Opportunities for High Energy Density Science

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• UK-FEL Meeting, Royal Society, 16th July 2019

Summary

- "High Energy Density Science" (HEDS) broadly encompasses matter with energy densities exceeding ~ 10^{11} Jm^{-3} : i.e. 'cold' solid matter at Mbar pressures, or dilute matter at millions of Kelvin.
- Effectively these are the conditions met deep in the cores of planets, stars, and within other astrophysical objects.
- The research field allows us to pursue fundamental science (e.g. astrophysics in the laboratory), but also has potential application (high pressure superconductivity, novel material synthesis, understanding of deformation at the atomic level…).
- X-Ray FELs have revolutionised this field both by providing means to, on their own, create such conditions, but also, in conjunction with high power optical lasers, to probe conditions made by other means with exquisite resolution.
- The UK has led this field at existing FELs, but is uniquely placed to construct its own facility with capabilities unparalleled worldwide.

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A sample of topics being studied

- Solids heated isochorically by an x-ray laser to millions of Kelvin can mimic conditions half way to the centre of the sun - the FEL heats the sample before it has time to expand.
- Plasmas in these conditions are poorly understood - at high density and temperature where do bound states 'end' and the continuum starts?
- What are the transport coefficients, and what is the equation of state when these plasmas are strongly coupled (thermal effects and coulomb energies are comparable).
- Optical lasers can, via ablation, subject matter to pressures far greater than possible by any other means. Compression only lasts a few nanoseconds, but the femtosecond FEL can then obtain high-quality diffraction patterns in 100 femtoseconds, recording the new phases. We thus can explore conditions deep within the planets in our own solar system and beyond.
- Tracking new phases in real time may allow us to generate new materials with new properties - optical, electrical, mechanical…
- Material deformation occurs by the generation and movement of defects - can we track these in real time during 'impact physics'?

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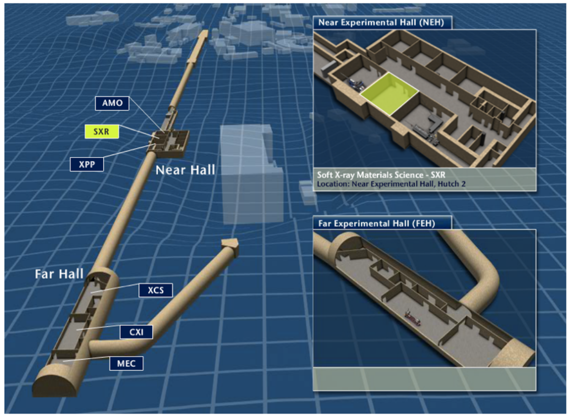
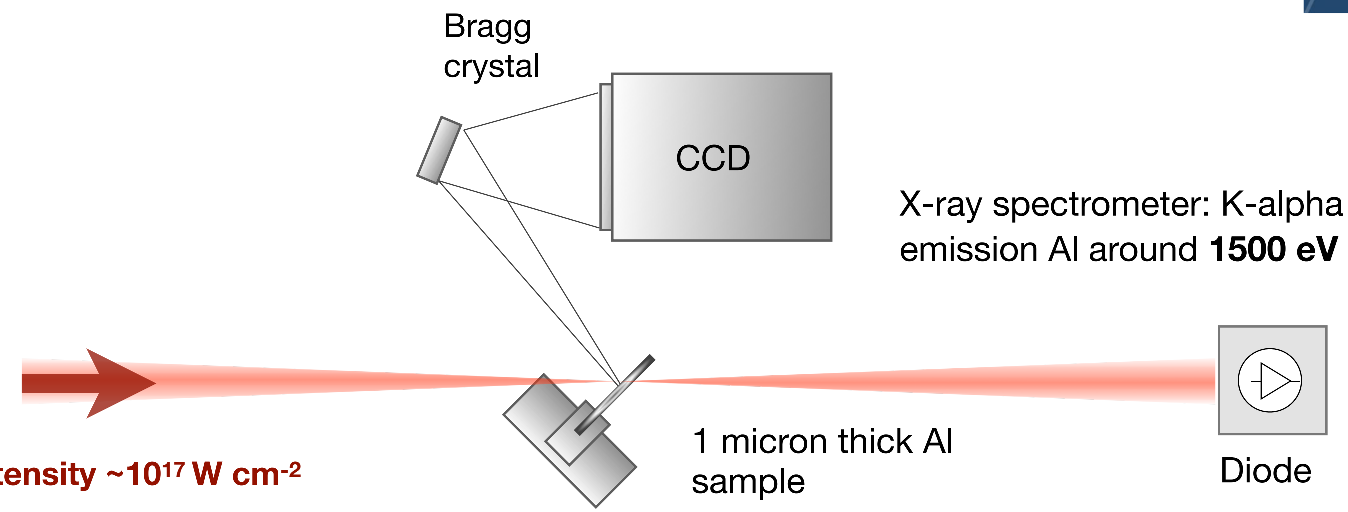
The experiment at the Linac Coherent Light Source X-ray Free-Electron Laser

LCLS pulse

Photon energy: 1460–1830 eV
Pulse length < 60 fs
Pulse Energy ~1.5 mJ
Bandwidth ~ 0.4%

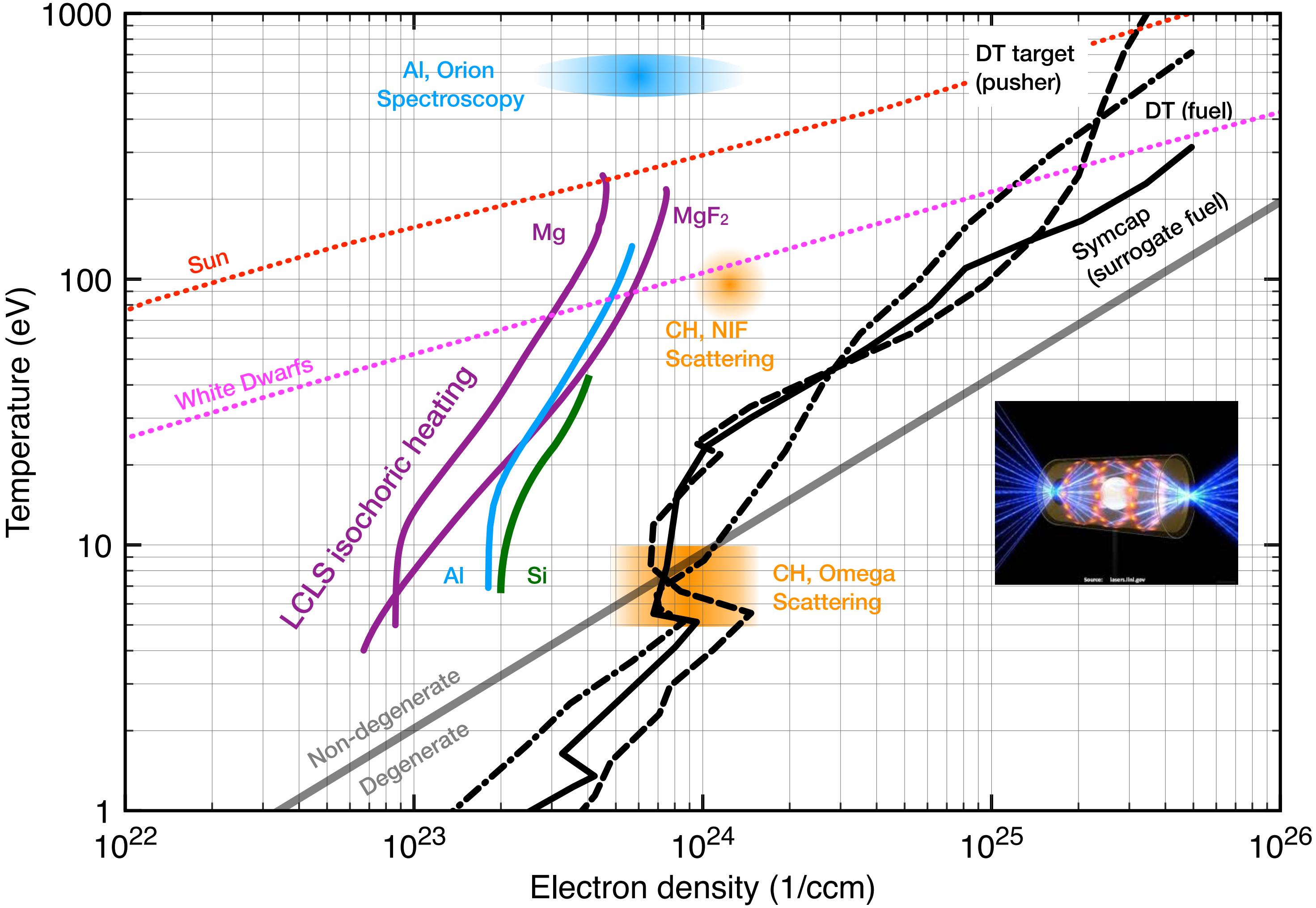




Peak Intensity ~10^{17} W cm^{-2}

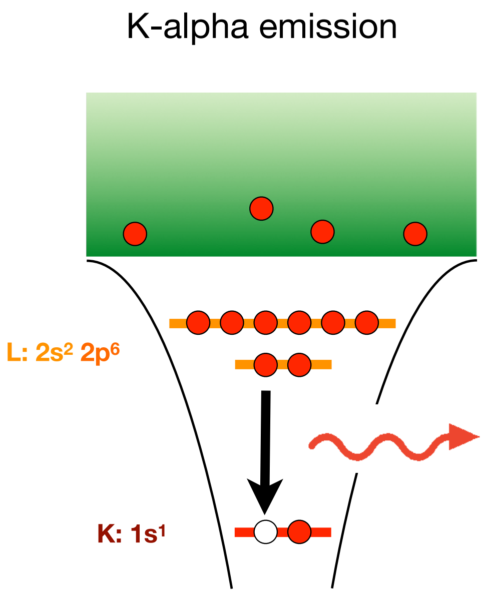
Vinko et al., Nature **482**, 59 (2012)
Ciricosta et al., PRL **109**, 065002 (2012)

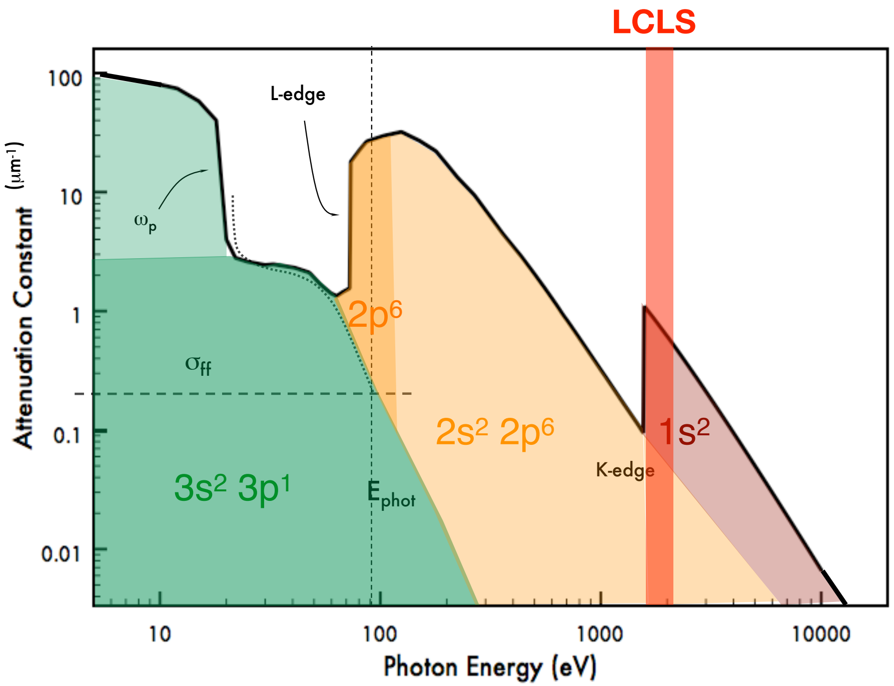
FELs can isochorically create high energy density plasmas



Electronic structure of Aluminium

Neutral Al

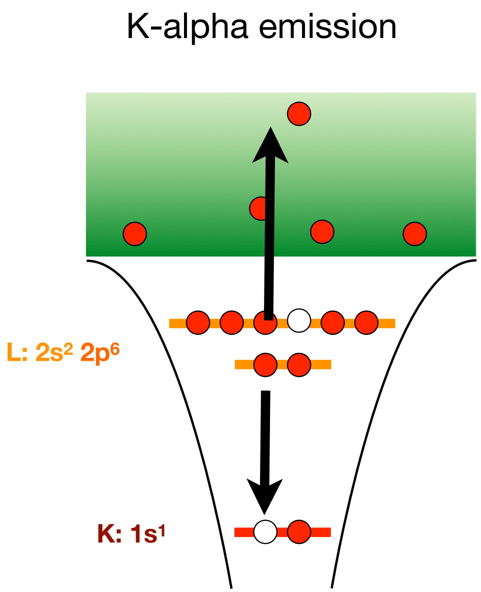


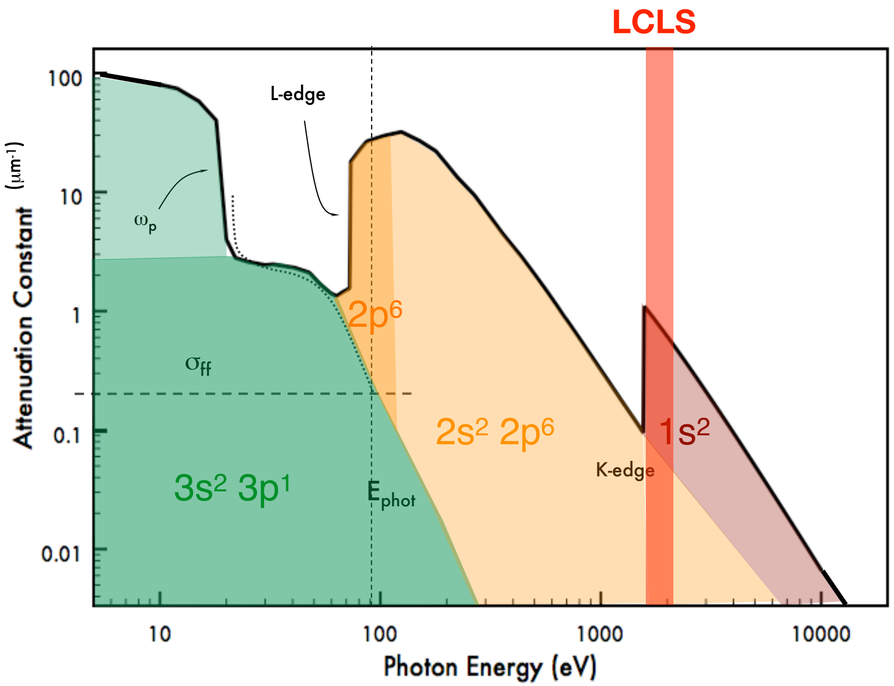


Core-hole lifetime ~1fs, although we diagnose via observing K-alpha, it is not the dominant decay mechanism.

Electronic structure of Aluminium

Neutral Al



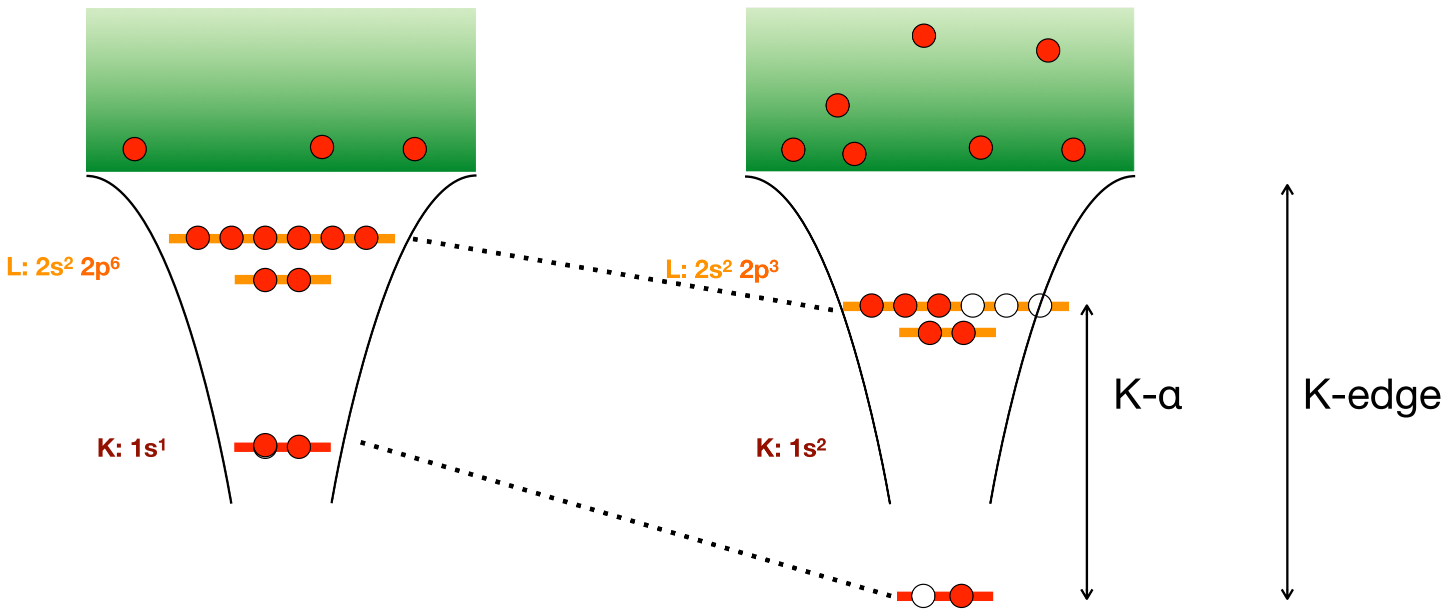


Radiationless Auger decay is 30 times more probable, ejecting L electrons into the continuum, that heat the other electrons within ~fsec

Photo-ejection of electrons, and Auger heating strips the Al ions

Neutral Al:

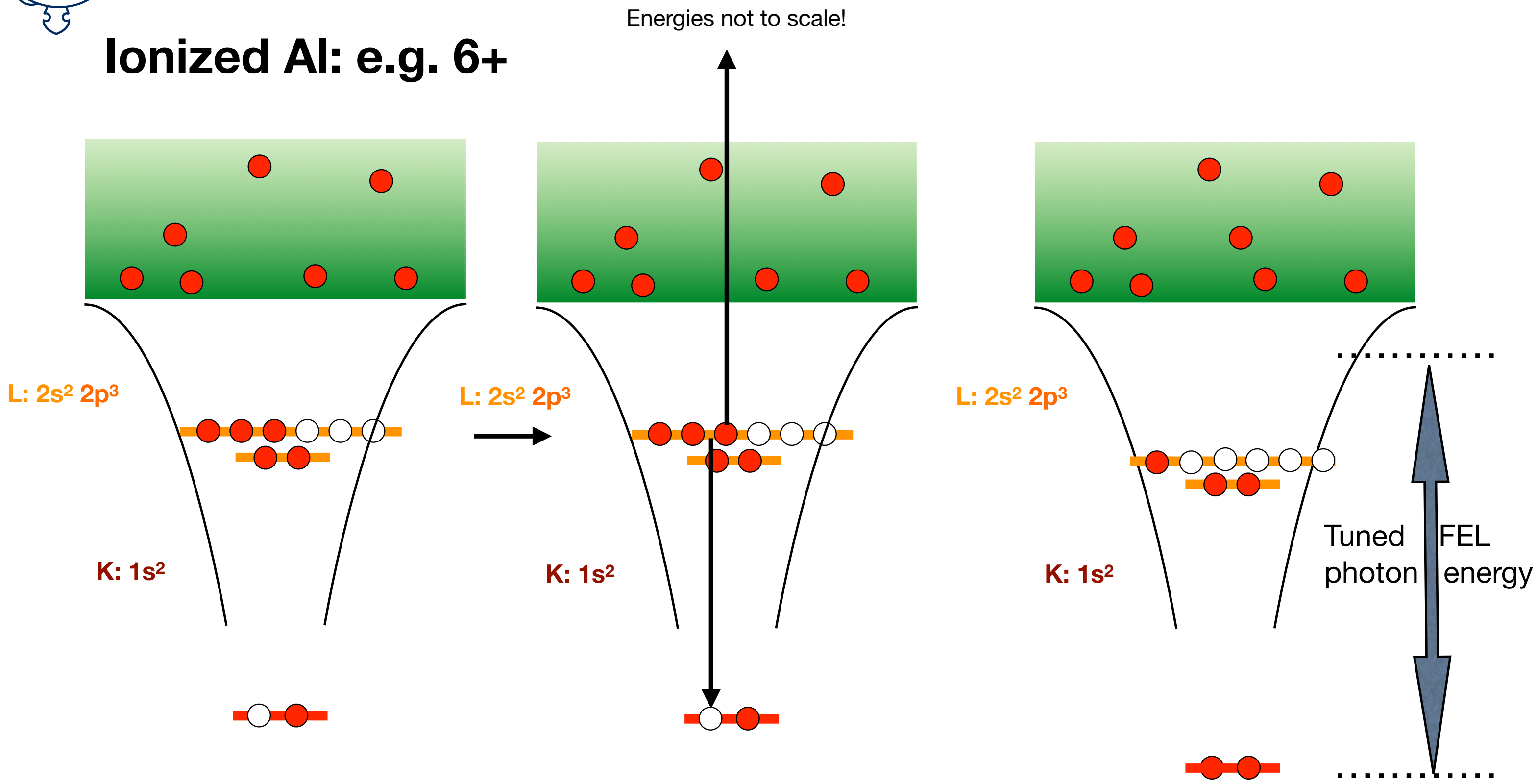
Ionized Al: e.g. 6+



As ionisation proceeds, note that both the K-edge energy, and the K-α energy increase with increasin
there are fewer L electrons to provide shielding.

If the FEL photon energy is too low, no K-α generated

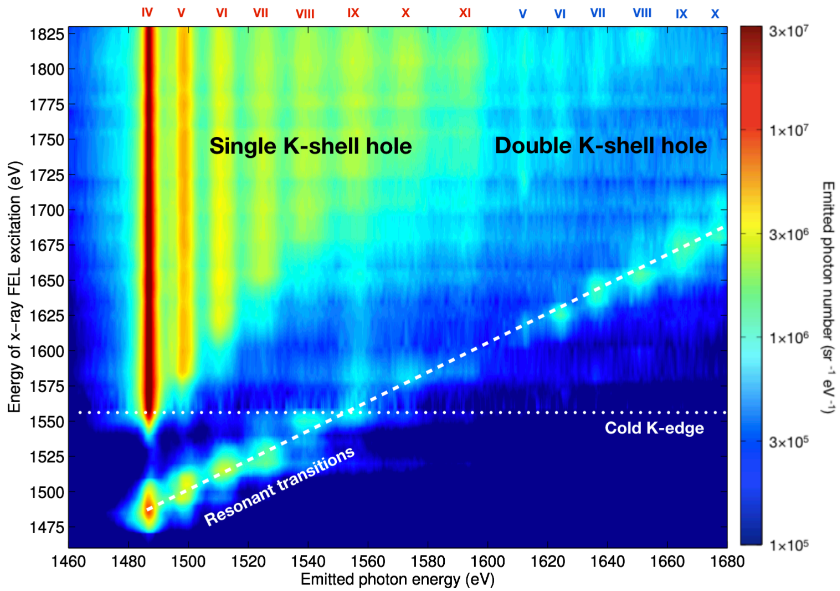
Ionized Al: e.g. 6+



Important to note: the heated continuum - many tens of eV, can further collisionally ionise the system.
No K-α will be seen if the K-edge energy of an ion exceeds the photon energy of the X-Ray Laser.

How do we model ionization at high densities, where screening and or Pauli exclusion forces are strong

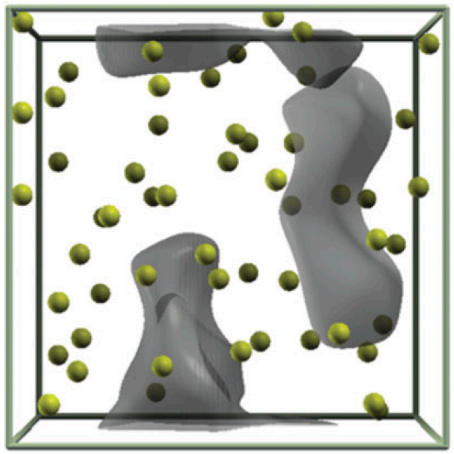
Continuum lowering models are challenged at high density



Physical Review Letters **109** 245003 (2012).

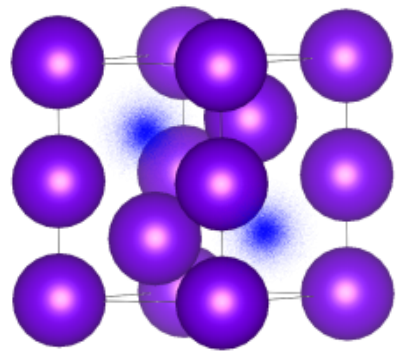
Screening/fluctuations/equilibration

Insulating plasma



Dai PRL 14

Transparent Na



Pauli exclusion/fluctuations

Publications on IPD since 2012

PRL 119, 065001 (2017) PHYSICAL REVIEW LETTERS week ending 11 AUGUST 2017

Continuum Lowering and Fermi-Surface Rising in Strongly Coupl[ed] and Degenerate Plasmas

S. X. Hu (胡素兴)*

PRL 110, 265003 (2013) PHYSICAL REVIEW LETTERS

Observations of the Effect of Ionization-Potential Depression in Hot Dense Plasma

D. J. Hoarty,[1] P. Allan,[1] S. F. James,[1] C. R. D. Brown,[1] L. M. R. Hobbs,[1] M. P. Hill,[1] J. W. O. Harris,[1] J. Morton,[1] M. G. Brookes,[1] R. Shepherd,[2] J. Dunn,[2] H. Chen,[2] E. Von Marley,[2] P. Beiersdorfer,[2] H. K. Chung,[3] R. W. Lee,[4] G. Brown,[3] and J. Emig[3]

nature COMMUNICATIONS — ARTICLE

Density functional theory calculations of continuum lowering in strongly coupled plasmas

S.M. Vinko,[1] O. Ciricosta[1] & J.S. Wark[1]

nature COMMUNICATIONS — ARTICLE — OPEN

Measurements of continuum lowering in solid-density plasmas created from elements and compounds

PHYSICS OF PLASMAS 23, 012708 (2016)

Monte Carlo simulations of ionization potential depression in dense plasmas

M. Stransky

High Energy Density Physics

A study of density effects in plasmas using analytical approximations for the self-consistent potential

M. Poirier

PRL 109, 065002 (2012) PHYSICAL REVIEW LETTERS week ending 10 AUGUST 2012

Direct Measurements of the Ionization Potential Depression in a Dense Plasma

O. Ciricosta,[1] S. M. Vinko,[1] H.-K. Chung,[2] B.-I. Cho,[3] C. R. D. Brown,[4] T. Burian,[5] J. Chalupský,[5] K. Engelhorn,[3] R. W. Falcone,[3,6] C. Graves,[7] V. Hájková,[5] A. Higginbotham,[1] L. Juha,[5] J. Krzywinski,[7] H. J. Lee,[7] M. Messerschmidt,[7] C. D. Murphy,[1] Y. Ping,[8] D. S. Rackstraw,[1] A. Scherz,[7] W. Schlotter,[7] S. Toleikis,[9] J. J. Turner,[7] L. Vysin,[5] T. Wang,[7] B. Wu,[7] U. Zastrau,[10] D. Zhu,[7] R. W. Lee,[7] P. Heimann,[3] B. Nagler,[7] and J. S. Wark[1,*]

PRL 112, 145004 (2014) PHYSICAL REVIEW LETTERS week ending 11 APRIL 2014

Observations of Continuum Depression in Warm Dense Matter with X-Ray Thomson Scattering

L. B. Fletcher,[1,2] A. L. Kritcher,[3] A. Pak,[3] T. Ma,[3] T. Döppner,[3] C. Fortmann,[3] L. Divol,[3] O. S. Jones,[3] O. L. Landen,[3] H. A. Scott,[3] J. Vorberger,[4] D. A. Chapman,[5,6] D. O. Gericke,[6] B. A. Mattern,[7] G. T. Seidler,[7] G. Gregori,[8] R. W. Falcone,[2] and S. H. Glenzer[1]

J. Phys. B: At. Mol. Opt. Phys. 48 (2015) 224003

Ionization potential depression for non equilibrated aluminum plasmas

A Calisti, S Ferri and B Talin

Quantum-Mechanical Calculation of Ionization-Potential Lowering in Dense Plasmas

Sang-Kil Son (손상길),[1,2,*] Robert Thiele,[1,2,†] Zoltan Jurek,[1,2] Beata Ziaja,[1,2,3] and Robin Santra[1,2]

(Received 19 July 2013; revised manuscript received 17 February 2014; published 8 July 2014)

High Energy Density Physics

Fluctuations and the ionization potential in dense plasmas

PHYSICAL REVIEW E 87, 013104 (2013)

Electronic and ionic structures of warm and hot dense [...]

PHYSICAL REVIEW E 94, 011202(R) (2016)

X-ray scattering measurements on imploding CH spheres at the National Ignition Facility

D. Kraus, D. A. Chapman, A. L. Kritcher, R. A. Baggott, B. Bachmann, G. W. Collins, S. H. Glenzer, J. A. Hawreliak, D. H. Kalantar, O. L. Landen, T. Ma, S. Le Pape, J. Nilsen, D. C. Swift, P. Neumayer, R. W. Falcone, D. O. Gericke, and T. Döppner

PHYSICAL REVIEW A 87, 062502 (2013)

Effect of screening on spectroscopic properties of Li-like ions in a plasma environment

Pradip Kumar Mondal,[1] Narendra Nath Dutta,[1] Gopal Dixit,[2,*] and Sonjoy Majumder[1,†]

(Received 6 March 2013; published 4 June 2013)

PHYSICAL REVIEW E 92, 011101(R) (2015)

Role of the ionization potential in nonequilibrium metals driven to absorption saturation

R. Mincigrucci, F. Bencivenga, F. Capotondi, E. Principi, E. Giangrisostomi, A. Battistoni, M. Caputo, F. Casolari, A. Gessini, M. Manfredda, E. Pedersoli, and C. Masciovecchio

High Energy Density Physics

Density effects in plasmas: Detailed atomic calculations and analytical expressions

A validation of a simple model for the calculation of the ionization ene[rgy] in X-ray laser-cluster interactions

Jeff White and Edward Ackad

Ionization Potential Depression in Hot Dense Plasmas Through a Pure Classical Model

A. Calisti*, S. Ferri, and B. Talin

Received 27 October 2014, revised 23 January 2015, accepted 23 January 2015. Published online 17 February 2015

PHYSICAL REVIEW A 91, 042515 (2015)

Nonrelativistic structure calculations of two-electron ions in a strongly coupled pl[asma]

S. Bhattacharyya,[1,*] J. K. Saha,[2] and T. K. Mukherjee[3]

(Received 19 March 2015; published 30 April 2015)

High Energy Density Physics

A plea for a reexamination of ionization potential depression measurements

Carlos A. Iglesias

Ionization-potential depression and othe[r] plasma statistical property studies - Application [to] spectroscopic diagnostics.

Annette Calisti, Sandrine Ferri, Caroline Mossé, Bernard Tali[n]

Reduction of the ionization energy for 1s-[...] dense aluminum plasmas

C Lin[1], H Reinholz[1,2] and G Röpke[1]

PHYSICAL REVIEW A 93, 052513 (2016)

Plasma screening effects on the electronic structure [of] Al ions using Debye and ion-sphere m[odels]

Madhulita Das,[1,*] B. K. Sahoo,[2,†] and Sourav [...]

(Received 6 April 2016; published 23 May 2016)

PHYSICAL REVIEW E 96, 013202 (2017)

Ionization-potential depression and dynamical structure factor in [...]

Chengliang Lin,[1,*] Gerd Röpke,[1,†] Wolf-Dietrich Kraeft,[1,‡] and Heidi Rei[nholz]

(Received 9 March 2017; published 6 July 2017)

PHYSICAL REVIEW B 93, 115114 (2016)

Link between K absorption edges and thermodynamic properties of warm dense plasmas established by an improved first-principles method

Shen Zhang,[1,2] Shijun Zhao,[1,2] Wei Kang,[1,2,*] Ping Zhang,[1,3] and Xian-Tu He[1,4,†]

(Received 31 October 2014; revised manuscript received 21 February 2016; published 7 March 2016)

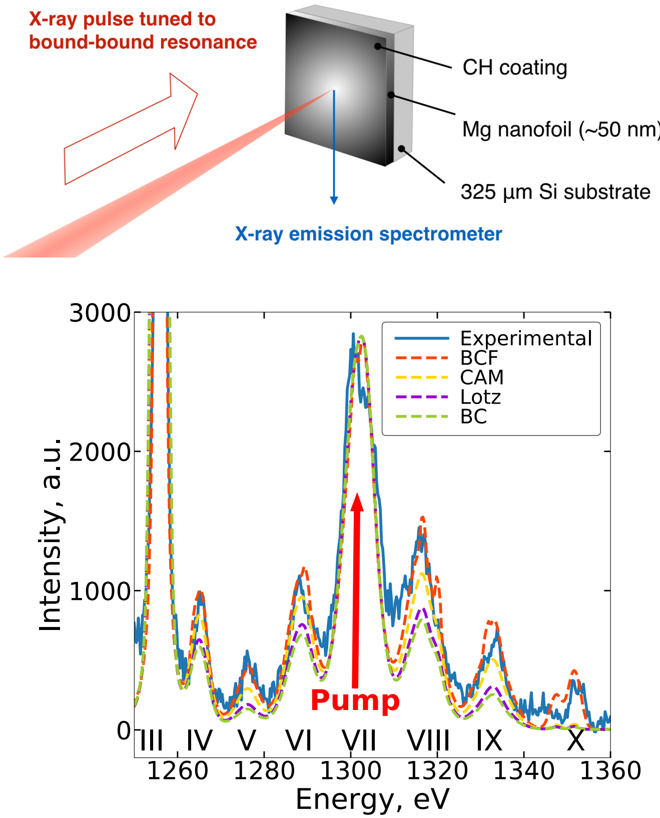
High Energy Density Physics — Review

A review of environment-dependent processes within FEL excited matter

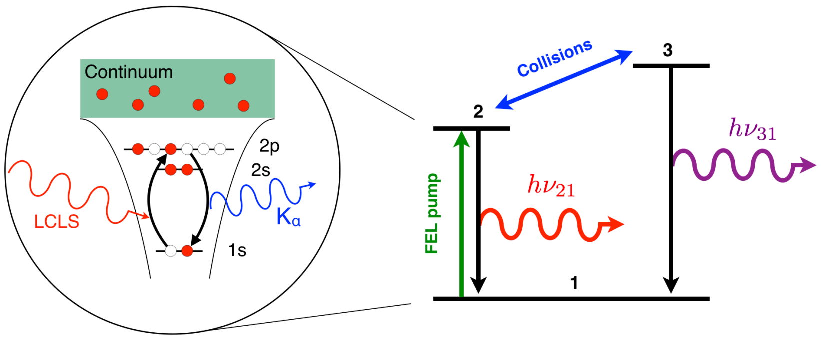
B. Ziaja, Z. Jurek, N. Medvedev, R. Thiele, S. Toleikis

XFELs can clock sub-femtosecond electron collisional dynamics

- How quickly do electrons collisionally ionize in hot-dense plasmas?
- What are the timescales for electron 'damage' in dense systems?



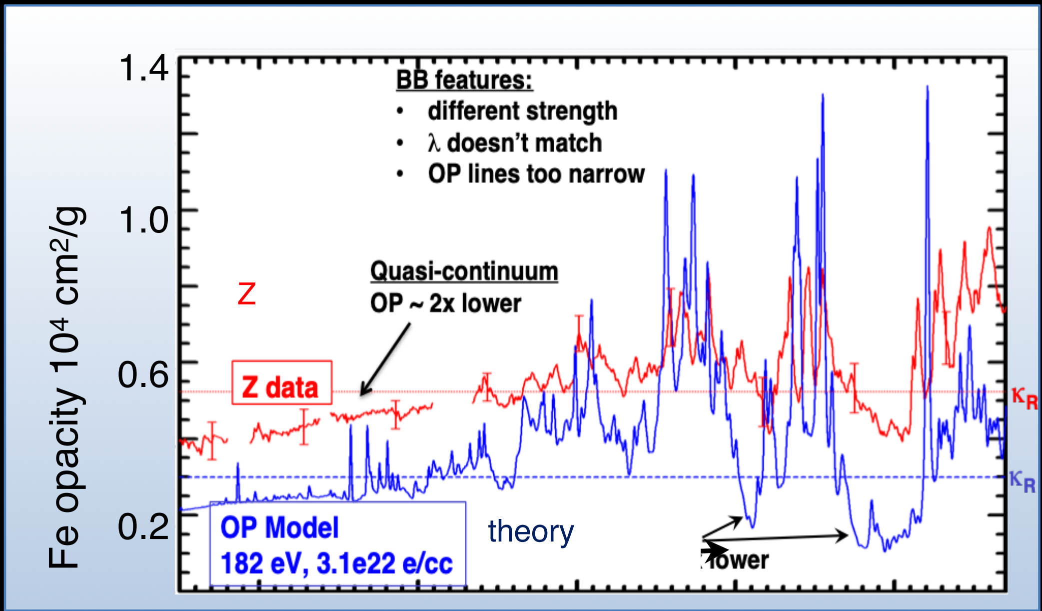
Collisions are 'clocked' by the Auger decay: Auger clock for collisional dynamics.



$$R_{\text{Collisions}} = R_{\text{Auger}} \cdot \left[\frac{I(\nu_{21})}{I(\nu_{31})} - 1 \right]^{-1}$$

Vinko et al., Nature Commun. 6, 6397 (2015)
van den Berg et al., PRL 120, 055002 (2018)

Recent Fe opacity data from Bailey suggest a need to explore radiation transport mechanisms in stars

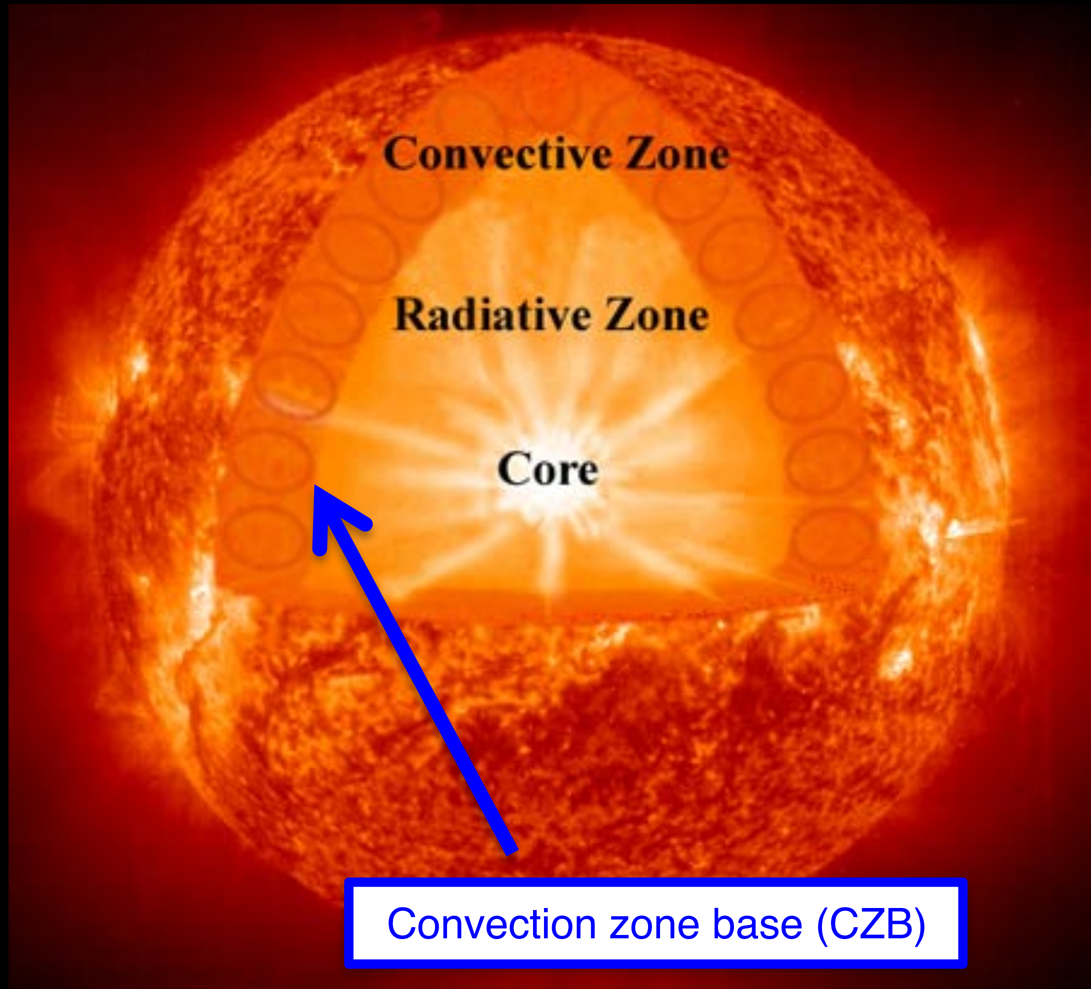


LETTER

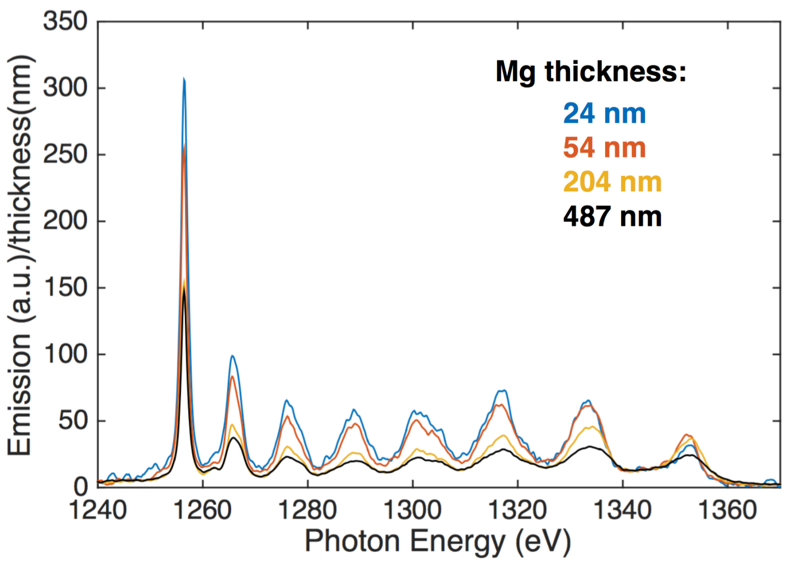
doi:10.1038/nature14048

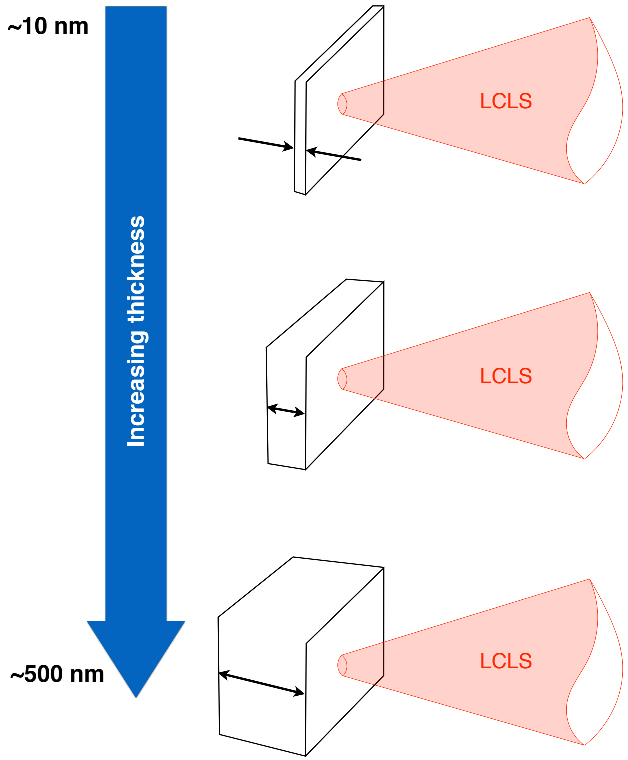
A higher-than-predicted measurement of iron opacity at solar interior temperatures

J. E. Bailey[1], T. Nagayama[1], G. P. Loisel[1], G. A. Rochau[1], C. Blancard[2], J. Colgan[3], Ph. Cosse[2], G. Faussurier[2], C. J. Fontes[3], F. Gilleron[2], I. Golovkin[4], S. B. Hansen[1], C. A. Iglesias[5], D. P. Kilcrease[3], J. J. MacFarlane[4], R. C. Mancini[6], S. N. Nahar[7], C. Orban[7], J.-C. Pain[2], A. K. Pradhan[7], M. Sherrill[3] & B. G. Wilson[5]



A new way to look at radiation transport and opacity in solid density systems via emission spectroscopy

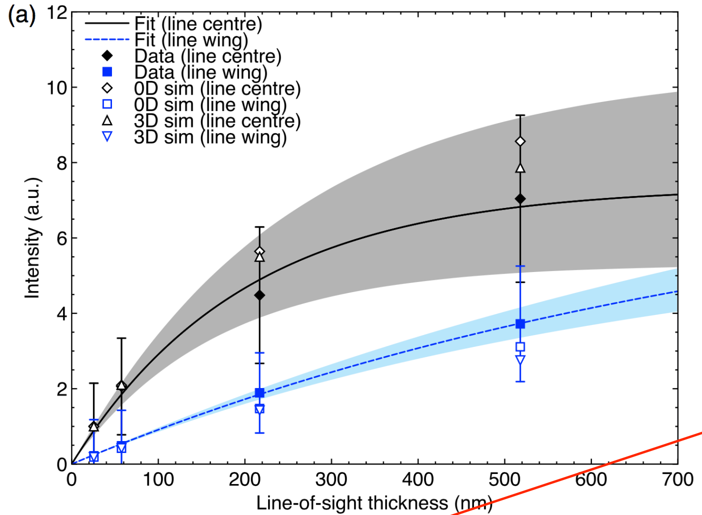


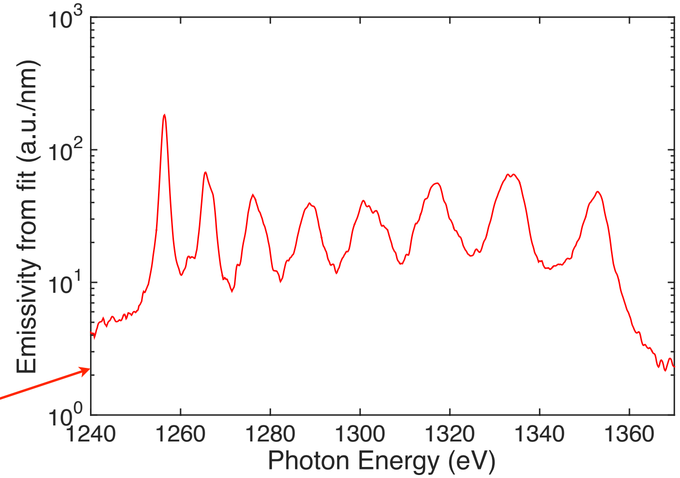


Volumetric photo-absorption on foils of different thicknesses, all thinner than 1 absorption depth

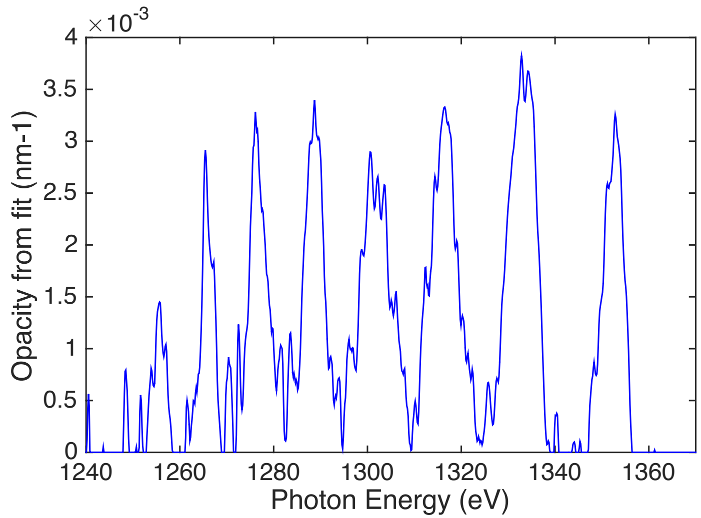
sam.vinko@physics.ox.ac.uk

A new way to look at radiation transport and opacity in solid density systems via emission spectroscopy





$$I(d) = \frac{\epsilon(\omega)}{\kappa(\omega)}\left[1 - \exp(-\kappa(\omega)d)\right]$$



Can measure absorption spectrum using a narrow-bandwidth X-ray source exploiting self emission!

T. Preston *et al.*, Physical Review Letters 119 085001 (2017).

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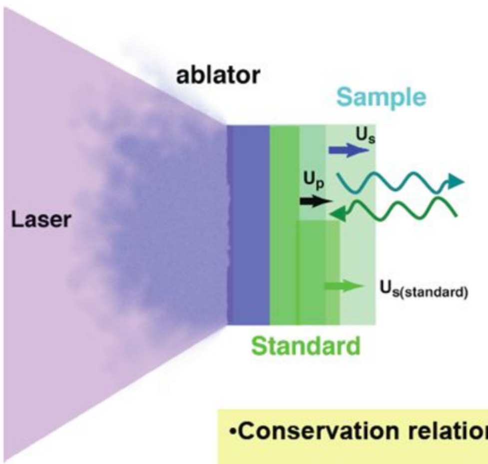
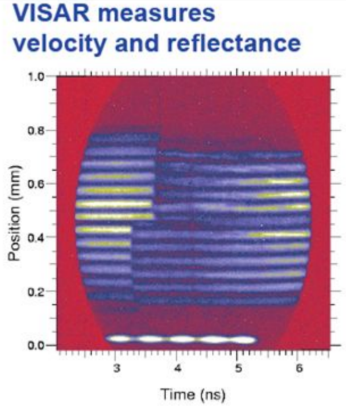
Laser Ablation

- Nanosecond laser irradiates an ablation and launches a pressure wave (or shock).
- The FEL records the diffraction pattern during the compression.
- Interferometry from the rear surface motion provides pressure diagnosis

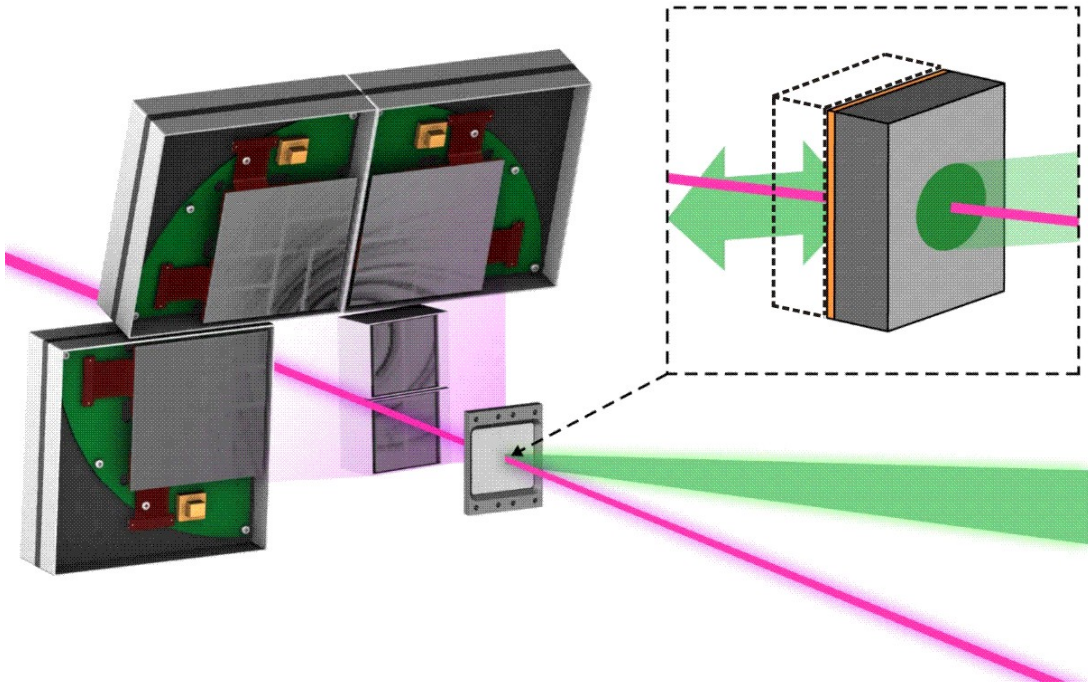




•Conservation relations => $P = \rho_0 U_s U_p$

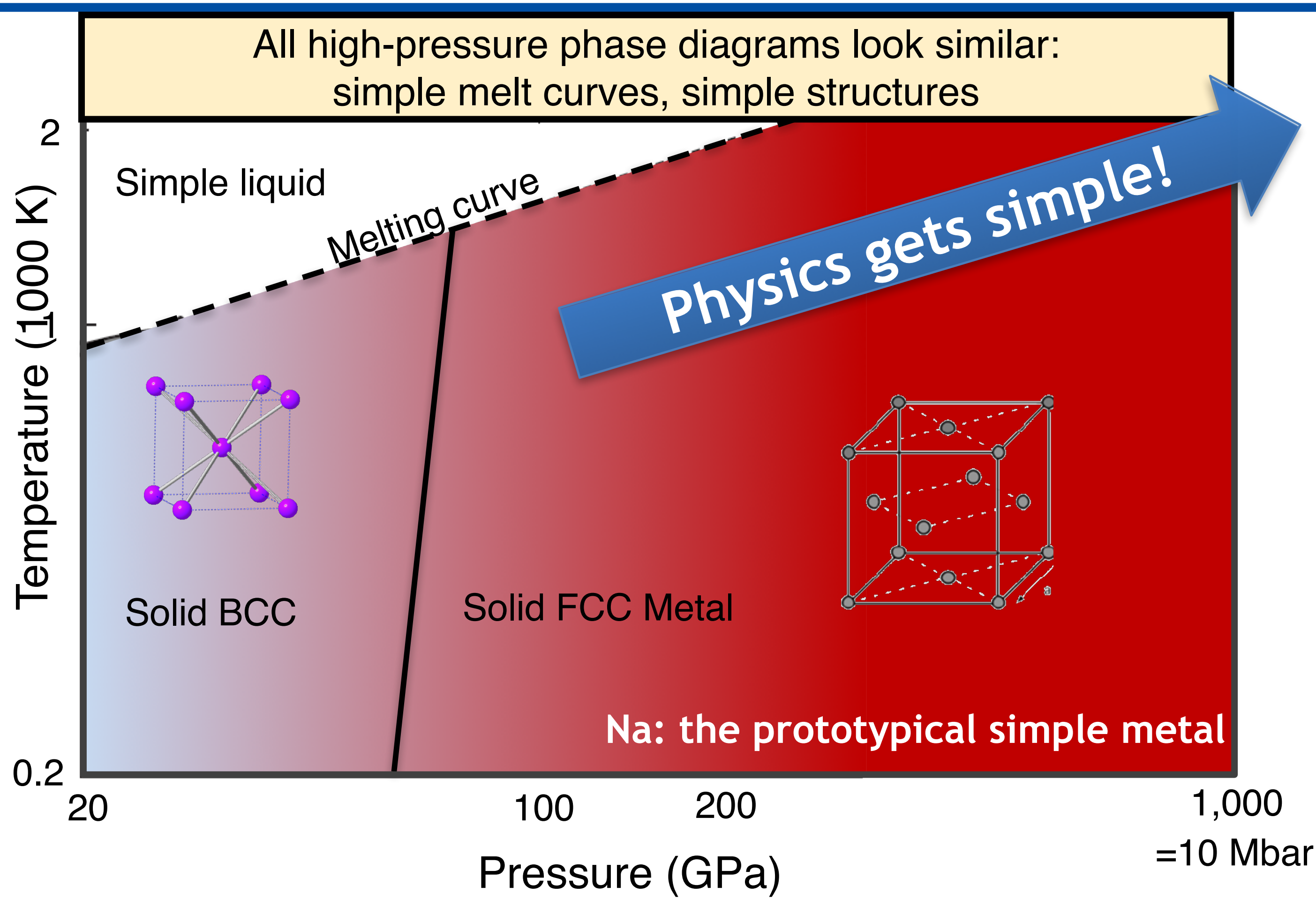
$\rho/\rho_o = 1/(1-U_p/U_s)$

•Temperature needs to be measured separately



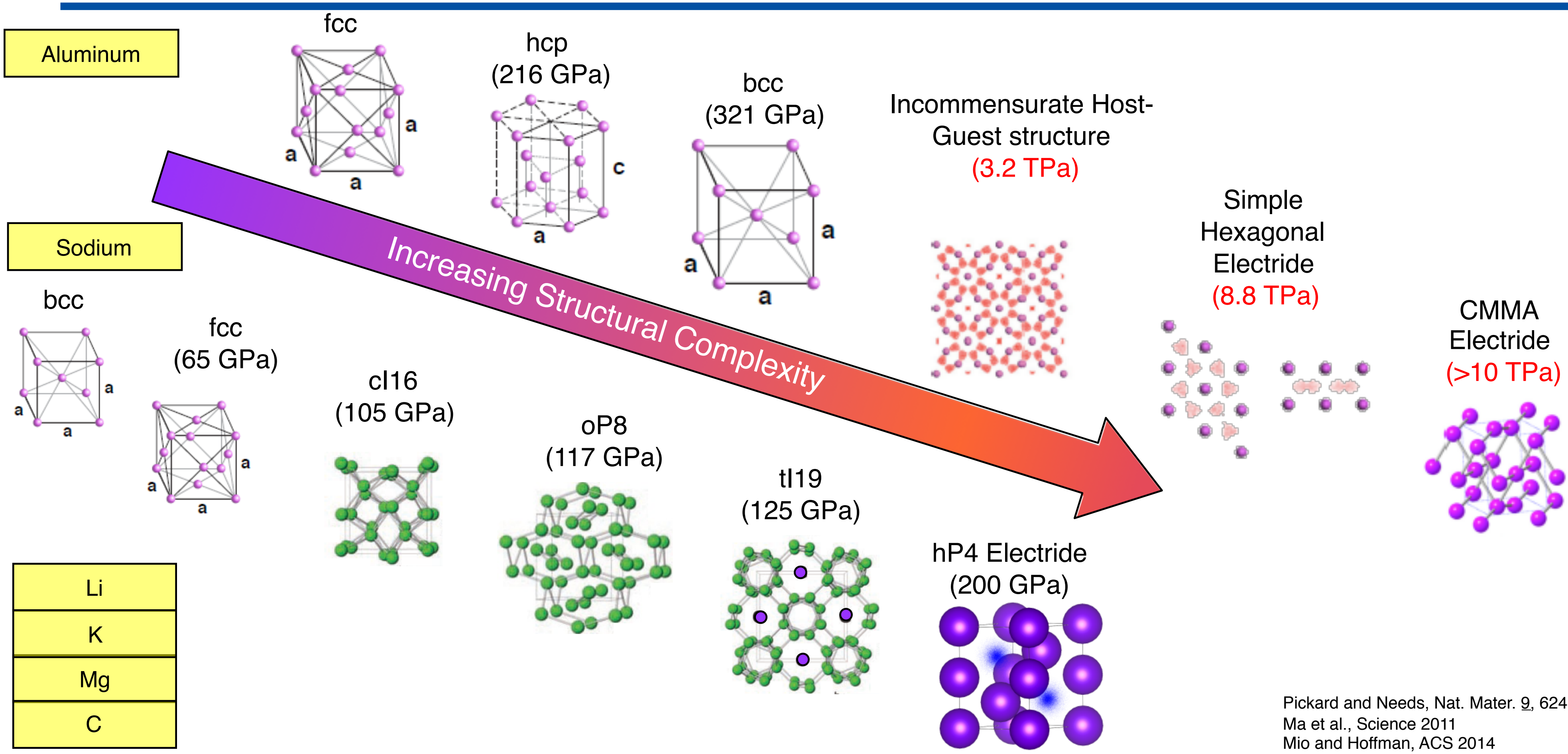
Nanosecond lasers can induce multi-TPa pressures for times of a few nanoseconds in

Just a few years ago, ultrahigh-pressure phase diagrams, for matter with core electrons, were very simple



* M. Marques et al., PHYSICAL REVIEW B 83, 184106 (2011)

Many materials are now predicted to exhibit exotic behavior at HED pressure

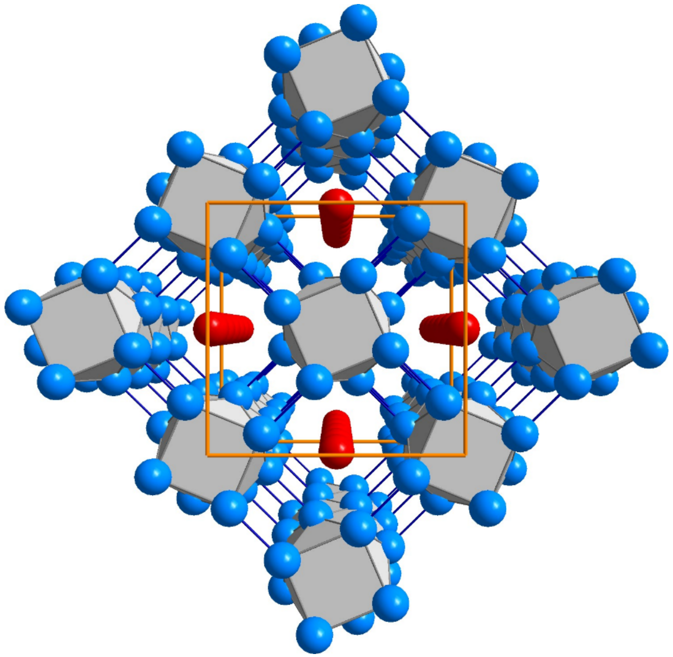


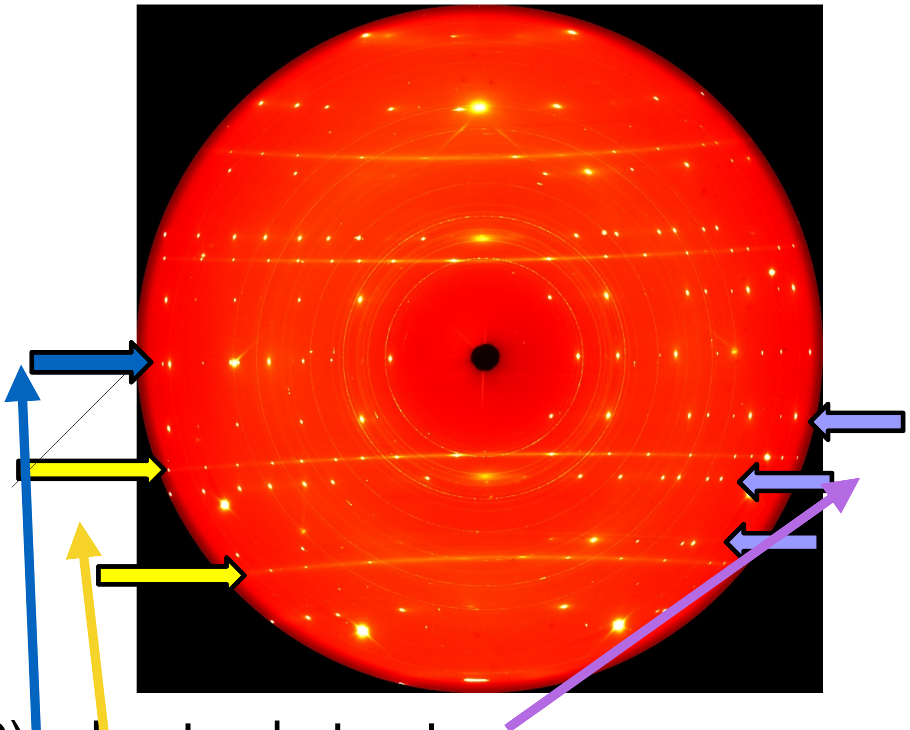
Pickard and Needs, Nat. Mater. 9, 624 (2010)
Ma et al., Science 2011
Mio and Hoffman, ACS 2014

THE UNIVERSITY *of* EDINBURGH

Creation of Host-Guest Structures

UNIVERSITY OF OXFORD





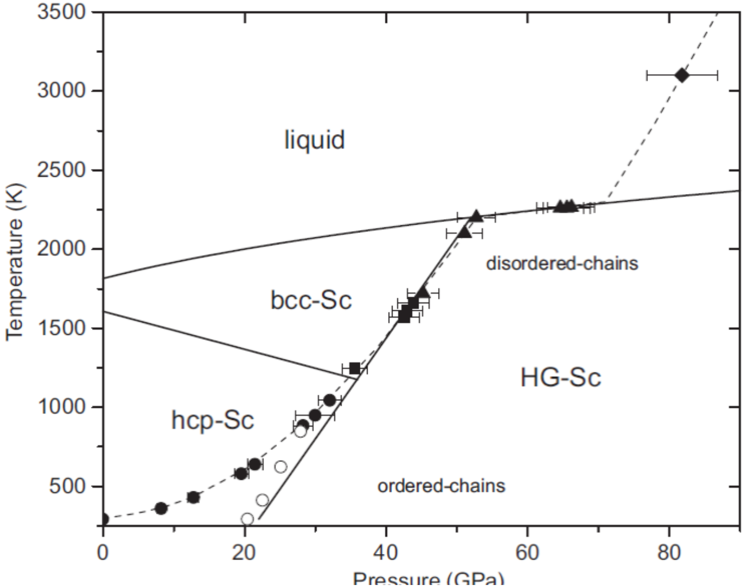
Miller Indices: (hkl0) – host substructure

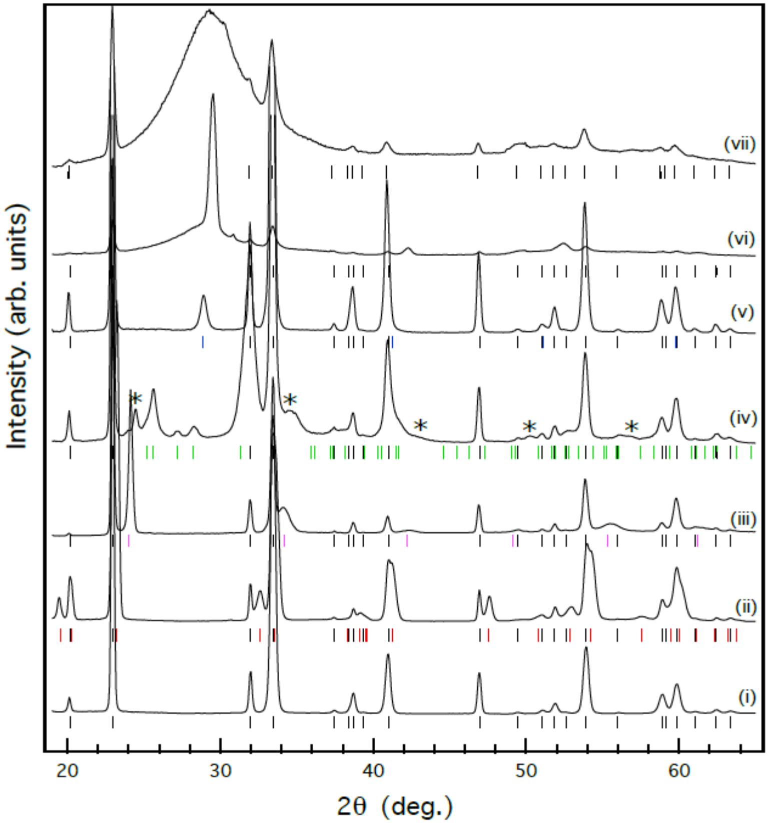
(hk0m) – guest substructure

(hk00) – common to both

No of atoms/cell = $16 + 2\times(c_H/c_G)$

Creation of Host-Guest Structures on nanosecond timescales via shock compression





Liquid – 57 GPa

Sb-V – bcc + liquid – 38 GPa

Sb-V – bcc – 19 GPa

Sb-III – incommensurate - 12 GPa

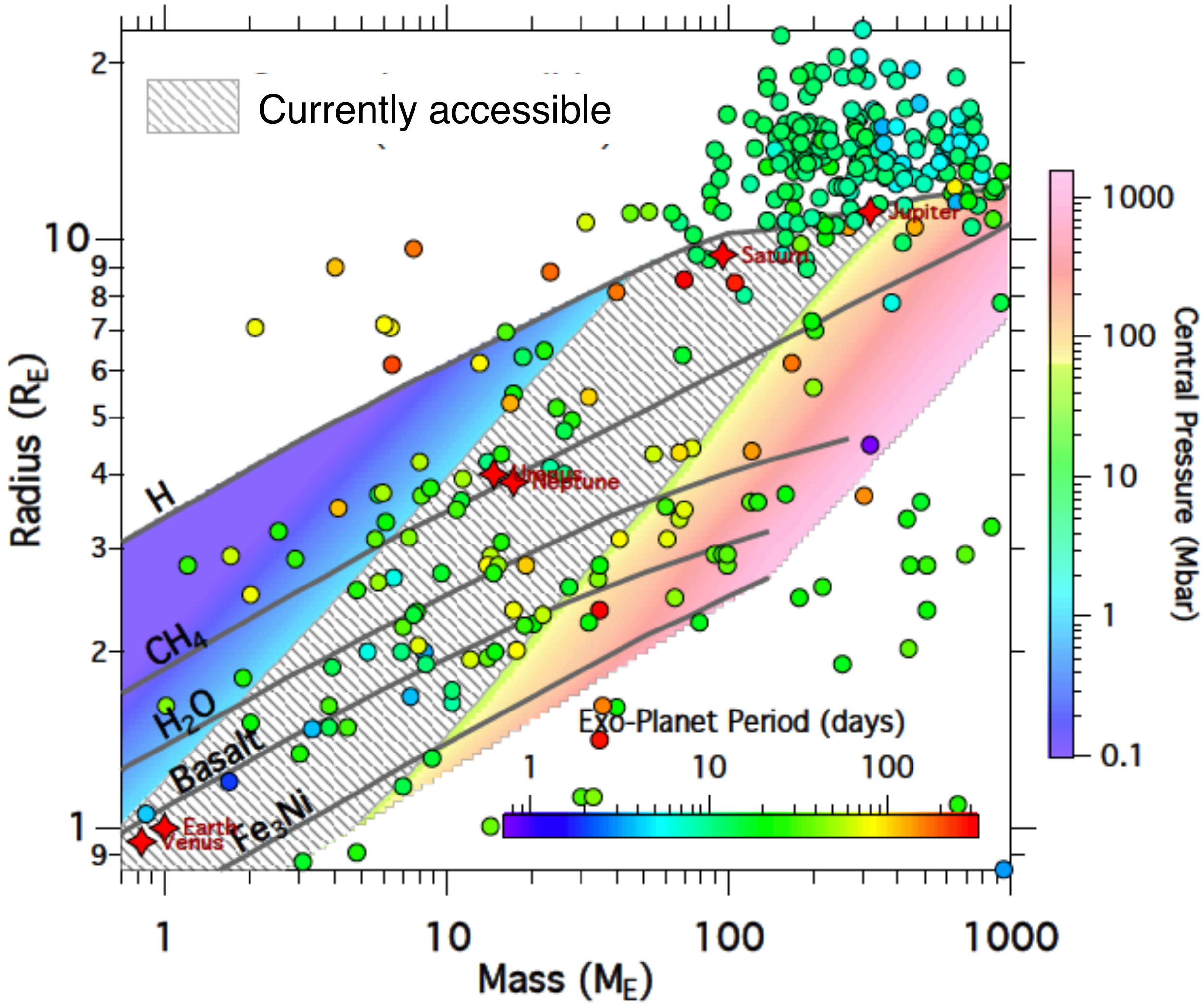
Sb-I – 8 GPa

Sb-I – 2 GPa

Sb-I - AP

- Sc: R. Briggs et al., Phys. Rev. Lett., **118** 025501 (2017).
- Sb: A.L. Coleman *et al.*, Phys. Rev. Lett., **122** 255704 (2019).

Recently discovered planets contain matter at millions (100's GPa) to billions (100's TPa) of atmosphere pressure, this is HEDS



Each circle is a planet

Observational data are limited

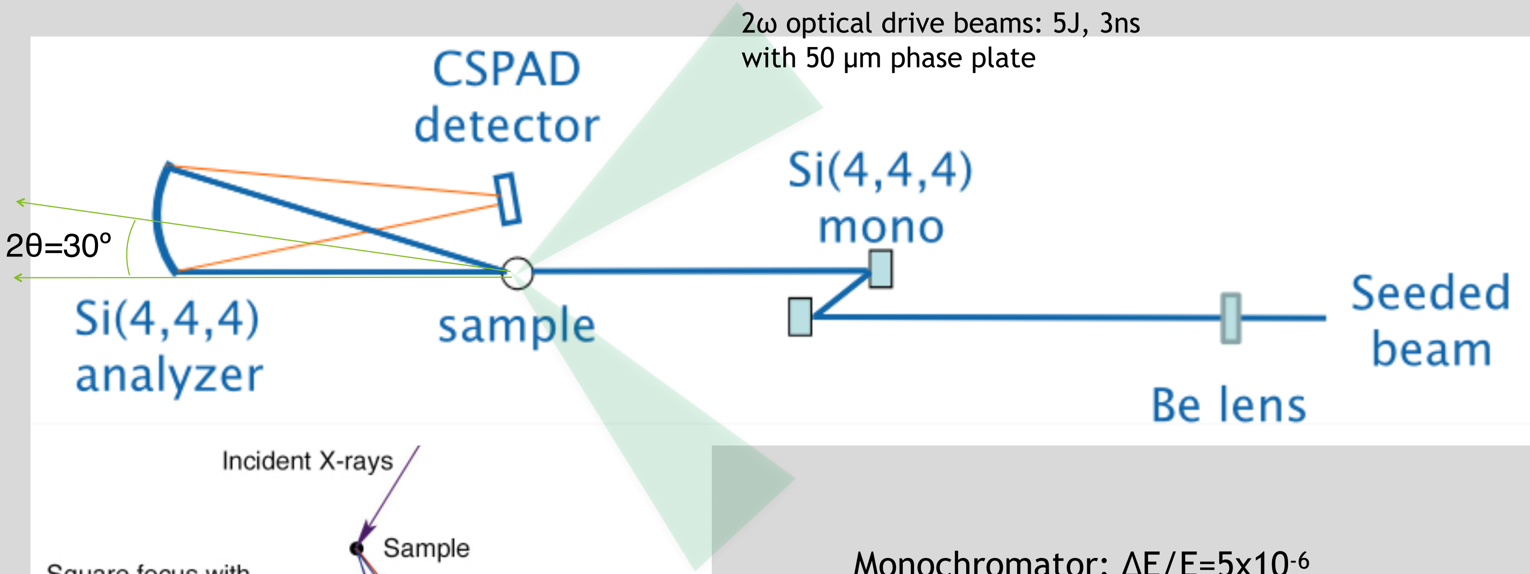
Need EOS and transport data/theory

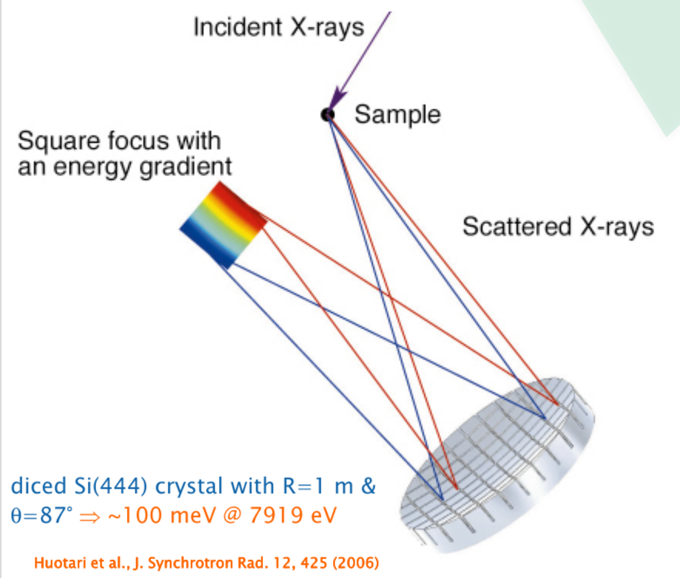
Transport properties and temperature can in principle be provided by inelastic scattering from ion fluctuations (phonons)

D. Swift, et al., 2012
S. Seager 2007
J. Eggert
exoplanet.eu/catalog/

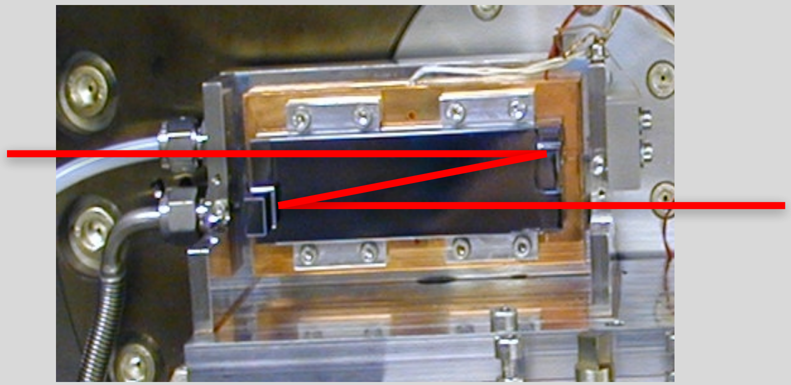
First experiments to measure ion-acoustic dynamics performed at LCLS

2ω optical drive beams: 5J, 3ns
with 50 μm phase plate



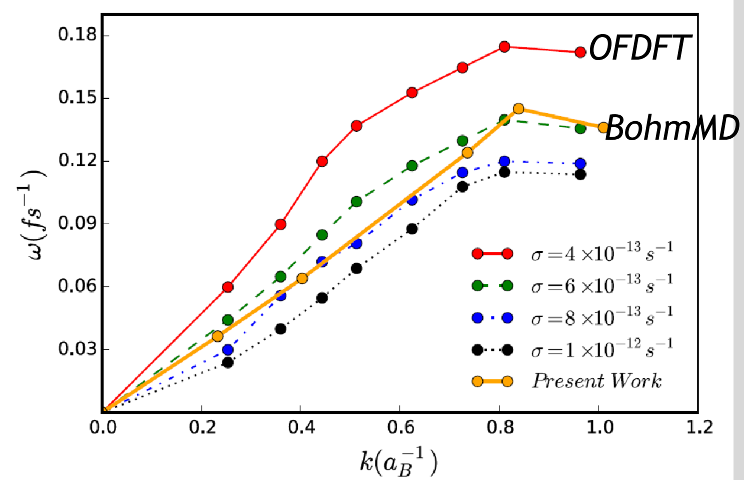


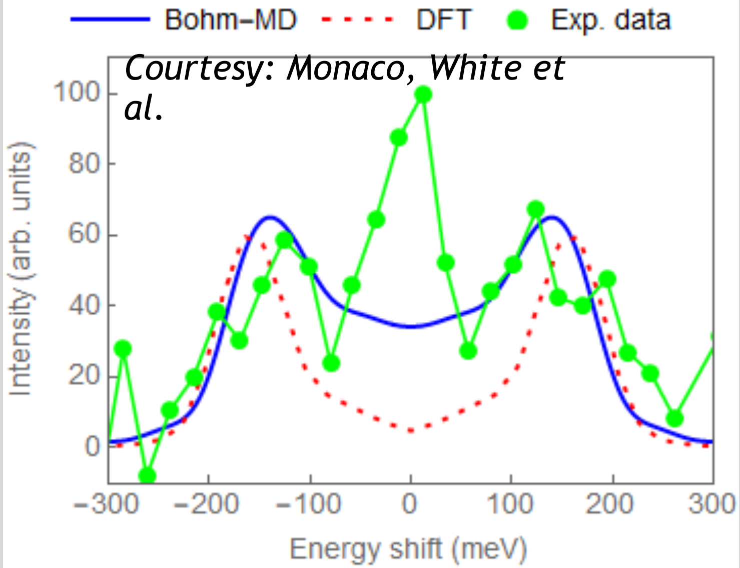
Monochromator: $\Delta E/E=5\times10^{-6}$



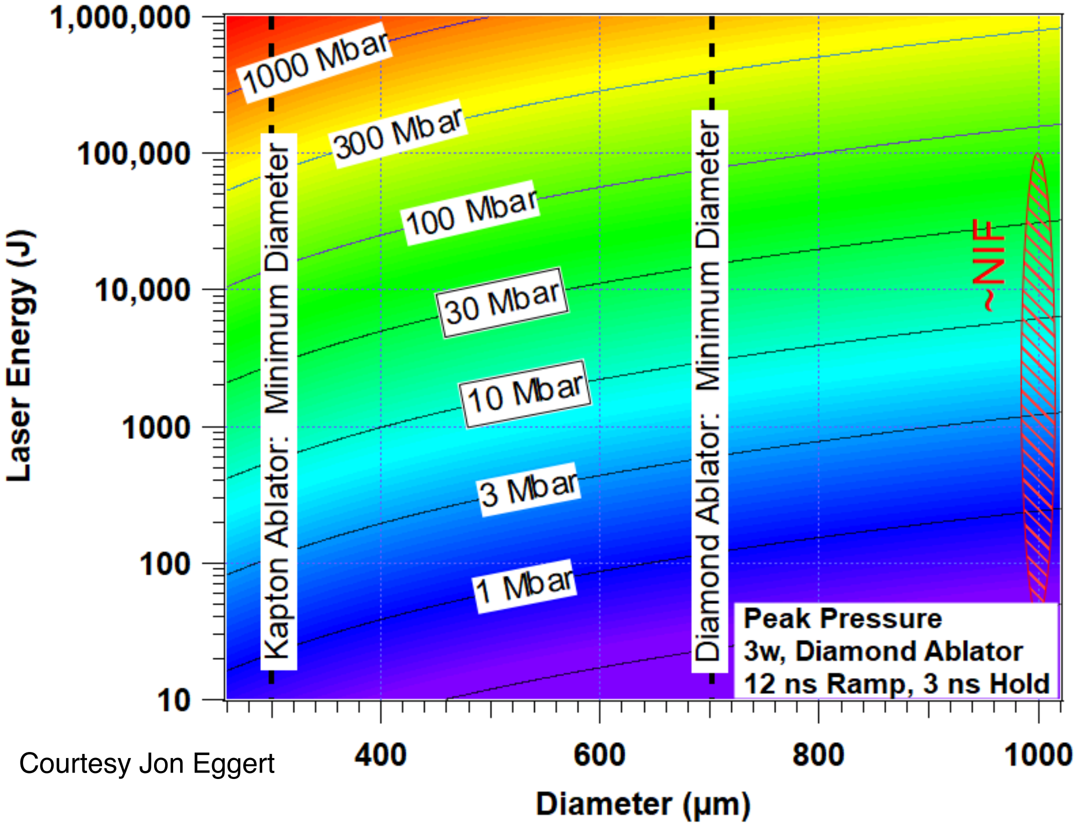
Observation of ion acoustic waves in dense plasmas (modelled with Bohm-MD

- Quantum bodies are treated as an ensemble of classical trajectories, but with the addition of a non-local potential, giving full electron and ion dynamics
- No need to introduce an unknown parameter (electron-ion collision frequency)
- Bohm-MD simulations performed with 1024 atoms (on a laptop), giving $>10^4$ increase in speed with comparable TDDFT simulations!
- Bohm-MD can be implemented in a fitting algorithm to predict plasma conditions

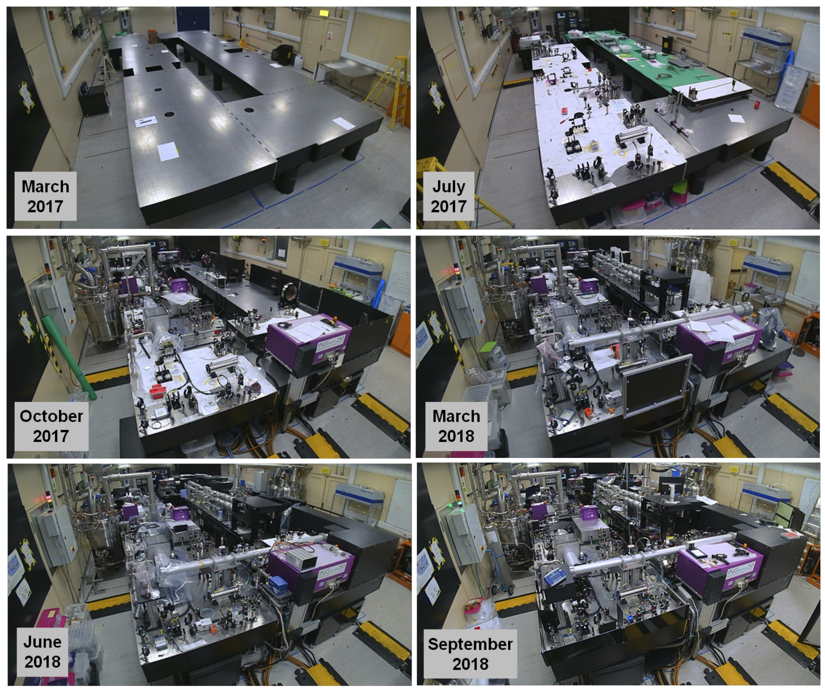




A 100J laser (DiPOLE) gets us to several Mbar easily - higher with convergent geometries. kJ systems get us to the TPa regime



Courtesy Jon Eggert

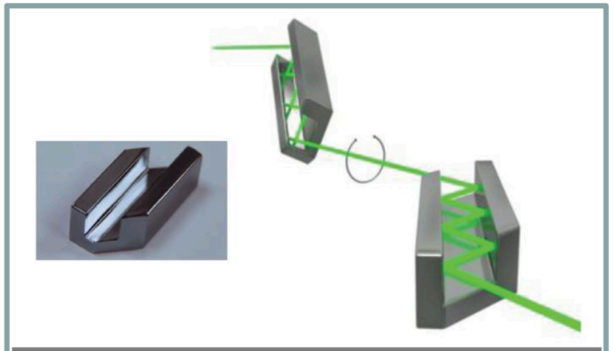


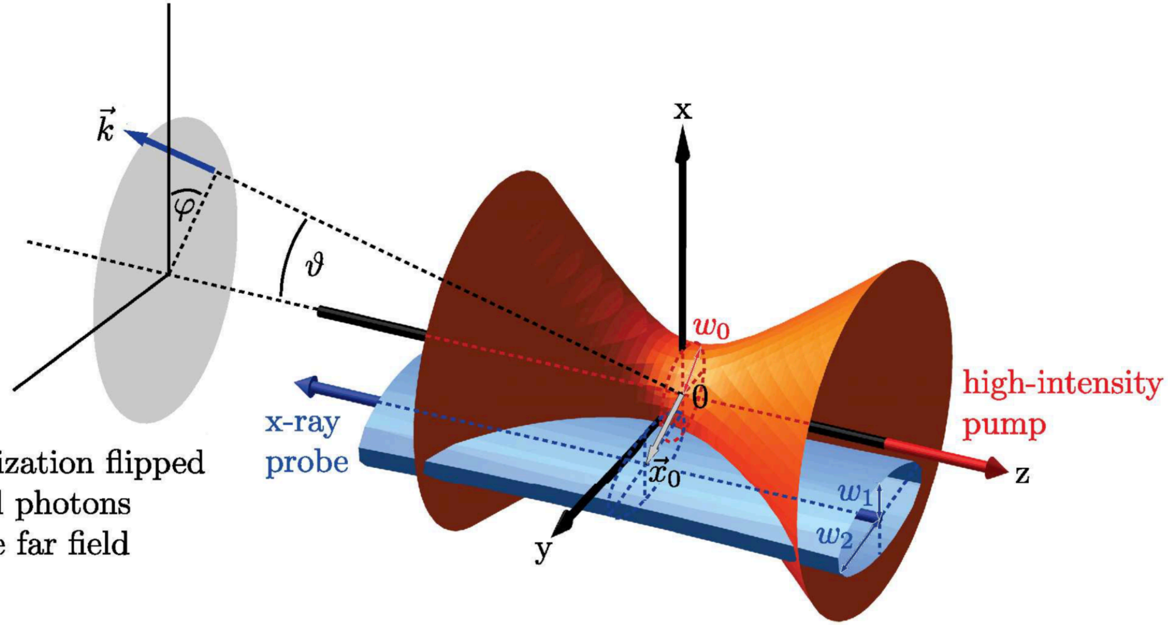
- 100 J, 10 Hz, nanosecond DiPOLE laser now commissioned and ready to be shipped to European XFEL

Short-Pulse Physics

- Thus far we have been looking at x-ray only experiments, and interactions with matter compressed with nanosecond optical lasers.
- There is also a plethora of physics that can be pursued with femtosecond optical lasers in the high intensity regime.
- The European XFEL has a 100-200 TW (40-fsec) optical laser alongside the x-ray laser.
- A variety of fundamental physics experiments have been proposed…

Measurements of Vacuum Birefringence


Si channel-cut Bragg polarimeter
I. Uschmann et al, Jena



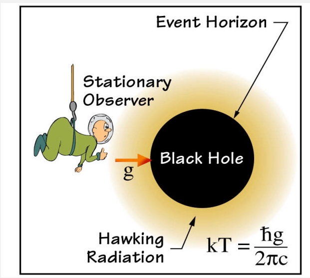
- Highly polarised x-ray beams can be generated from multiple diffraction in channel cut crystals
- Rotation of some of the x-ray photons in an intense optical pulse measures the birefringence of the vacuum.
- The effect is highly non-linear in optical laser energy and x-ray wavelength.

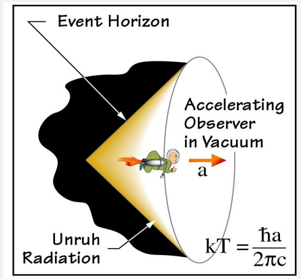
- Figure from Felix Karbstein, Jena

Gravity analogues and strong field QED

Electrons accelerated by lasers provide means to test fundamental physics

- ➜ Photons scattered by accelerated electrons experience a frequency shift due to ponderomotive motion (mass shift)
- ➜ Accelerated detector (the electron) would see Unruh radiation
- ➜ $a=10^{25}$ g (laser intensity $\approx 10^{19}$ W/cm^2) corresponds to $T=10^4$ K
- ➜ Even if the laser intensity is below the Schwinger's limit, axion production is achievable (possible tests for dark matter theories)

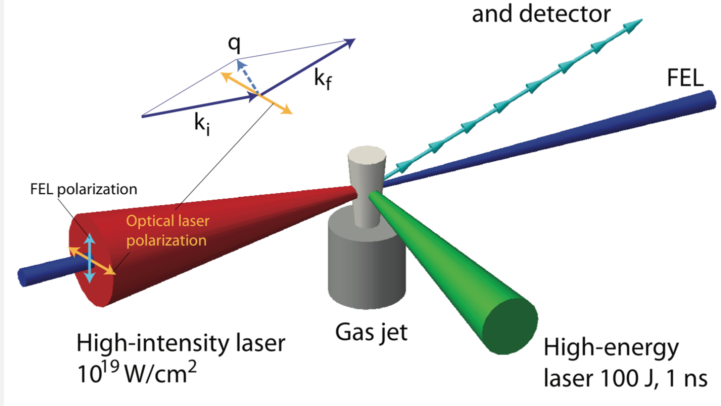




We have proposed an experiment to look for acceleration effects in scattering

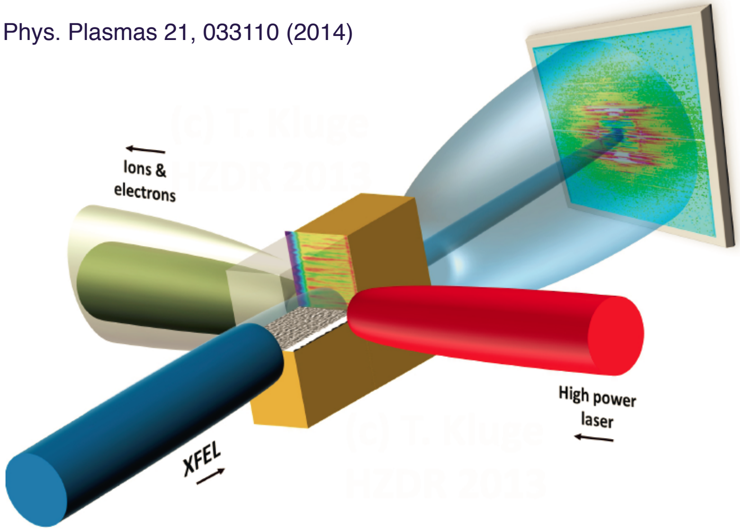
- ➜ For $I\approx 10^{19}$ W/cm^2, $E_{xray}\approx 500$ eV, $\theta\approx 15^o$ we get (T_{eff} -T) is a few hundred eV (measurable!)
- ➜ The original proposal required phase stabilized optical laser and FEL
  - Circularly polarized optical laser will relax this requirement and make the experiment technically feasible

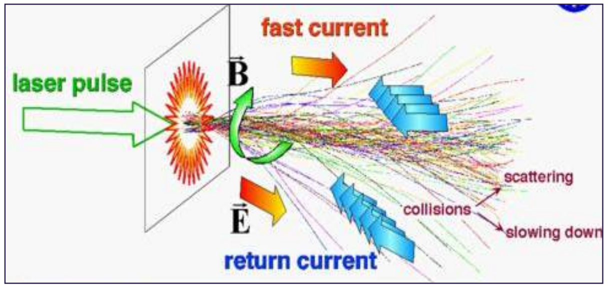
Crowley et al., Nature Sci. Rep. 2012



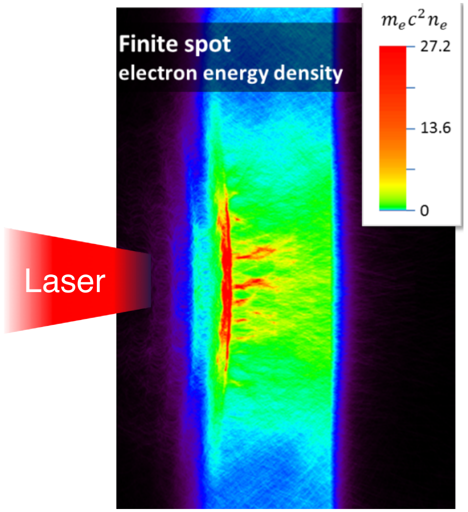
Relativistic laser-matter interactions: HI laser

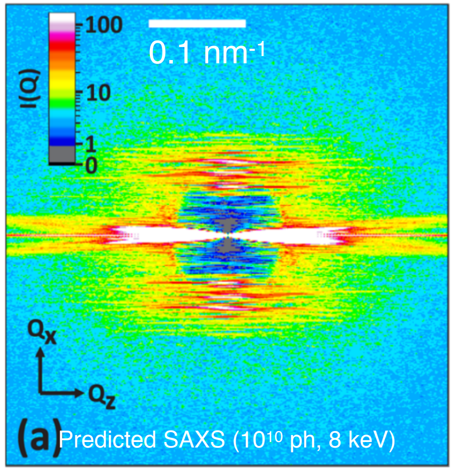
Phys. Plasmas 21, 033110 (2014)





10^{13} A/cm^2, > 1000 T, 10^{13} V/m,
~keV , solid density





- ionization dynamics, heating & resistivity
- electron transport, return current neutralization
- filamentation, hole boring
- e-e & e-i equilibration
- quasi-static fields

Opportunities for the UK

- The UK HED community has been at the forefront of the use of 4th generation light sources.
- To date, the optical lasers that have accompanied such FEL sources have, to a large degree, been ‘bolted on’ to a fixed end-station design.
- Whilst both the construction and possible siting of a UK-FEL have yet to be decided, there is real-estate at RAL which would clearly allow a UK-FEL to be co-located with the existing Central Laser Facility - allowing a fully integrated approach to HED science from the start.
- A personal view is that such thinking should be incorporated into the UK-FEL review process.
- We should be asking what new world-leading science is enabled by synergistically upgrading UK high power laser facilities to be compatible with a UK-FEL capability (e.g. multi-kJ long pulse systems at high repetition rate, co-location of FEL with Petawatt lasers etc. etc.).

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Summary

- "High Energy Density Science" (HEDS) broadly encompasses matter with energy densities exceeding ~ 10^{11} Jm^{-3} : i.e. 'cold' solid matter at Mbar pressures, or dilute matter at millions of Kelvin.
- Effectively these are the conditions met deep in the cores of planets, stars, and within other astrophysical objects.
- The research field allows us to pursue fundamental science (e.g. astrophysics in the laboratory), but also has potential application (high pressure superconductivity, novel material synthesis, understanding of deformation at the atomic level…).
- X-Ray FELs have revolutionised this field both by providing means to, on their own, create such conditions, but also, in conjunction with high power optical lasers, to probe conditions made by other means with exquisite resolution.
- The UK has led this field at existing FELs, but is uniquely placed to construct its own facility with capabilities unparalleled worldwide.
- Come to the workshop (October 2nd, University of Edinburgh) - please get involved.

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