High Energy Density Science Workshop

Summary Report

Justin Wark

University of Oxford

European XFEL

International workshop on the High Energy Density Science Endstation and associated Instrumentation at the European XFEL

30 March – 01 April 2009

St Catherine's College University of Oxford, UK

The capability to produce material at ultra high energy densities is one of the prioritized areas of science for the upcoming European XFEL facility as described in the Technical Design Report (available at www.xfel.eu). Matter at such energy densities is of relevance to a number of fields of science, including basic plasma physics, materials in extreme environments, and planetary physics and astrophysics.

The workshop will bring together scientists interested in using the HEDS instrument at XFEL in order to review the present state of the field, potential experiments on XFEL, and the requirements for the facility in terms of beam characteristics, chamber configuration, diagnostics, and associated instrumentation and data acquisition technology.

The workshop will feature a series of invited lectures providing an overview of scientific and technical ideas for the endstation. Group sessions will build on the ideas presented, providing the opportunity for specific input on endstation design and capability from potential users.

Young scientists bursaries
Deadline 06 February 2009
(for details see website)

The workshop is co-funded by the European Commission through the Pre-XFEL grant. This will allow free of charge access to the workshop.
Hosting the workshop and support by the Photon Science Research Institute of the UK Science and Technology Facilities Council is gratefully acknowledged.

Local Organizer

Science & Technology Facilities Council

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University of Oxford & STFC, UK

International programme committee

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www.xfel.eu/hed-workshop-2009
Deadline 06 February 2009

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THEN THE HOUSING BUBBLE BURST AND WE LOST OUR FUNDING.
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Participants

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- Patrick Audebert LULI
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- Robert Donovan Edinburgh
- Ladislav Drska Prague
- Gyula Faigel Budapest
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- Richard Lee LLNL
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- Bob Nagler Oxford
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- Justin Wark Oxford
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- Beata Ziaja-Motyka DESY
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- Ulf Zastrau Jena
- Jaromir Chalupsky Prague
- Muhammad Baig Siegen
- Stefan Michalik Kosice
- Vladimir Kolesar Kosice
- Vladimir Girman Kosice
- Nikita Medvedev Kaiserslautern
- Lauren Gartside York


Comparison: Experiment – ESTHER output
Heated target: Al 5 µm
Heated target: Al 10 µm

What is ‘High Energy Density Science’

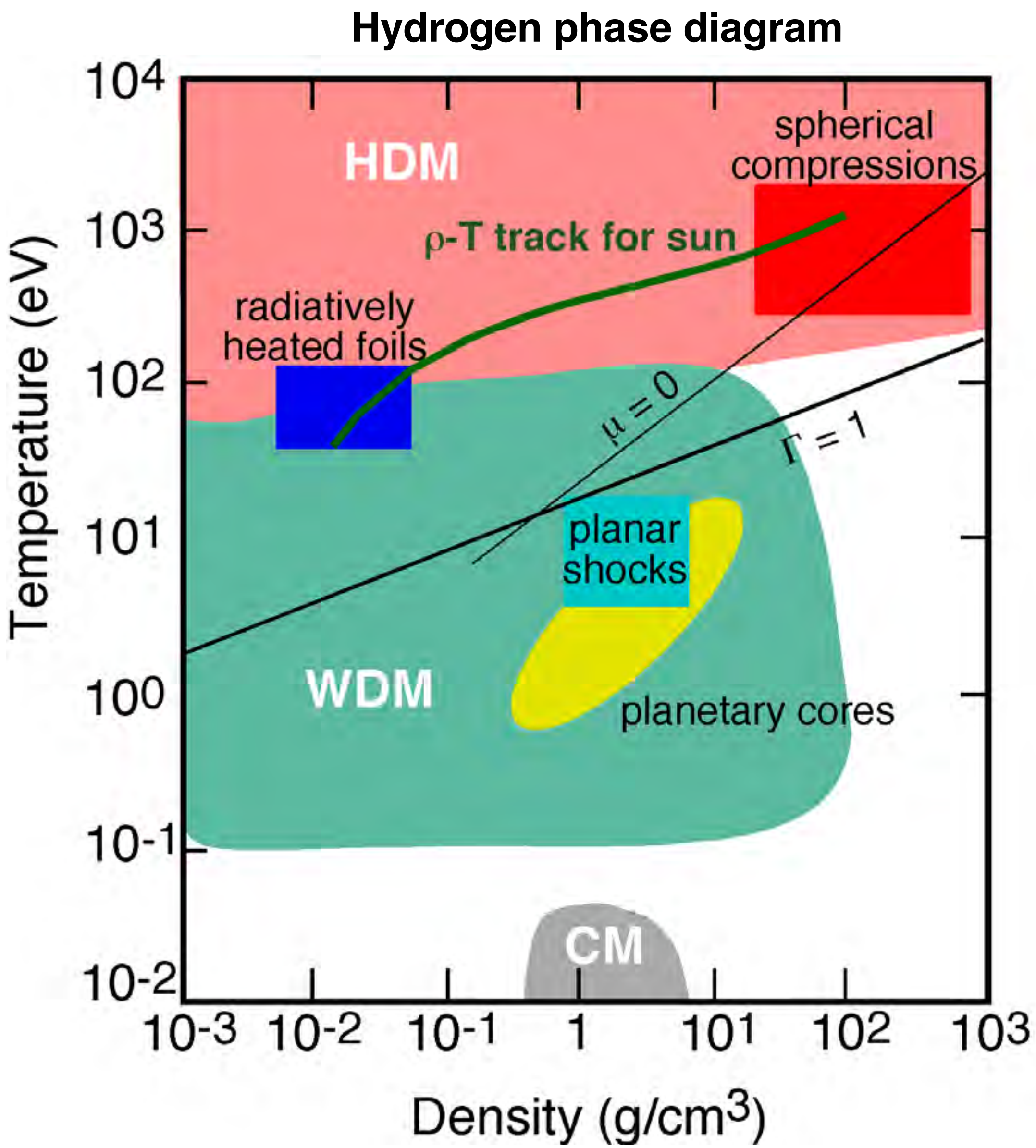
- ‘Rough’ definition is the study of matter with energy density exceeding of order 10^{11} Jm^{-3}.
- Why this definition?:
  - This is about the point where the temperature of solid density matter is such that the thermal energy competes with the potential (Coulomb) energy.
  - It is also about the regime where cold matter is compressed by of order a factor of two - and close to pressures that greatly exceed those attainable in any diamond anvil cell.

So What? Why is this interesting?

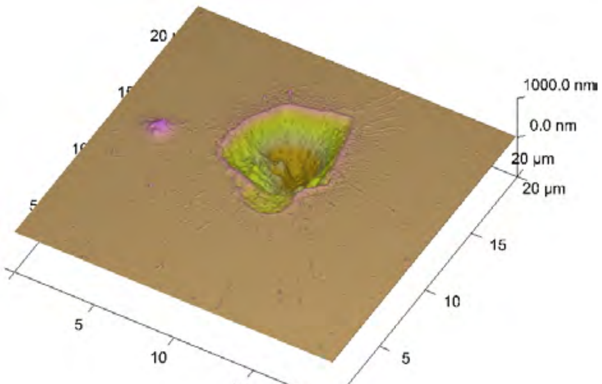
- The focussed beam from XFEL impinging on a solid target will invariably create such states…
  - Matter with thermal energies comparable to coulomb energies (‘strongly coupled’) is very poorly understood, yet is wide-spread throughout the universe (e.g. centres of giant planets). We don’t know the equation of state or transport properties.
  - Current synchrotron-based/diamond anvil cell ‘high pressure’ research ‘gives up’ at about 3.5Mbar (the pressure at the centre of the earth). Novel pulsed (nanosecond) laser techniques offer the potential to access up to 30 Mbar solid crystalline material - but we need sub-nanosecond diffraction to observe and diagnose.
  - This means that a HEDS end-station will produce such matter by the XFEL itself (mainly isochorically), *but we will also need optical lasers for compression and/or heating for other classes of experiments*.

High Energy Density matter is interesting because it occurs widely

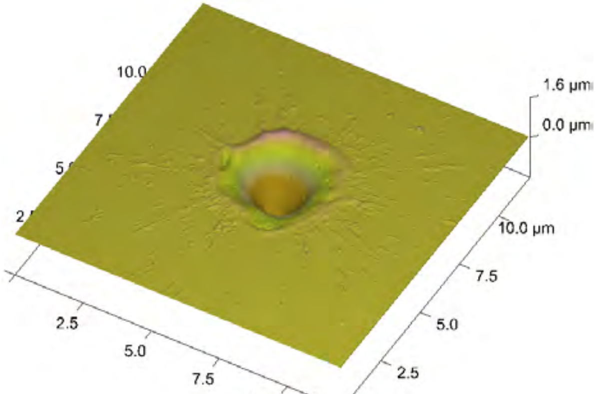
- **Hot Dense Matter (HDM) occurs in:**
  - Supernova, stellar interiors, accretion disks
  - Plasma devices: laser produced plasmas, Z-pinches
  - Directly and indirectly driven inertial fusion experiments
- **Warm Dense Matter (WDM) occurs in:**
  - Cores of large planets
  - Systems that start solid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



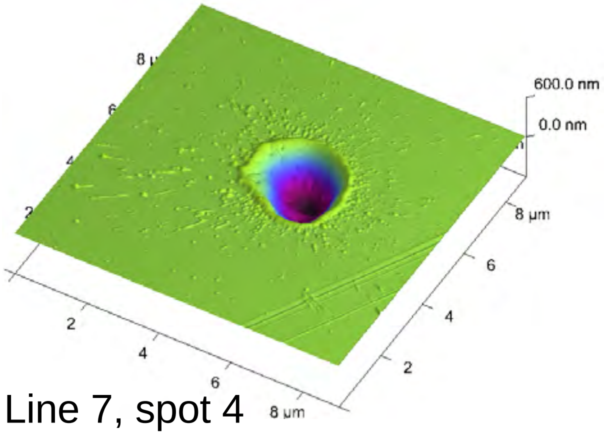
An extract of some spots from microscopy analysis (Czech IOP):



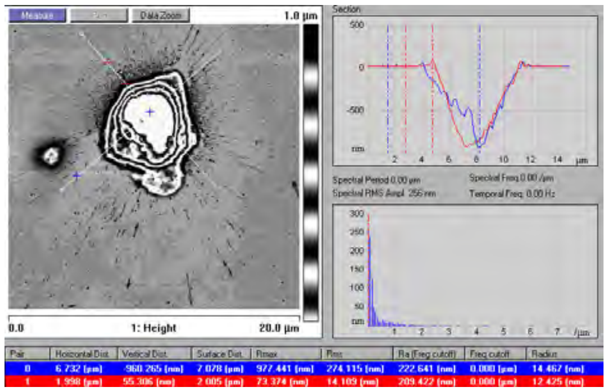
Line 2, spot 1



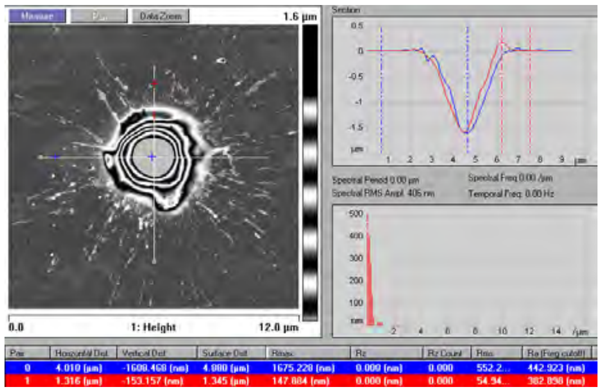
Line 5, spot 1



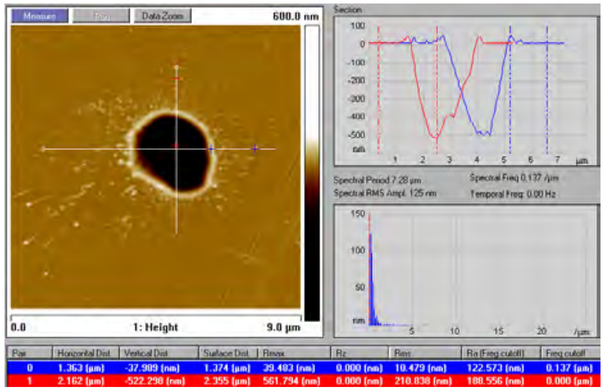
Line 7, spot 4



FWHM ≈ 4 µm



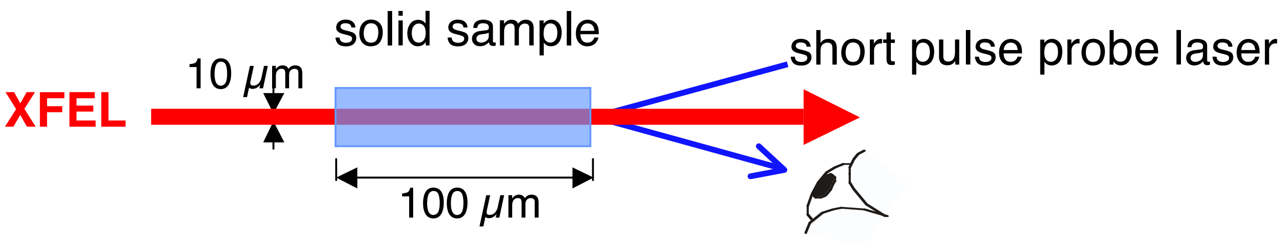
FWHM ≈ 1.5 µm



FWHM ≈ 1.5 µm

- Assuming the average energy on target (10 µJ) this corresponds to ≈ 4 10^{16} W/cm^2.
- Peak energies of 2-3 times higher also observed – intensities in the 10^{17} W/cm^2 range!

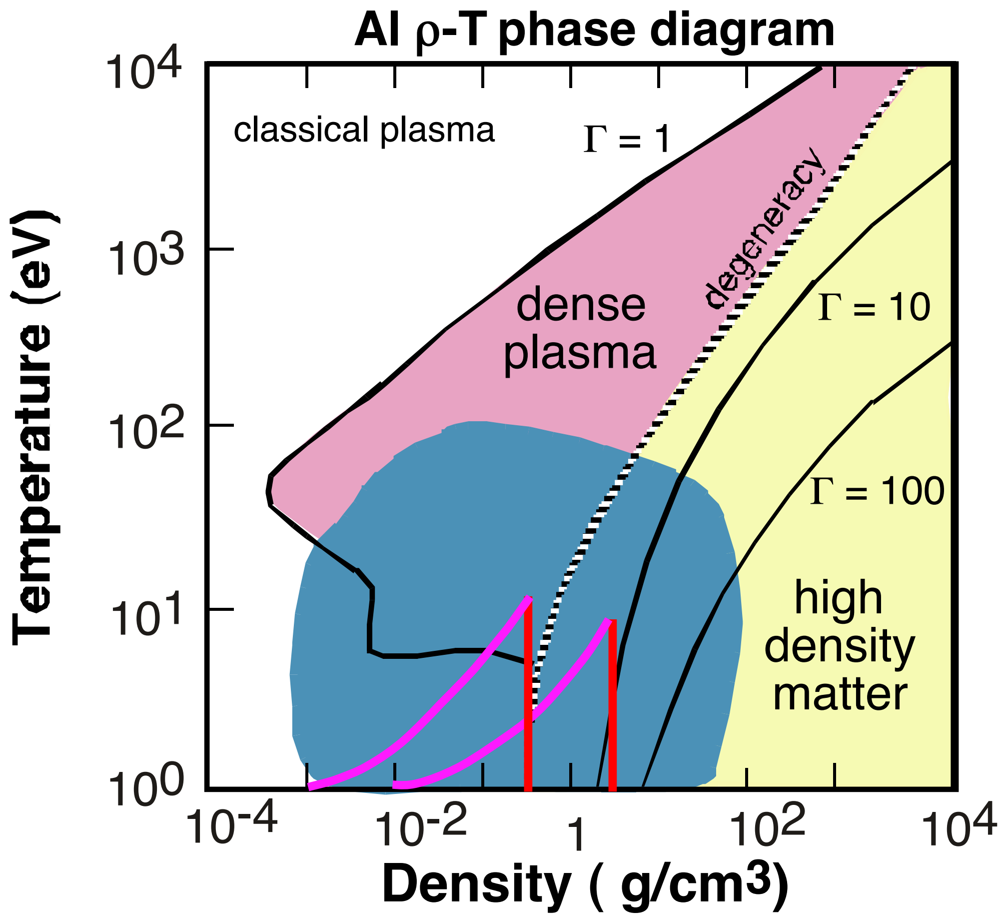
WDM created by isochoric heating will expand isentropically



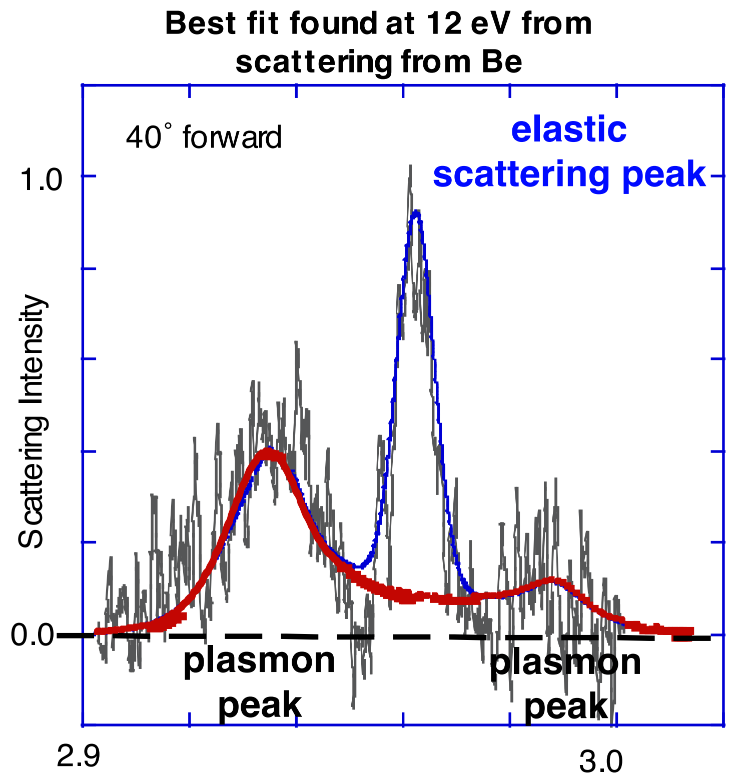
- **Concept is straightforward**
  - 10x10x100 μm Al sample
  - 10ev, Z* = 0.3, at 2 Mbar
- **XFEL heats matter rapidly and uniformly to create:**
- **Using underdense foams allows fuller sampling**

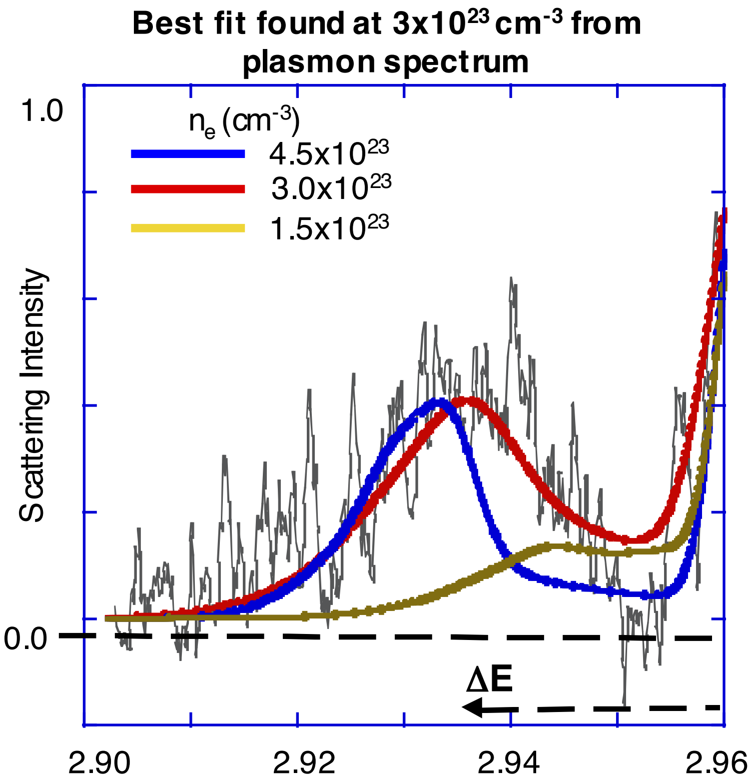
$$\Gamma = \frac{V_{ii}}{T} = \frac{Z^2 e^2}{r_o T}$$

where $r_o \propto \frac{1}{\rho^{1/3}}$



Thomson forward scattering from collective regime: plasmons provides additional data

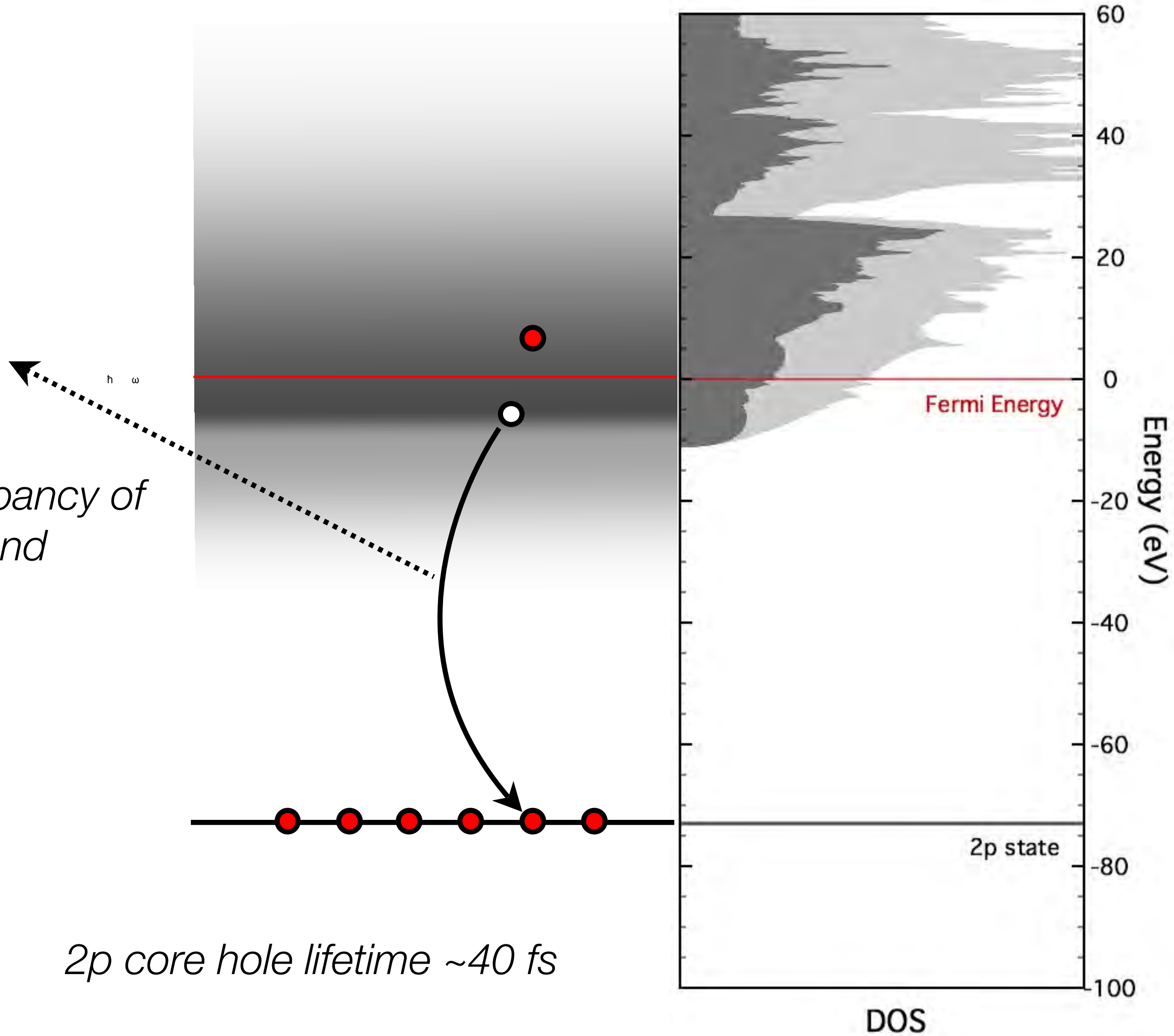




- Plasmon peak intensity related by detailed balance, i.e., $e^{-(2\Delta E/T)}$

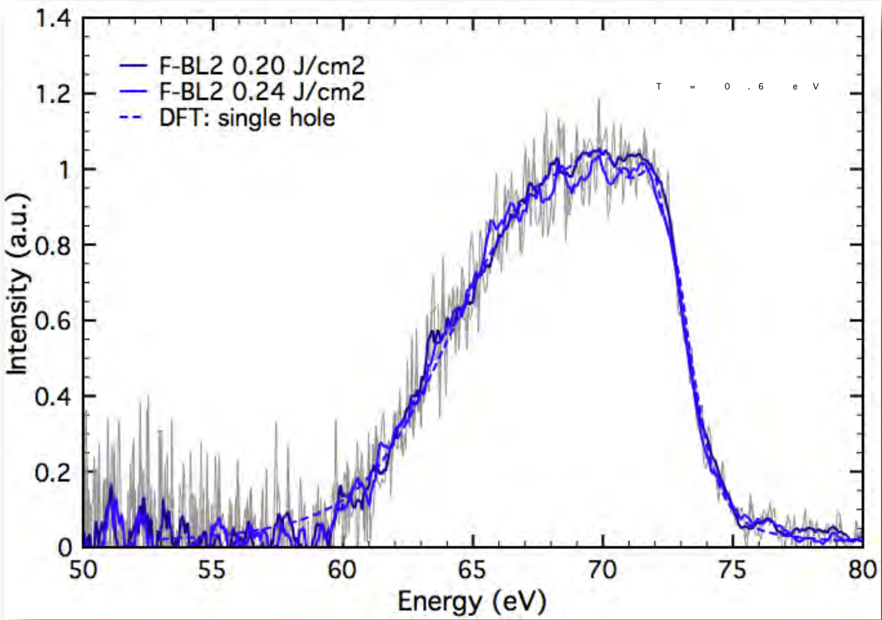
- Experiments with independent T_e measurement are needed to determine correct approximation for collisions

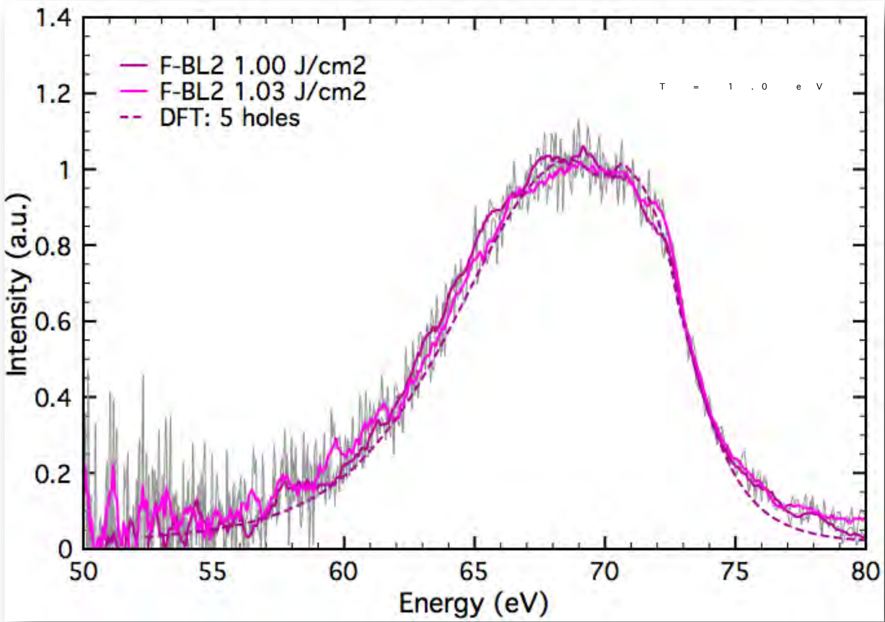
Mapping the electronic structure of WDM

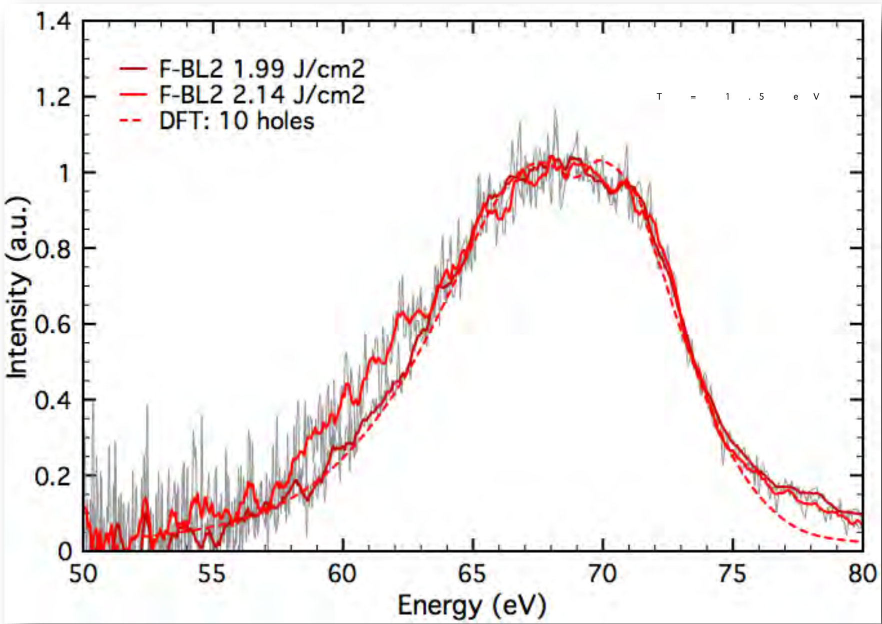


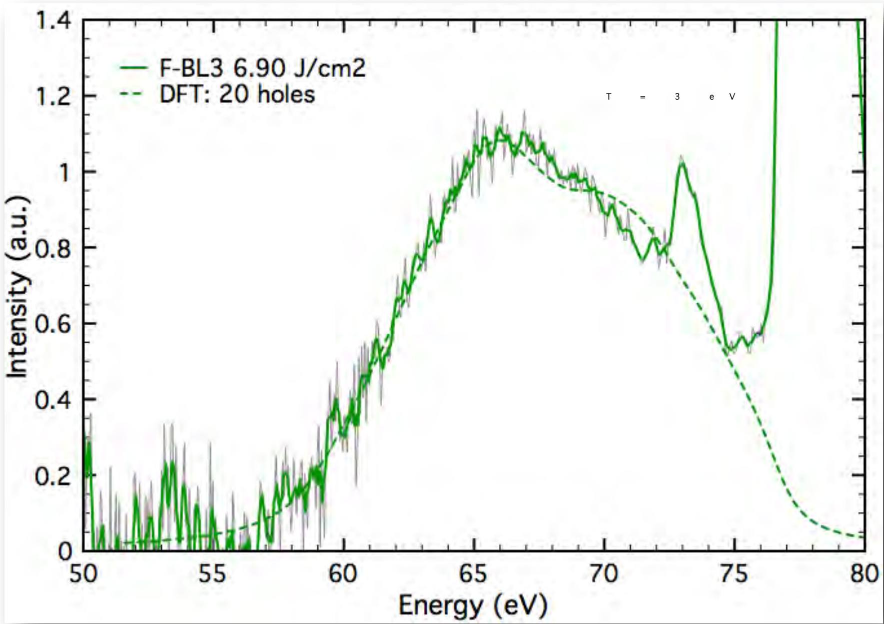
Map the occupancy of the valence band

2p core hole lifetime ~40 fs



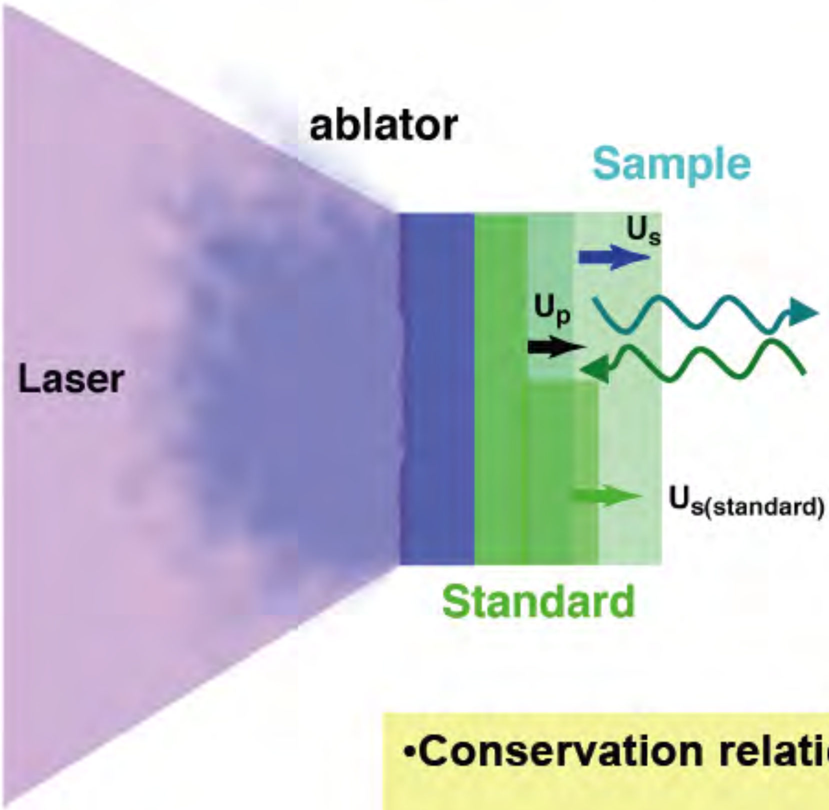




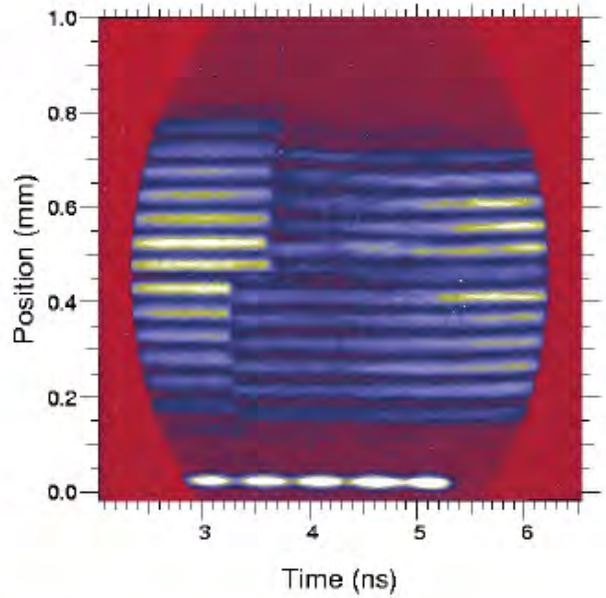


sam.vinko@physics.ox.ac.uk

How do we measure the equation of state and transport properties



VISAR measures velocity and reflectance



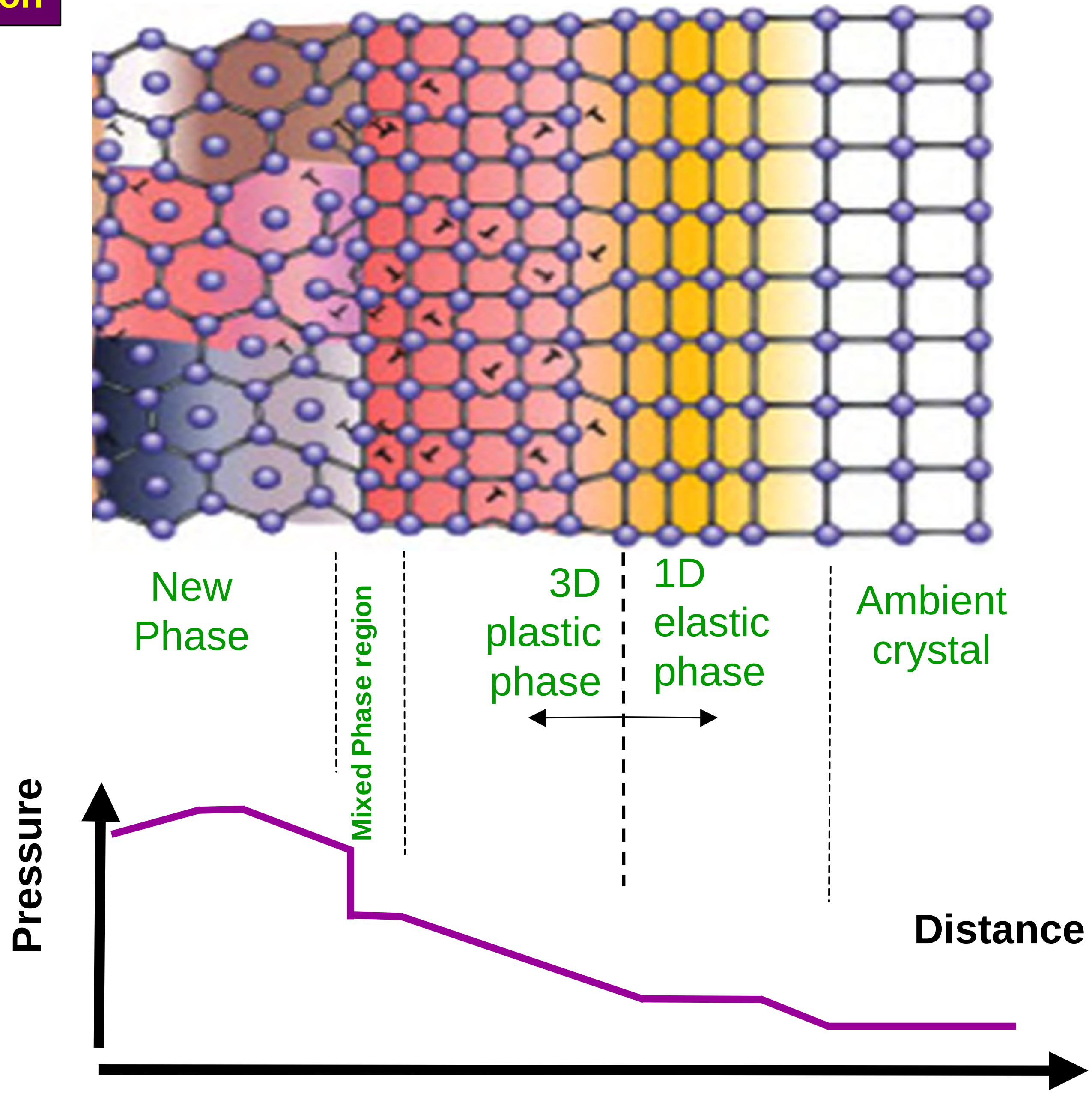
- **Conservation relations =>** $P = \rho_0 U_s U_p$

  $\rho/\rho_o = 1/(1-U_p/U_s)$

- **Temperature needs to be measured separately**

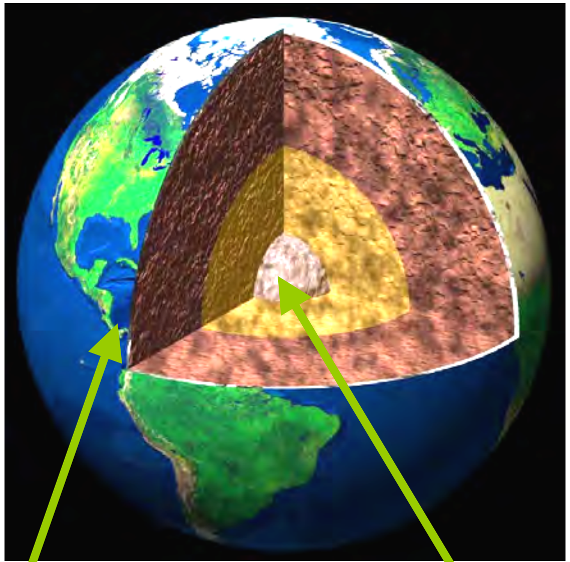
Slide from Rip Collins

Motivation



New Phase
Mixed Phase region
3D plastic phase
1D elastic phase
Ambient crystal
Pressure
Distance

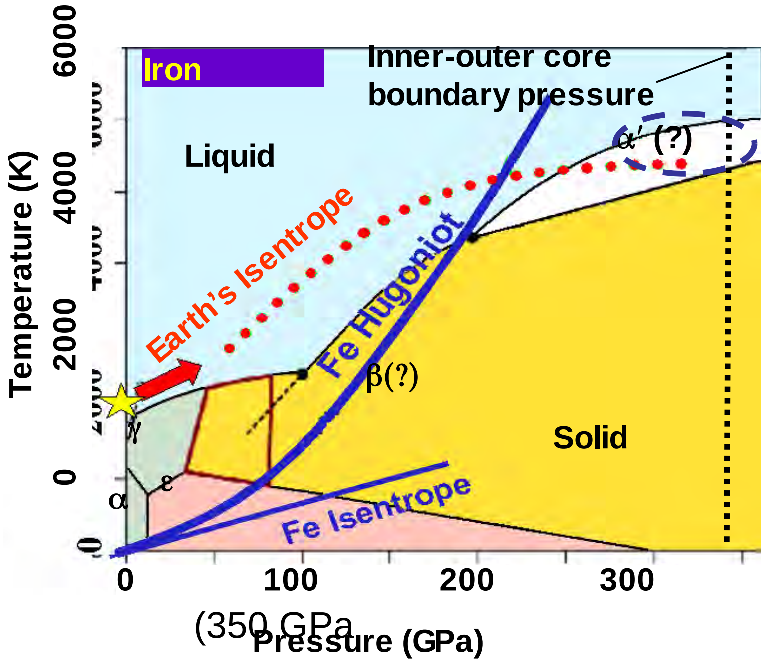
Phase Transitions in Iron - so far only resolved with nsec resolution

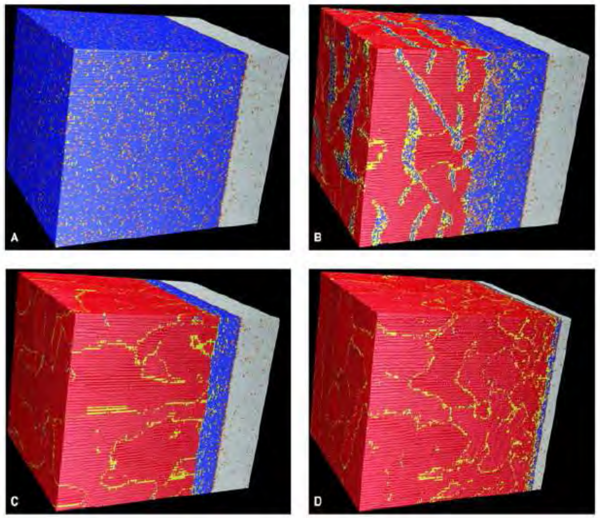


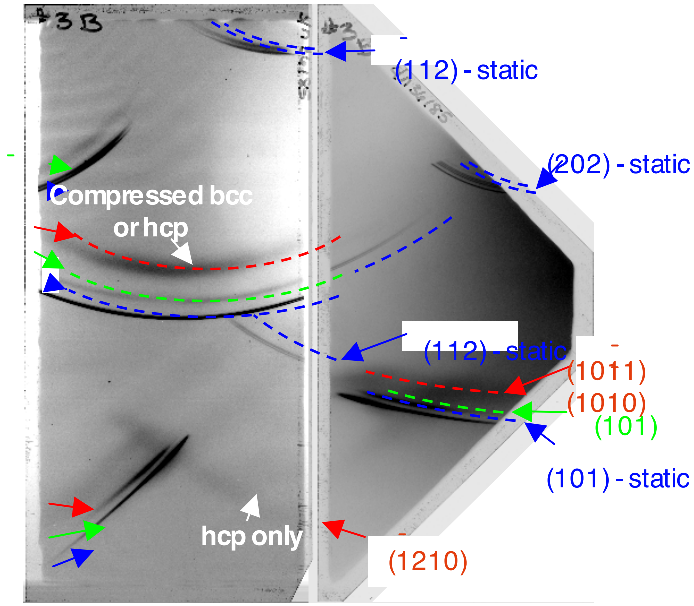
Outer liquid core

Inner solid core
= 3.5×10^6 atmospheres)

(350 GPa

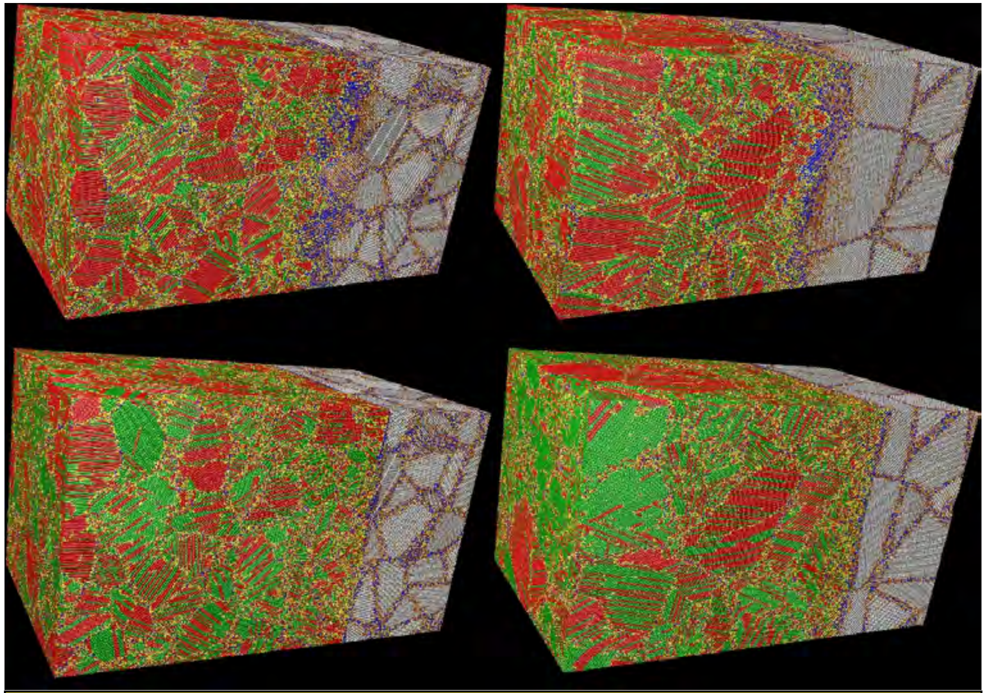




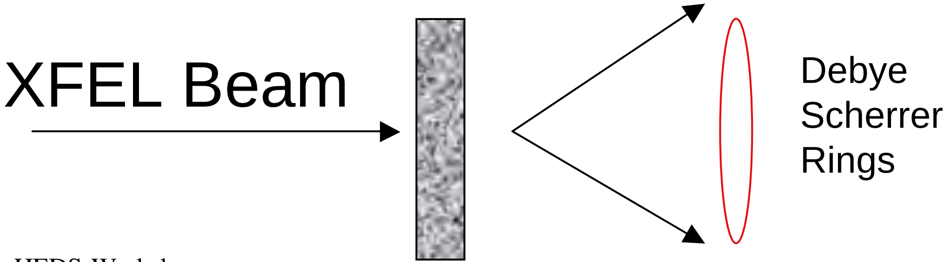


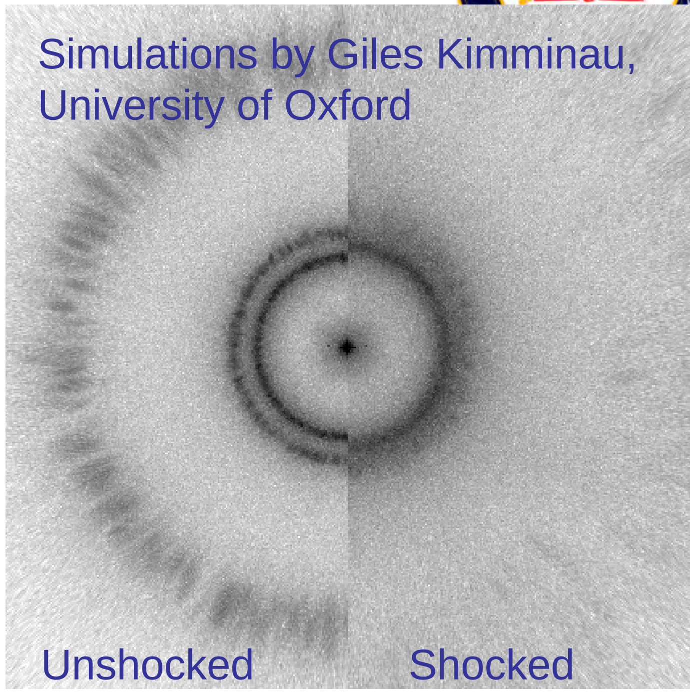
XFE
Apri

XFEL bright enough to allow powder diffraction of shocked samples



Investigate elastic-plastic response and phase transitions at the granular level in polycrystalline materials.



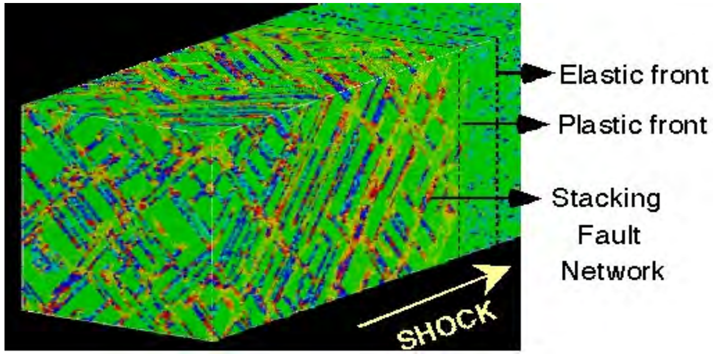


- MD Simulations of powder diffraction fro unshocked and shocked polycrystalline copper (NB MD shown left is polycrystalline *Iron*).
- 30 million atoms ($72nm^3$)
- 3000 grains
- Calculate 'absolute' intensities

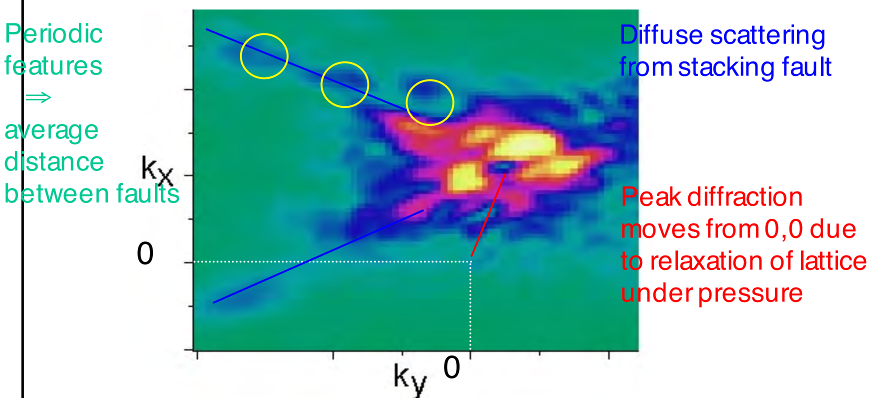
Defects alter the diffraction

Current Status

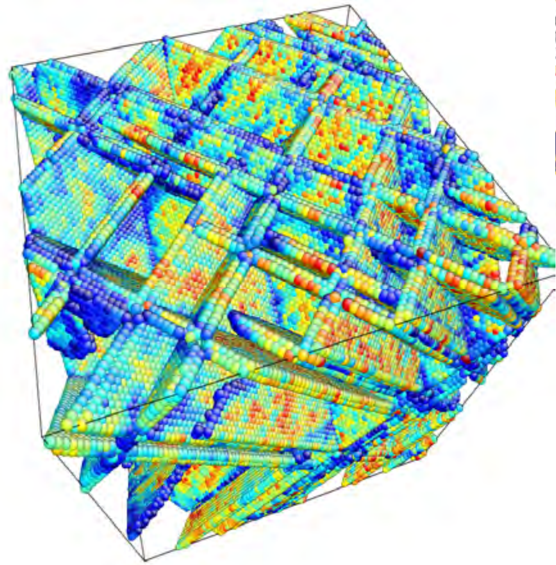
Simulation Classical scattering



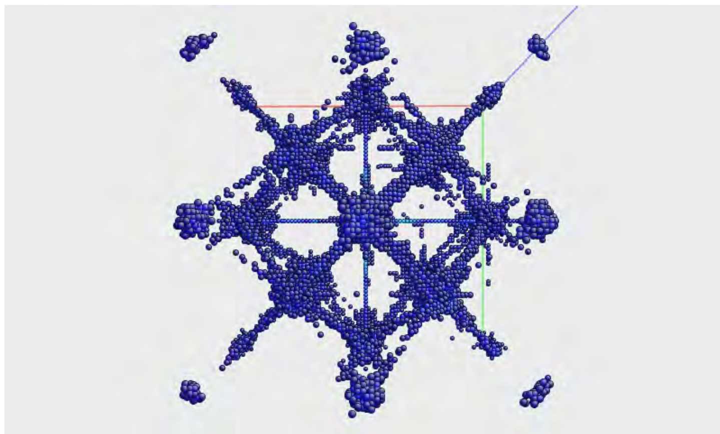
- MD simulation of FCC copper (E. Bringa)



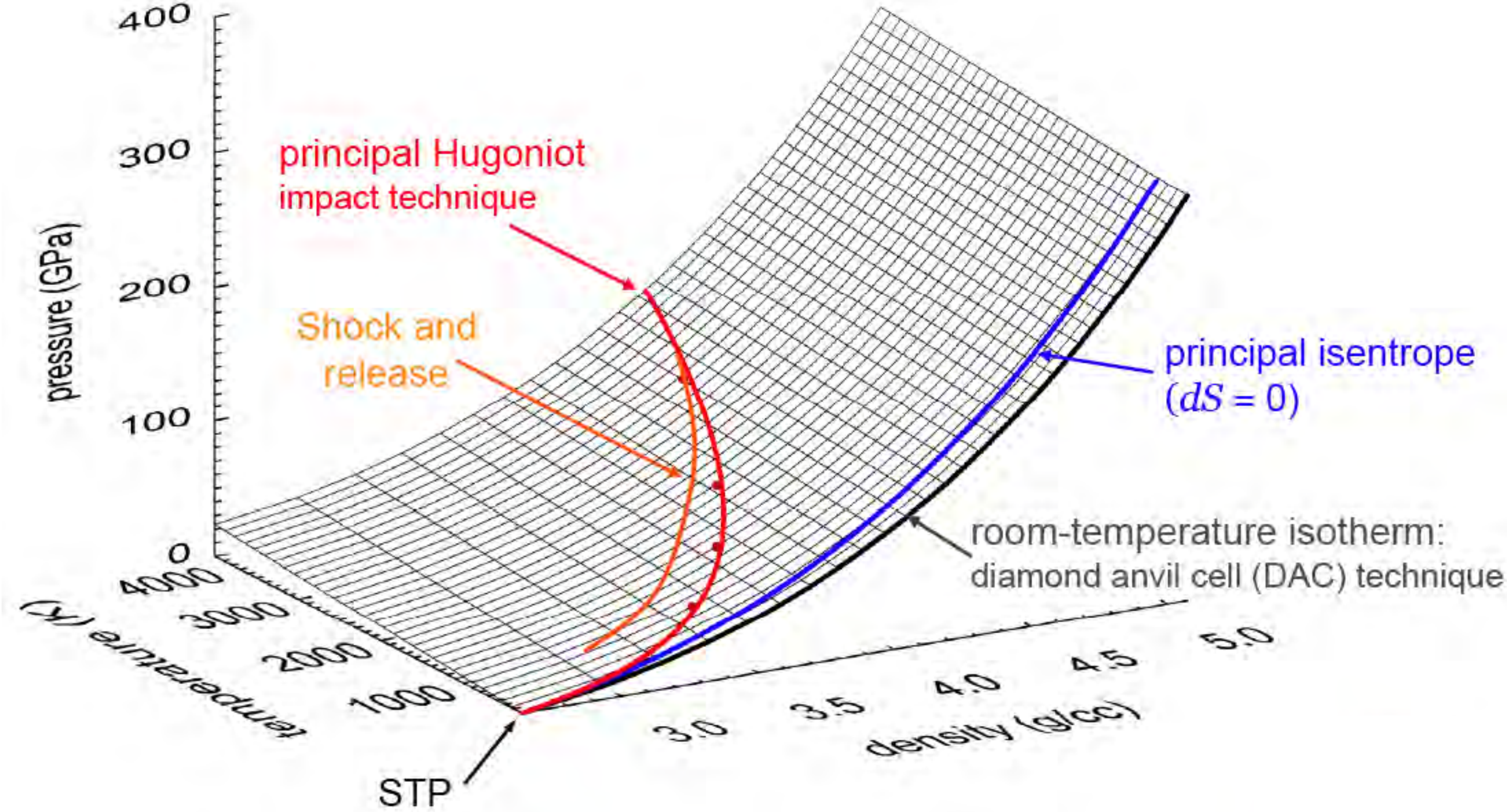
- ***Simulatec*** X-ray diffraction image using XFEL probe of the (002) shows *in situ* stacking fault information (Rosolankova and Wark)



Shocked Cu - real space



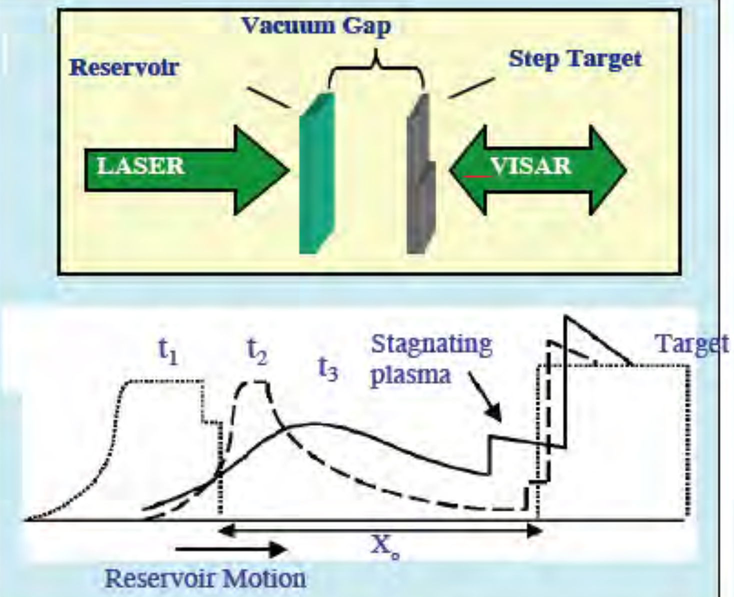
Shocked Cu - reciprocal space



pressure (GPa)
400
300
200
100
0
principal Hugoniot
impact technique
Shock and
release
principal isentrope
(dS = 0)
room-temperature isotherm:
diamond anvil cell (DAC) technique
4000
3000
2000
1000
temperature (K)
3.0
3.5
4.0
4.5
5.0
density (g/cc)
STP

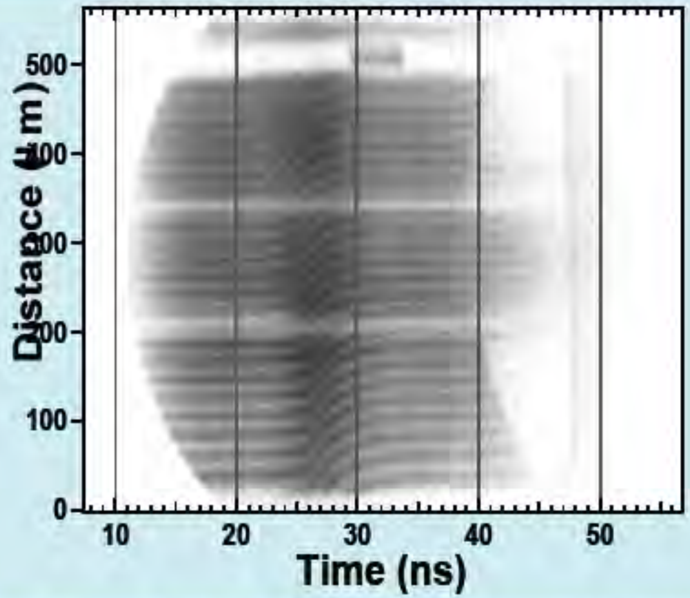
Laser produced isentrope is generated by a stagnating plasma and measured with line VISAR

Target design



•Design based on that of Edwards and Lorenz (PRL 04)

VISAR image



•Current direct drive design has ~ 800 µm planar region

Smith *et al.*, APS DPP, 2004

Working Groups

- Optical Laser Instrumentation
  - Chaired by Patrick Audebert (Ecole Polytechnique, France).
- X-ray Instrumentation
  - Chaired by Dave Riley (QUB, UK)

Issues Raised in Working Groups

– ‡ ***Experimental techniques***
- *x-ray scattering (elastic, inelastic, small-angle) (G. Gregori)*
- *plasma spectroscopy (XFEL pump ◊ x-ray emission) (F. Rosmej)*
- *WDM generation/Transmission (B. Nagler)*
- *(2-color) FEL/FEL pump-probe experiments (H. Sinn, K. Sokolowski-Tinten)*
- *studying strongly driven matter (K. Sokolowski-Tinten)*

– ‡ ***Laser issues***
- *Lasers for shock generation (J. Wark)*
- *Lasers for driving matter to excited states (P. Audebert, K. Sokolowski-Tinten)*

– ‡ ***Instrumentation***
- *Soft x-ray spectroscopy (D. Riley)*
- *Hard x-ray spectroscopy (E. Förster, F. Rosmej)*
- *Visible light & charged particle spectroscopy (L. Juha)*
- *Coherent diffraction imaging ◊ (LLNL) (I. Robinson)*
- *Bragg/Powder diffraction (A. Jephcoat, (Wark-group))*
- *Visible light diagnostics (FDI, tr optical probing) (C. Fourment, F. Dorchies)*

Optical Lasers

- Optical Lasers for Excitation
  - Low energy (0.1mJ), high rep rate (MHz), 10-fsec
  - Medium Energy (1J), TW, highest rep rate possible (few Hz?), 30-fsec
  - Large Energy (10s-500J), nanoseconds pulselengths, pulse shaping, what rep rates are possible? (diode pumping/ HiPER project indicates Hz technology is being developed). Can this be within budget (?). If not, what can be? Impact on shock/compression work (fsec lasers can generally only heat a system uniformly, not compress/rarify) - alternatives need to be discussed.
- Optical Lasers for Probing
  - Velocity Interferometry (Shock/Isentropic compression of matter)
  - Fourier domain interferometry (can be the low energy fsec laser).

X-ray Instrumentation

Table 2: Requirements to instrumentation at the HED instrument.

Purpose		**Short description**	**Comments**
X-ray techniques		Amorphous/liquid scattering, Bragg/Powder scattering, Imaging (Holography, CDI, Phase contrast), Absorption/XANES, inelastic scattering/emission spec. (resonant).	
OL techniques		FDI, VISAR,	
Sample environment		Vacuum chamber (Fast) Sample mover/exchanger Liquid jet	
Detector		Mostly 1 – 10 Hz Requirements acc. to other instruments	
Spectrometer		Optimize to emission angle Resolution 100 – 1000 Resolution 10000 (ion measurements)	

Parameter	Unit	Value (range)	Comments/Special
Photon energy	**keV**	**3.1 – 12.4**	**Lower energies for heating;** **Harder x-rays for probing**
Bandwidth	**%**	**10^-6 10^-3**	**Monochromate to see ion features**
Tunability	**%**	**+/- 3**	**Tune across edges**
Harmonics		**Yes**	**For 2-colour pump-probe experiments the 3^{rd} harmonics shall be available**
Focal spot size	**µm**	**1 - few 100**	
Polarization		**No**	**No particular request - but could affect geometry of Thomson scattering**
Coherence			**No particular requests at this stage**
Rep. rate	**Hz**	**10+**	**Use of pulsetrains requested in cases of flux limited techniques (e.g. IXS) and schemes in place for sample refreshment**
Pulse duration	**fs**	**30 - 100**	**Perhaps shorter to investigate k-shell lifetimes**
Synchronization	**fs**	**< 30**	**To optical lasers**
X-X delay	**ps**		**Delay generated using x-ray split&delay unit** **Delays >700 ps accessible by accelerator**

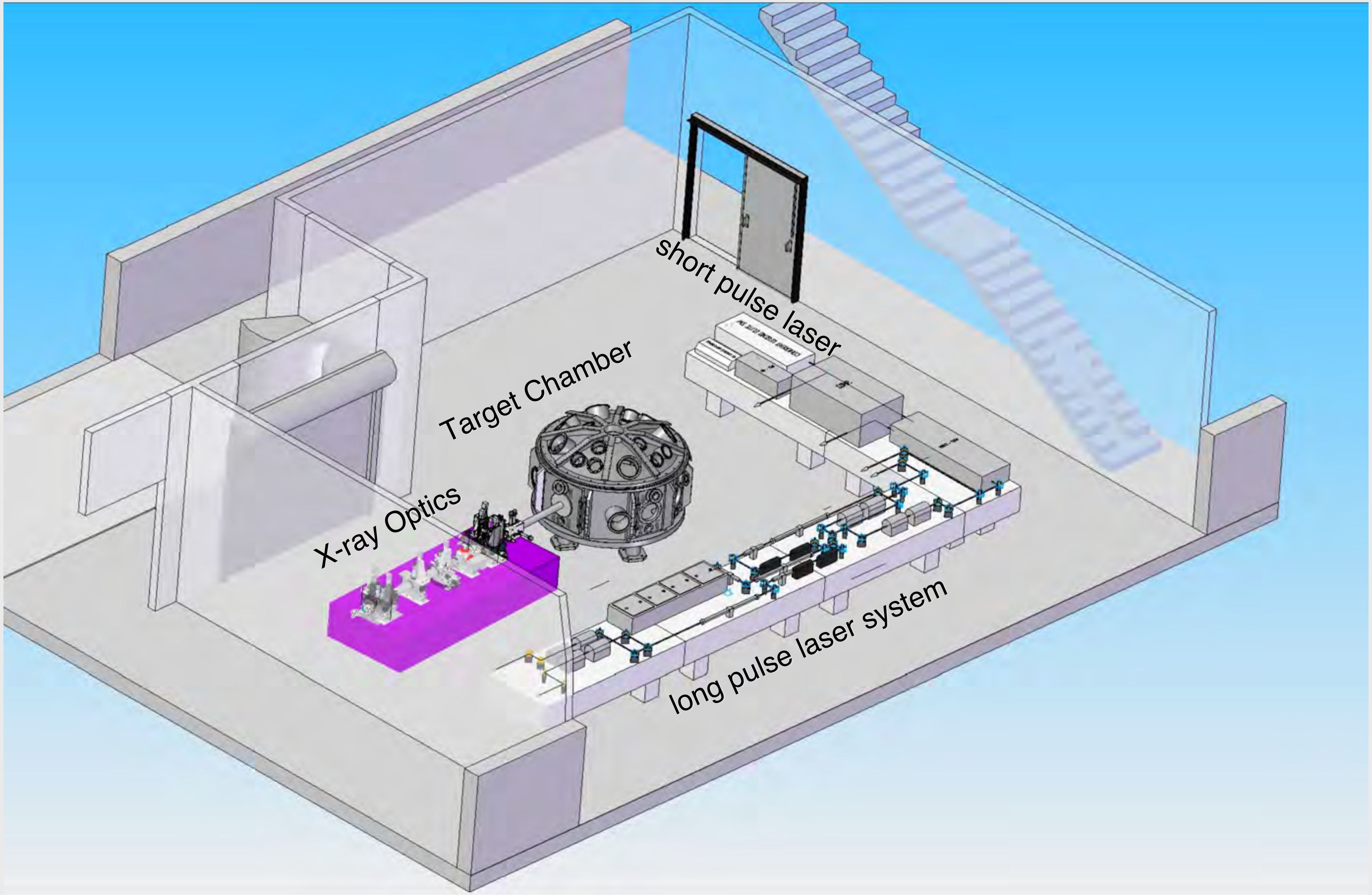
Report Contributions

- T. Tschentscher
- P. Audebert,
- F. Dorchies,
- C. Fourment,
- G. Gregori,
- A. Jephcoat,
- L. Juha,
- B. Nagler,
- D. Riley,
- F. Rosmej,

Further Work

- We need to hone down our analysis of required lasers that fit in the budget. The issues here are:
  - The field of isentropic compression to multi-Mbar pressures is itself in its infancy, and laser-pulse requirements will be material dependent.
  - Laser technology is rapidly evolving - we are trying to hit a moving target
- Detailed Instrument design and detectors.
- Monitor Progress at LCLS

MEC endstation configuration for HEDS



LCLS: *probe* solid density, WDM and high pressure matter; *create* HED matter; *photo-excite* selected transitions; *perform* x-ray Thomson scattering

Acknowledgements

- Organisational help from Andy Boyd, STFC
- Funding - XFEL, Gyula Faigel, Hungary
- Funding STFC/PSRI
- Writing up - *really* pulling everything together: Thomas Tschentscher - XFEL