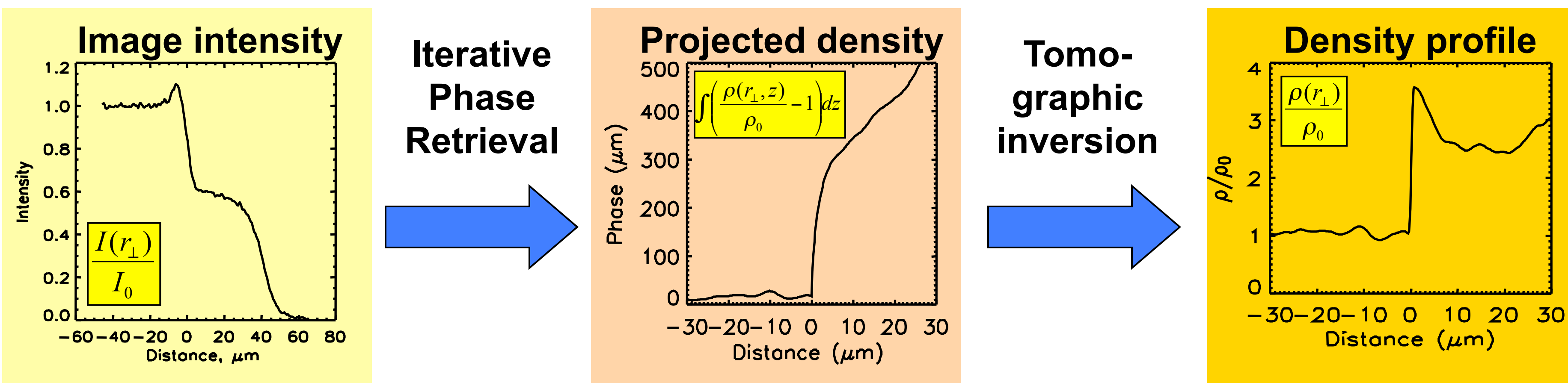
XFEL

as a

probe

Current x-ray *phase-contrast imaging* at ~ 5 μm resolution uses laser-plasma sources



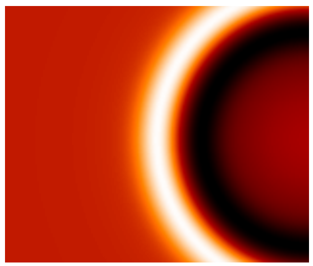


Current techniques are limited by spatial coherence & flux of laser-plasma x-ray source [D. G. Hicks 2006]

LCLS will enable coherent diffractive x-ray microscopy at the nanoscale

Shock front @ 2 μm resolution

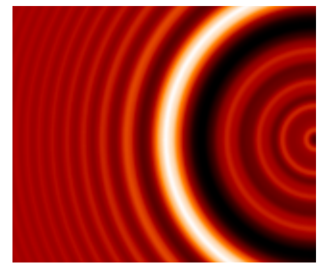
Phase-contrast imaging (near-field)



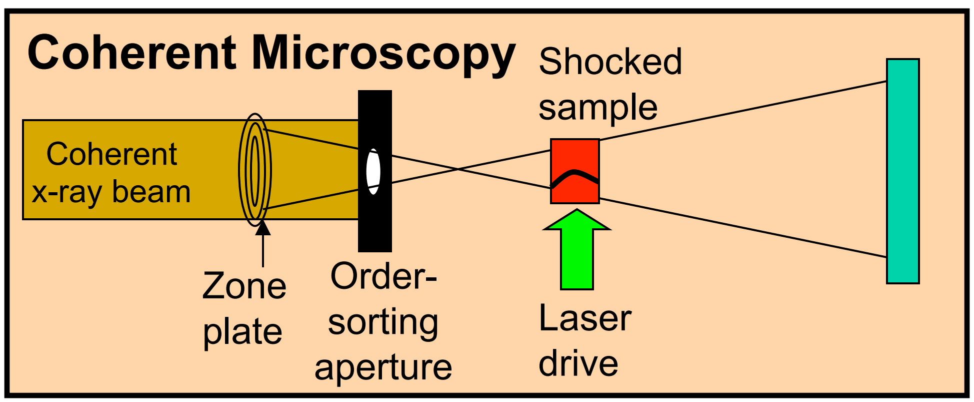
Coherent XFEL beam

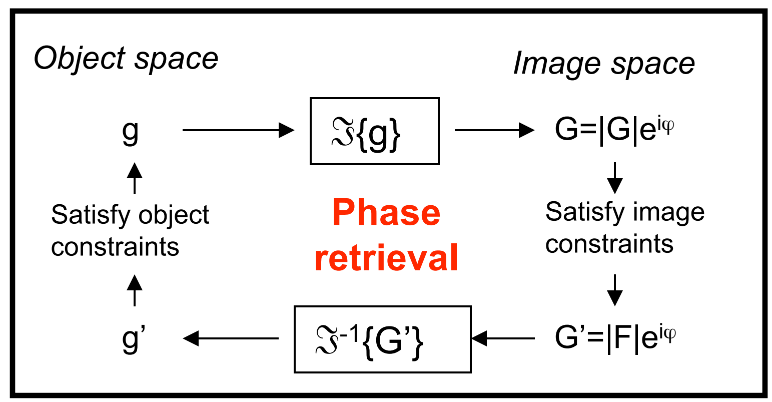
Single-pulse imaging: > 10^7 photons/pulse

Shock front @ 50 nm resolution



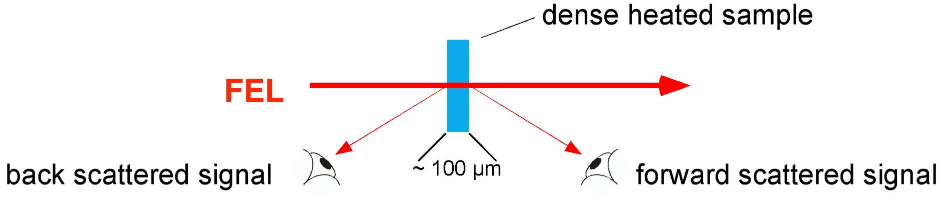
Coherent-diffractive imaging (far-field)





Dynamic processes on the nanoscale: shock front size (viscosity), phase transition kinetics, nucleation & growth, grain structure deformation

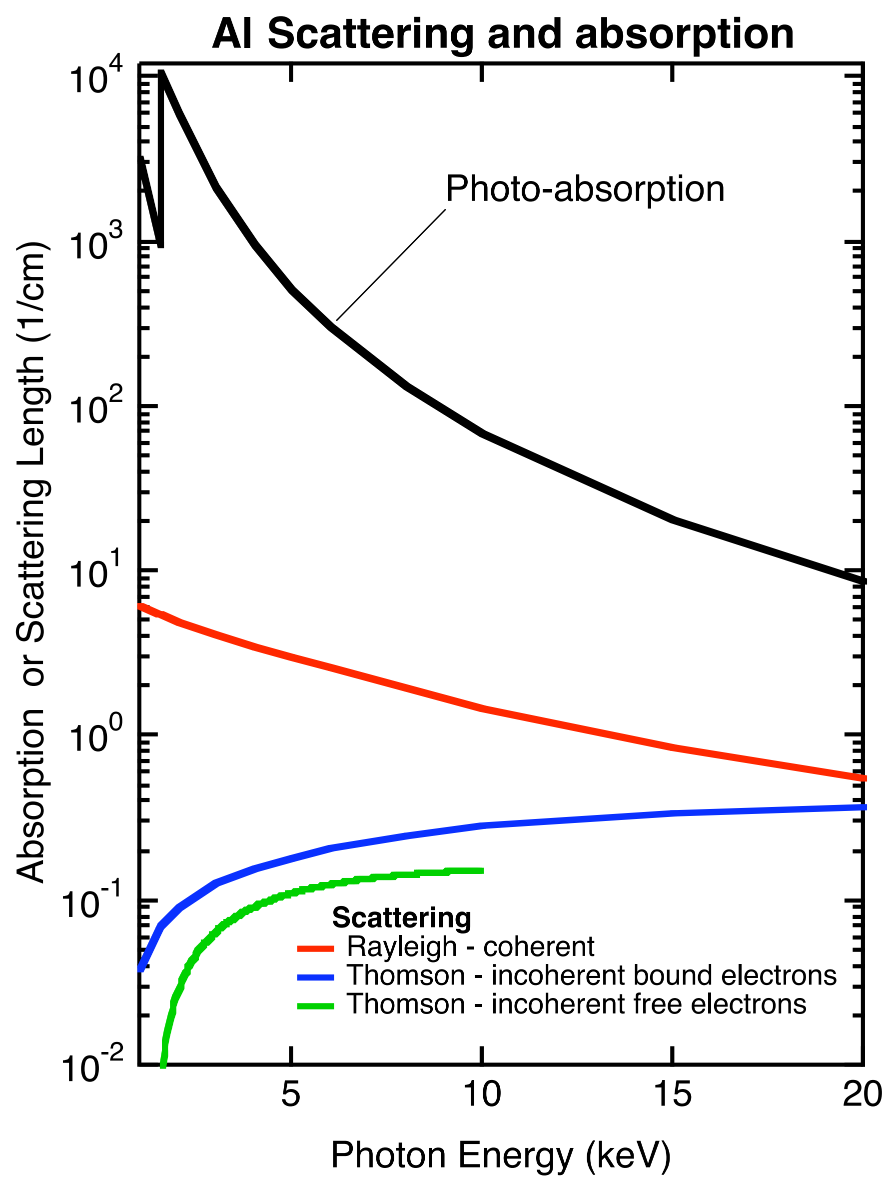
X-ray '*Thomson Scattering*' will provide a unique probe for HED matter



- Scattering from free electrons provides a measure of the T_e, n_e, f(v), and plasma damping
  - ⇒ structure alone ***not*** sufficient for plasma-like matter

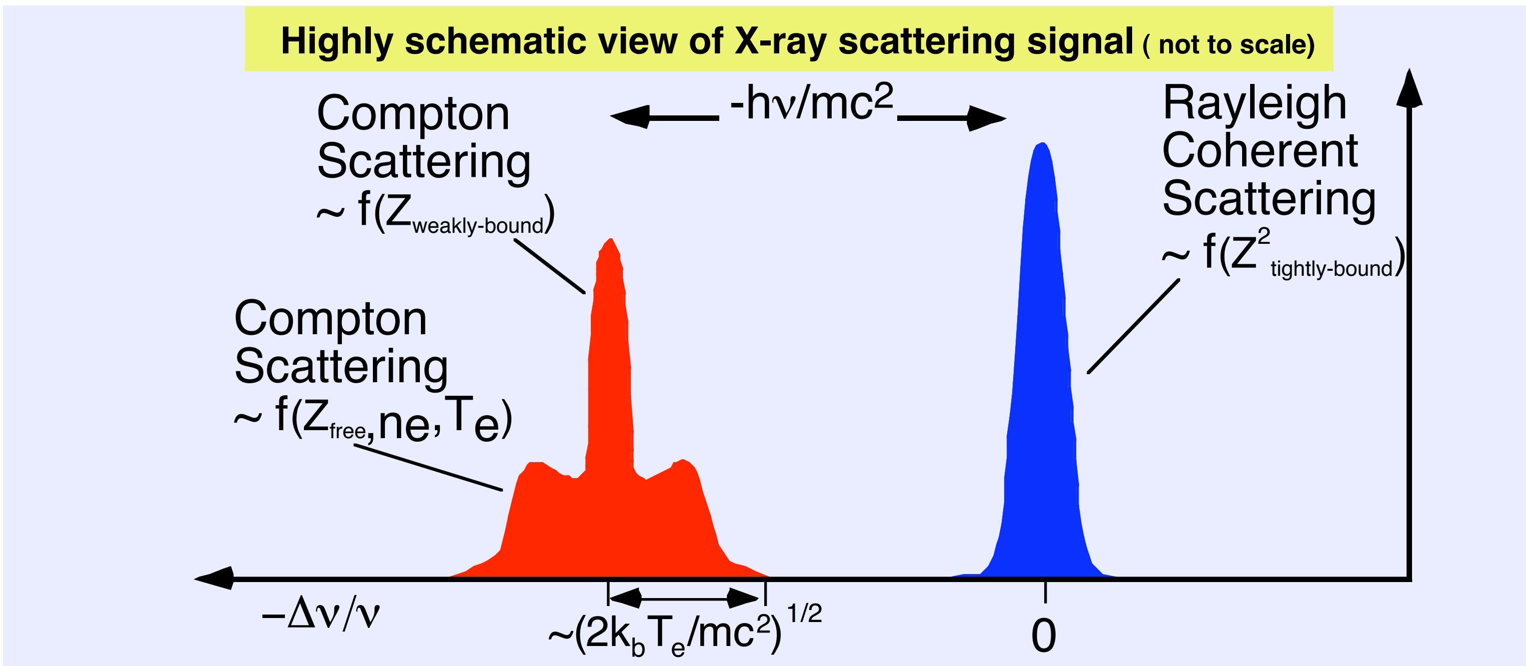
- Due to absorption, refraction and reflection neither visible nor laboratory x-ray lasers can probe high density
  - ⇒ little to no high density data

- FEL scattering signals will be well above noise for all HED matter



Scattering of the XFEL will provide data on free, tightly-, and weakly-bound electrons

- Weakly-bound and tightly-bound electrons depend on their binding energy relative to the Compton energy shift

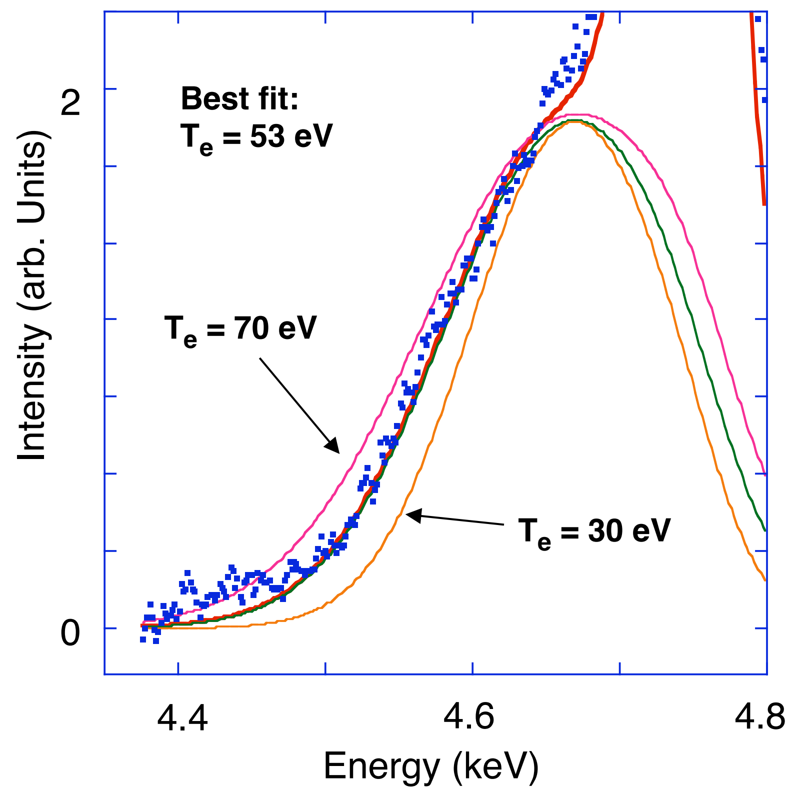


- For a 25 eV, $4x10^{23}$ cm^{-3} plasma the XFEL produces 10^4 photons from the free electron scattering

- Can obtain temperatures, densities, mean ionization, velocity distribution from the scattering signal

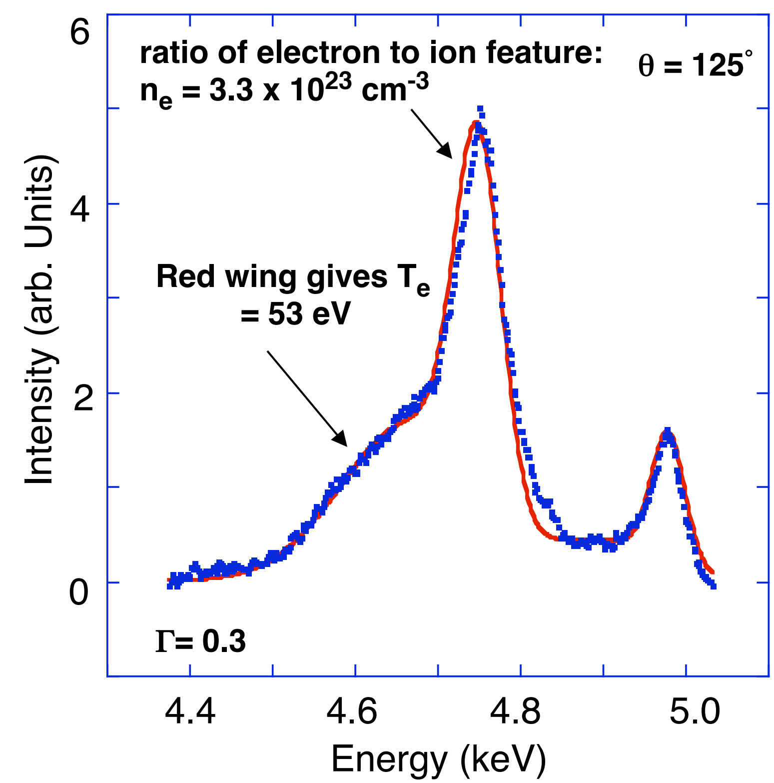
Thomson Backscattering diagnosis of solid density Be in WDM regime: $T_e \sim 55$ eV

A sensitivity analysis shows that T_e measured with an error of ~15%



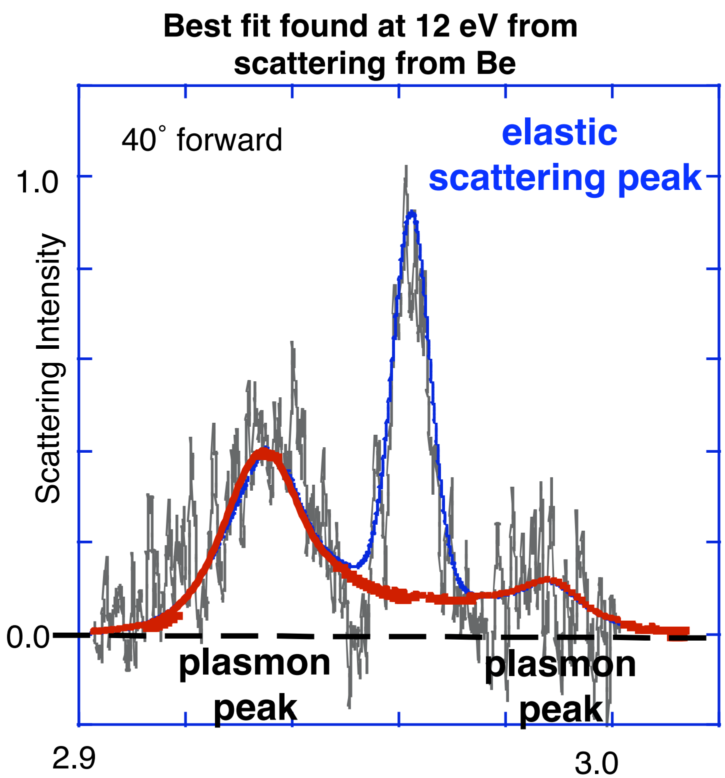
Comparison of the experimental data with the theoretical calculations for various electron temperatures

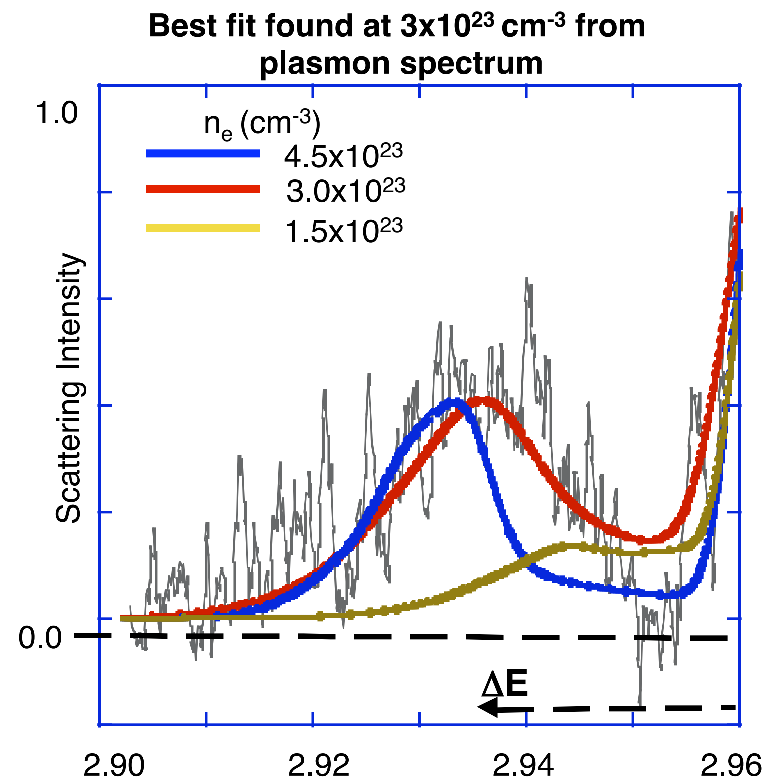
X-ray Thomson scattering spectra provide accurate data on T_e and n_e



From the theoretical fit to the data from the heated Be we obtain T_e = 53 eV and Z_{free} = 3.1 corresponding to $n_e = 3.8 \times 10^{23}$ cm^{-3}

Thomson forward scattering provides data from collective regime: plasmons yield information





- Plasmon peak intensity related by detailed balance, i.e., $\exp(-2\Delta E/T)$
- Experiments with independent T_e measurement are needed to determine correct approximation for collisions
- Experiments have now been performed with photon numbers consistent with LCLS capability.

Summary of HEDS using x-ray FELs

- For both the hot and warm dense matter regimes the possibilities opened up by x-ray FELs are important

- For WDM x-ray FELs provide
  - Fast uniform heating source to create WDM
  - Diagnostic potential: Thomson Scattering, K_α temperature measurement, fast absorption sources, phase contrast imaging, diffraction for high pressure states

- For HDM x-ray FELs provide:
  - Fast deposition creates hot, high pressure matter
  - Plasma spectroscopic probes of kinetic and radiative processes
  - Diagnostic potential: Thomson scattering

- The future looks bright!

Meetings where the MEC instrument at LCLS was planed

•	10/10/99	1st XFEL HEDS Talk	SLAC	1st workshop on next generation applications
•	3/1/01	LCLS Instruments	SLAC	
•	3/21/01	TESLA/XFL Colloq.	DESY	Official introduction of HEDS to Europeans
•	11/9/01	HEDS for VUV-FEL	DESY	
•	4/3/02	WDM Workshop	LLNL	Get LLNL, LANL, and SNL interested
•	6/18/02	WDM Expt planning	SLAC	1st focused planning meeting for MEC
•	2/15/03	XFEL HEDS Wkshp	DESY	
•	9/13/03	VUV/LCLS exp plan	Lisbon	
•	8/22/04	VUV-FEL PBC	DESY	Peak Brightness Collaboration
•	11/28/05	XFEL HEDS Mtg	Paris	
•	12/6/06	NNSA HEDS instr.	LLNL	Generated mission need document
•	1/24/07	XFEL PBC	DESY	
•	5/19/08	UK NLS on HEDS	Oxford	
•	10/5/08	PBC	DESY	
•	1/26/09	MEC workshop	RAL	
•	3/30/09	HEDS for XFEL	Oxford	
•	4/13/09	MEC Workshop	SLAC	
•	1/25/10	PBC	DESY	

BES Funding of LCLS

CONSTRUCTION

- LCLS Construction Project (includes AMO endstation) 420M$
- LUSI MIE (XPP, CXI, XCS endstations) 60M$

OPERATIONS: including 5000hrs of user time, all 6 endstations >100M$/yr

- Endstation Staffing
  - 2 scientific staff
  - 2 research associates
  - Engineering support
  - Technical support
- Facility support
  - Laser group
  - Data acquisition and controls group
  - ES&H
- Consumables

Summary

- LCLS is general user facility providing open access with operations fully funded by BES

- FES ARRA funding is constructing the MEC instrument focused on high energy density science

- FES funding is requested for a strong in-house research group and proposal driven peer reviewed single investigator grants

- FES funding is requested for laser systems upgrades

Thank you

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