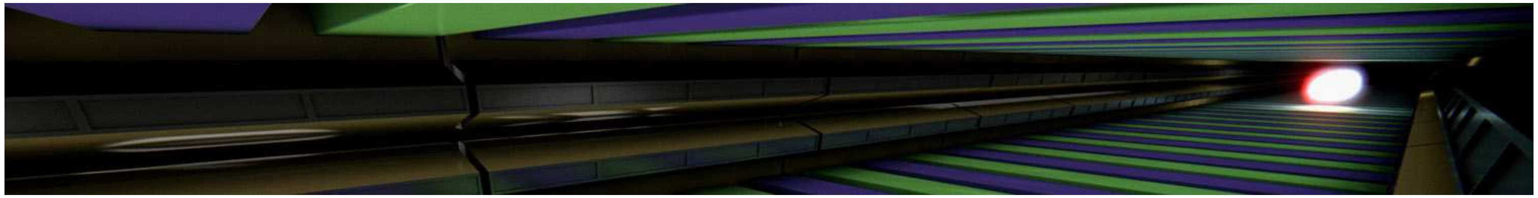


The High Energy Density Science Instrument at European XFEL

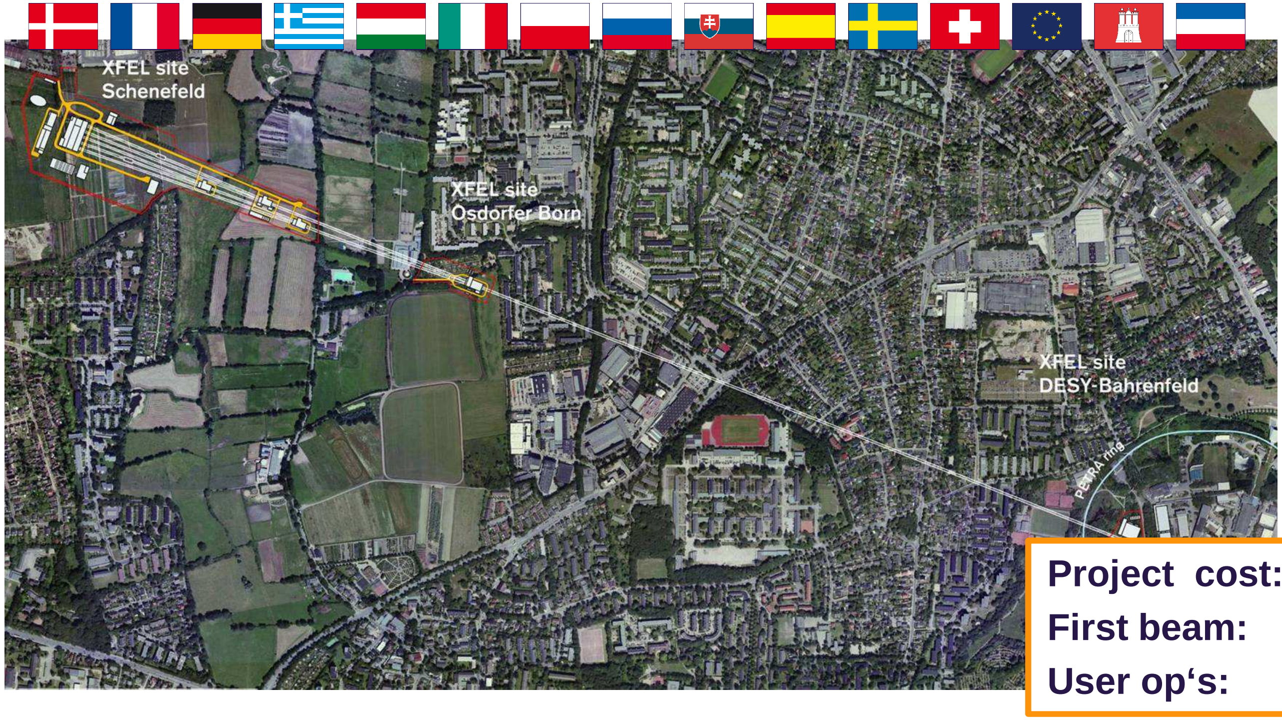
Instrumentation Seminar

DESY, Hamburg, October 17, 2014

Thomas Tschentscher, European XFEL
thomas.tschentscher@xfel.eu

European XFEL

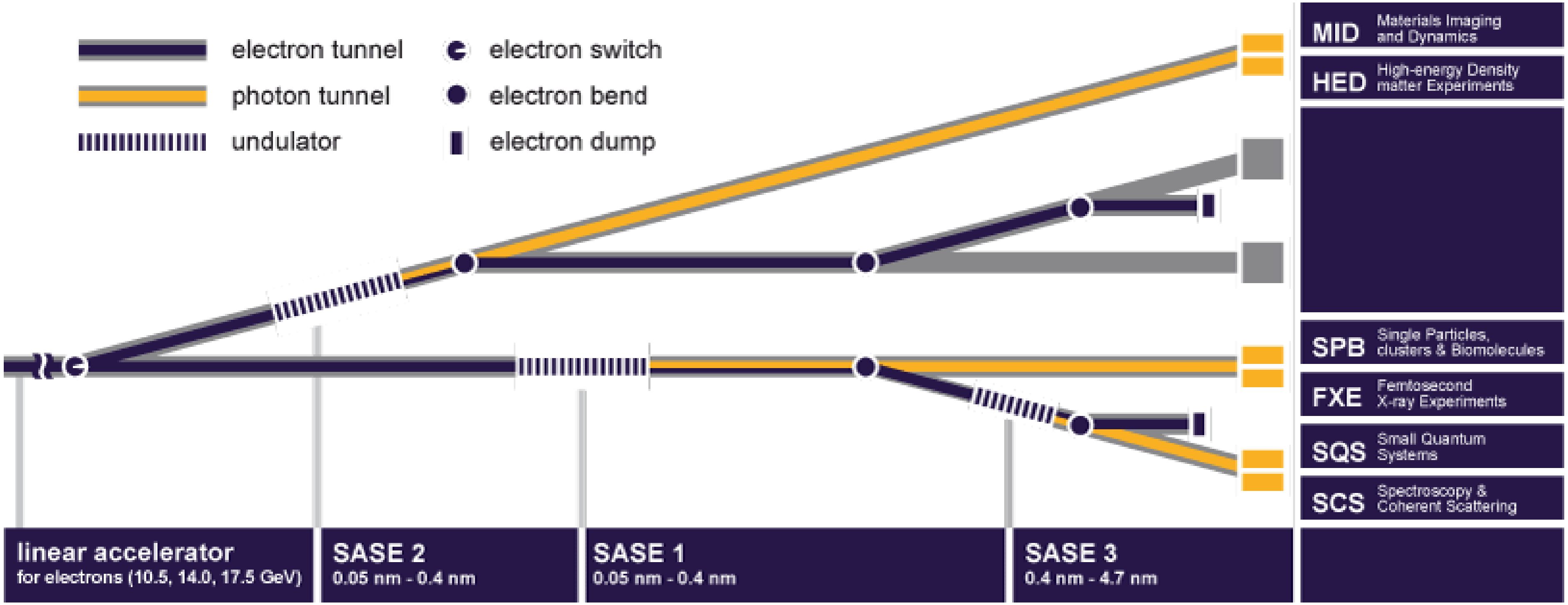
International user facility for FEL research by a multi-disciplinary science community using soft & hard X-ray FEL radiation.



Project cost:	**1147 B€**
First beam:	**end 2016**
User op's:	**2017**

- **Multidisciplinary:** physics, chemistry, biology, materials sciences, geo-sciences, ...
- **User proposed experiments:** peer-review, invitation, support
- **Basic science:** establish the foundations for future high tech applications

6 science instruments



Hard x-ray instruments (>3 – 25 keV)

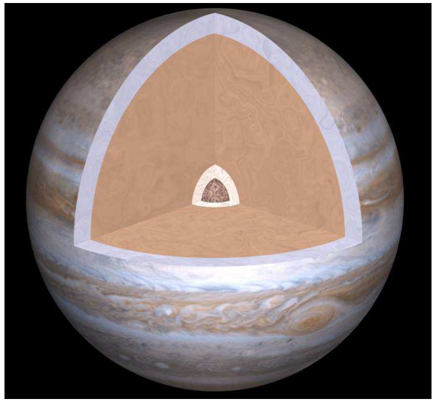
- MID – Materials Imaging & Dyna.
- HED – High Energy Density Sci.
- SPB – Single Particle & Biomolec.
- FXE – Femtosecond X-ray Exp.

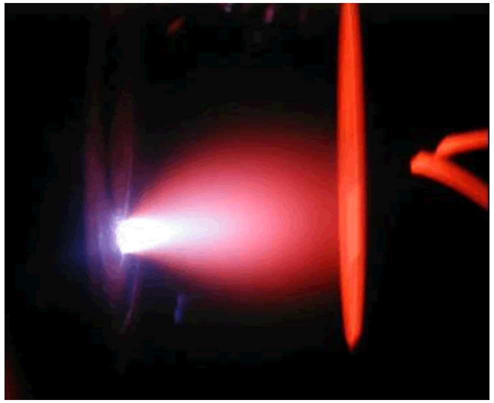
Soft x-ray instruments (270 – 3000 eV)

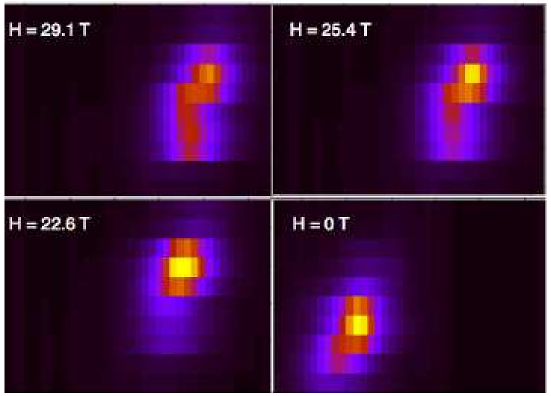
- SQS – Small Quantum Systems
- SCS – Spectroscopy & Coh. Scat.

Provision for 2 more FEL sources and up to 6-7 additional scientific instruments

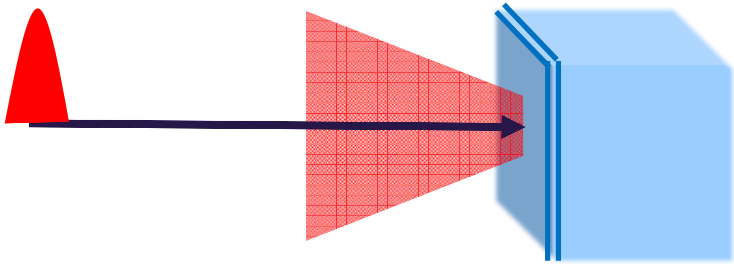
HED instrument: study matter at extreme states







In general: **Matter under extreme conditions of temperature, pressure, electric and/or magnetic field strength**



Dynamic, often irreversible processes:

1. **Condensed-matter at extremes**
2. **(Near) solid-density plasmas**
3. **Quantum states of matter**

Content

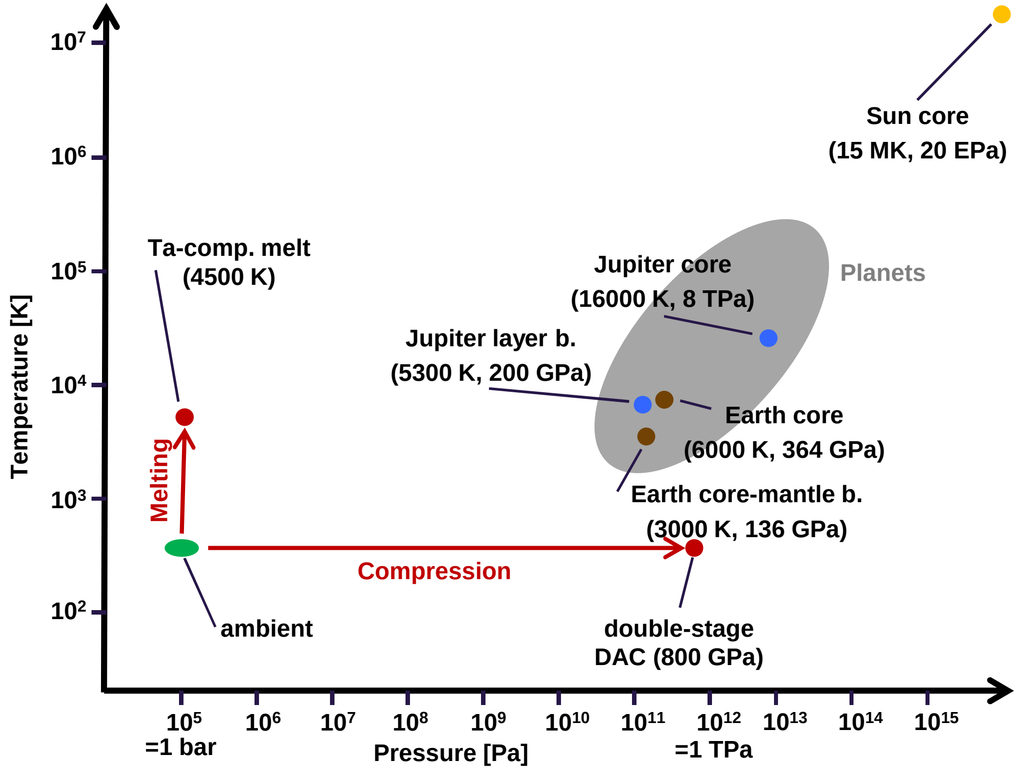
- Introduction to HED science with FELs
- The HED instrument at European XFEL
- Instrumentation challenges

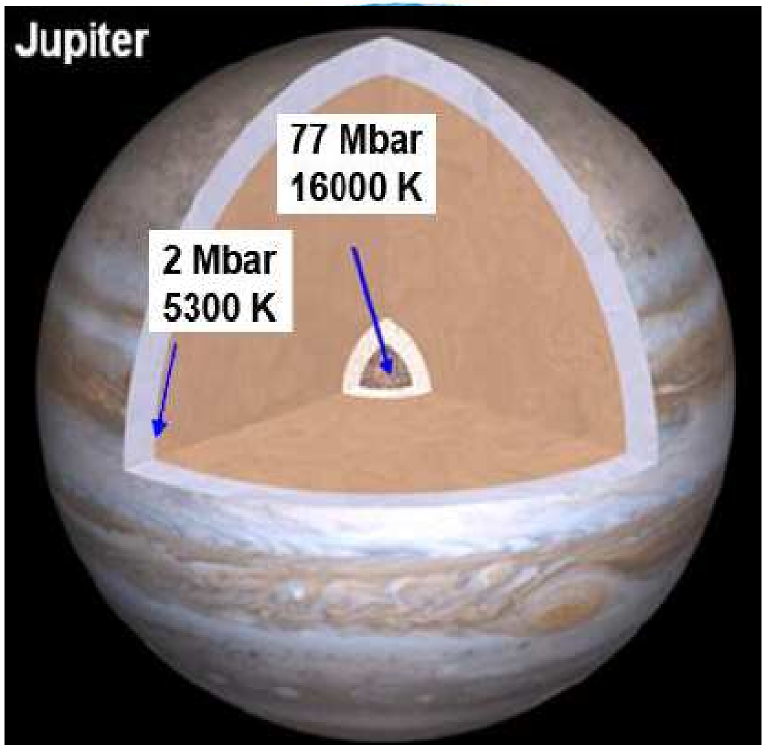
What do we mean by HED / extreme conditions

HED ≡ States with (additional) energy density of 10^{11} J/m^3 (=100 mJ/(100µm)^3**.**

≡ A pressure of 100 GPa or a temperature of 5 × 10^6 K or a radiation intensity of 3 × 10^{15}W/cm^2 or an elec. field strengths of 1.5 × 10^{11}V/m or a magn. field of 500 T

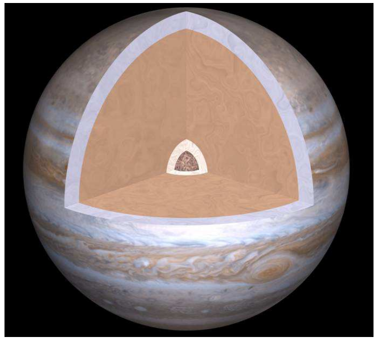
Matter at extreme states: P – T – ρ – ($\overleftarrow{E}$,$\overleftarrow{B}$)

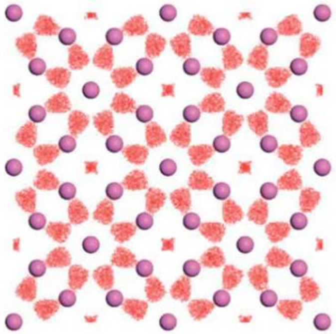




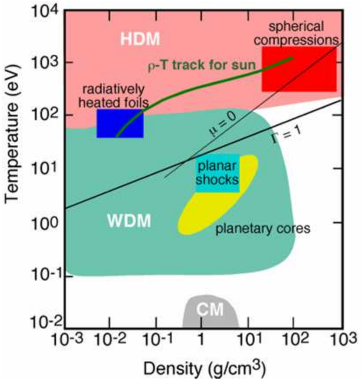
HED science relevant to x-ray FELs (a selection)

Matter at very high T, P, ρ

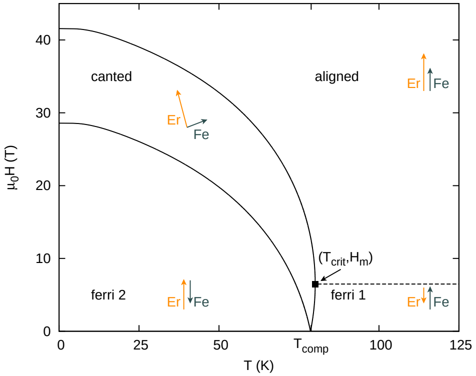




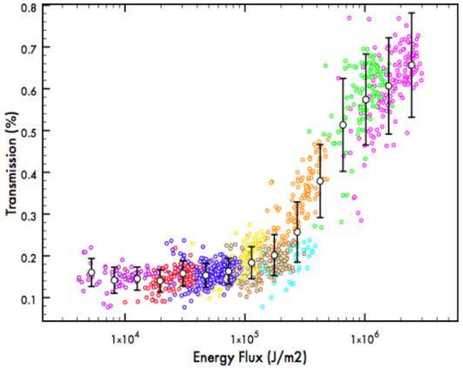
Beyond condensed matter



Complex solids in high fields



Intense x-ray matter interaction



Planets and planet models

The solar planets

Rocky planets

- Mercury, Venus, Earth, Mars

Gas/icy planets

- Jupiter, Saturn, Uranus, Neptune

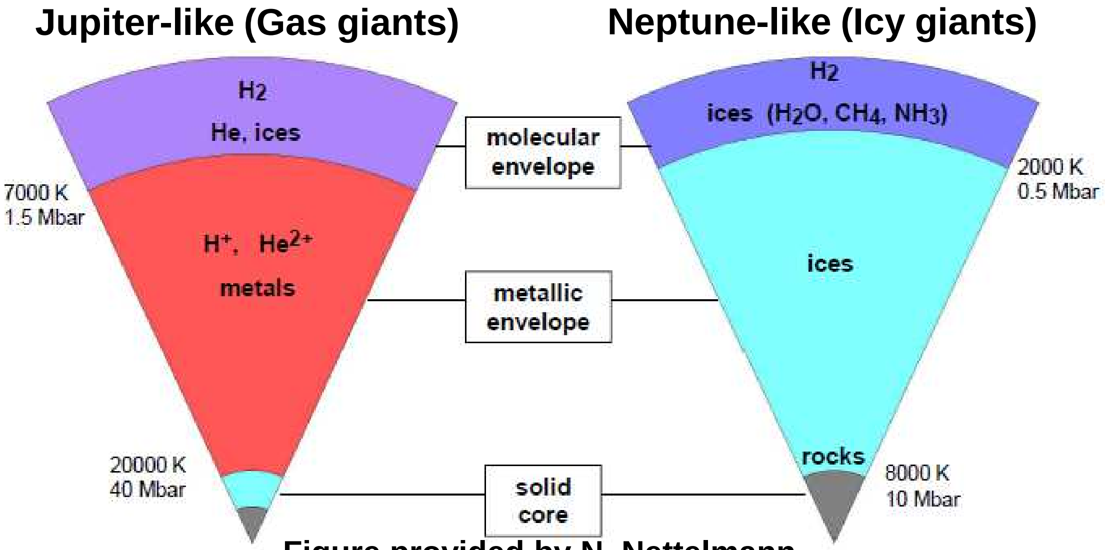
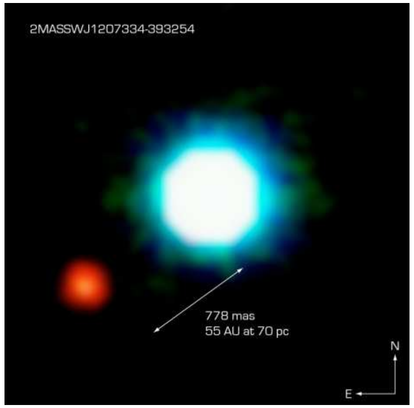


Figure provided by N. Nettelmann

Exoplanets



Copyright: ESO/VLT

First discovery in 1990s

- Typically by indirect observations
- Kepler, CoRoT, SuperWASP

Observation methods

- Indirect: Transit (→ Int. oscillation), Radial speed (fre. osc.)
- Direct observation (>2004): Hubble, VLT, VLA

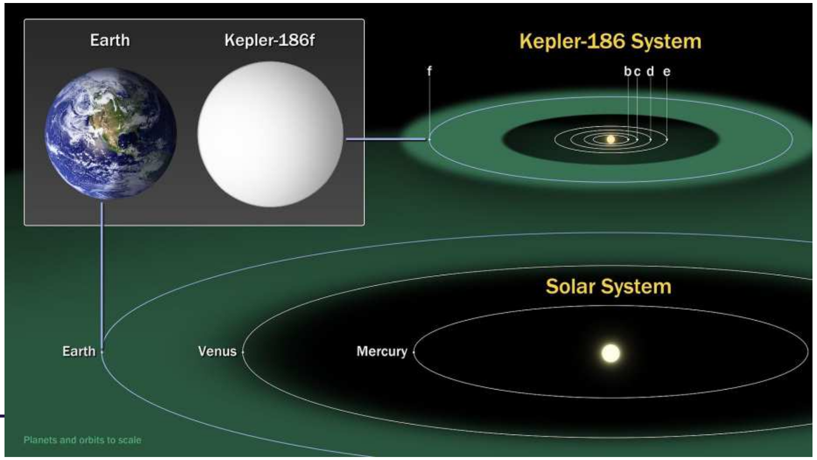
Today (Oct 02, 2014; NASA Exoplanet Archive)

- 1760 objects classified as extrasolar planets
- ~5000 candidates

‘Earth-like’ exoplanets

- e.g. Kepler-186f; few detected
- Conditions similar to Earth

Copyright: NASA



Open questions in planetary models

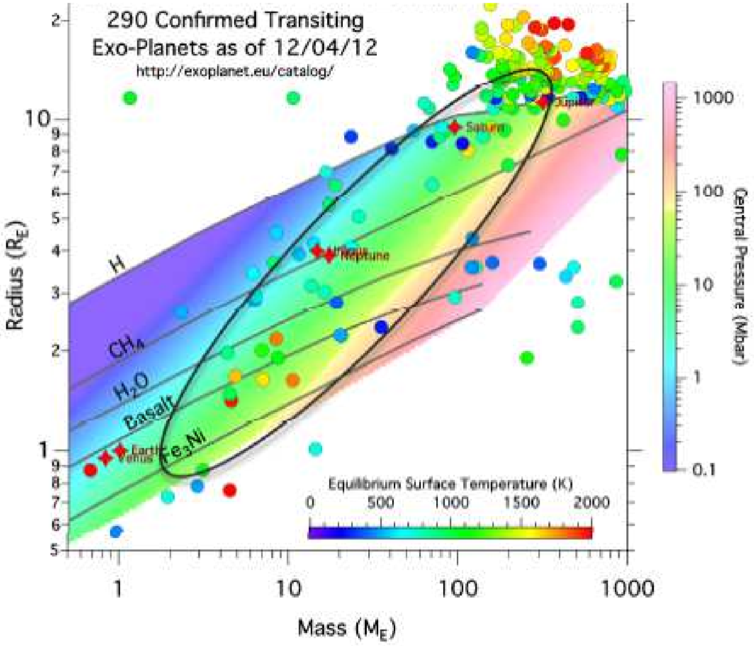
Interior structure of different classes of (exo-)planets

- Super-Earths
- Hot Jupiters
- Neptunes

Relevant parameters

- Size of core, layer boundaries
- Melting lines, solid-solid phase transitions
- Accurate equation-of-state data
- Material properties: viscosity, conductivity
- Mixing and new phases (e.g. metallic Hydrogen)

Combine with observation data to develop better models for planet formation and interior structure



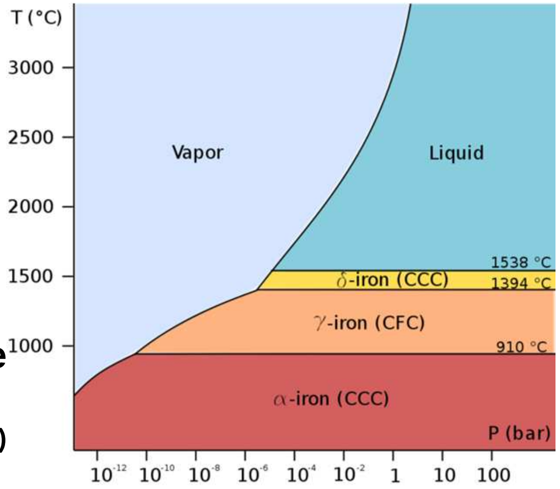
D.C. Swift et al., Astrophys. J. 744, 59 (2012)

Condensed matter at extreme conditions

Phase diagrams

- Structural rearrangement
- Solid-solid phase transitions
- Diff. macroscopic properties

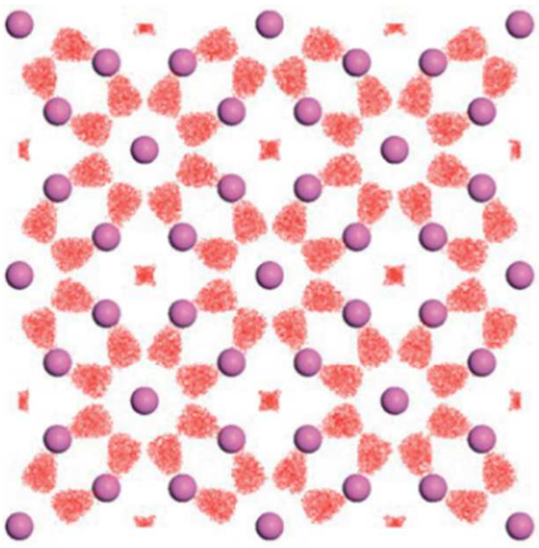
Fe



Copyright: Wikipedia (EN)

Surprisingly

- Structures become more complex at high pressure
- New structures that are un-known at ambient conditions
- Can these materials be recovered ?



Al at 3.2 TPa

C.J. Pickard, R.J. Needs, Nat. Mat.9, 624 (2010)

Plasmas

At very high P – T – ρ matter starts to ionize

⇒ plasma formation

- The “fourth state of matter,” in which the temperature is high enough that the electrons have been separated from their nuclei, leaving a gas of charged particles. (The atoms are said to be “ionized.”)
- The majority of stars, and hence most of the visible universe, is composed of plasma. It should really be called “the first state of matter.”

Ideal plasmas

- Ideal gas approximation
- Only smooth background field, no binary interactions
- low density & high temperature $\Gamma \ll 1$

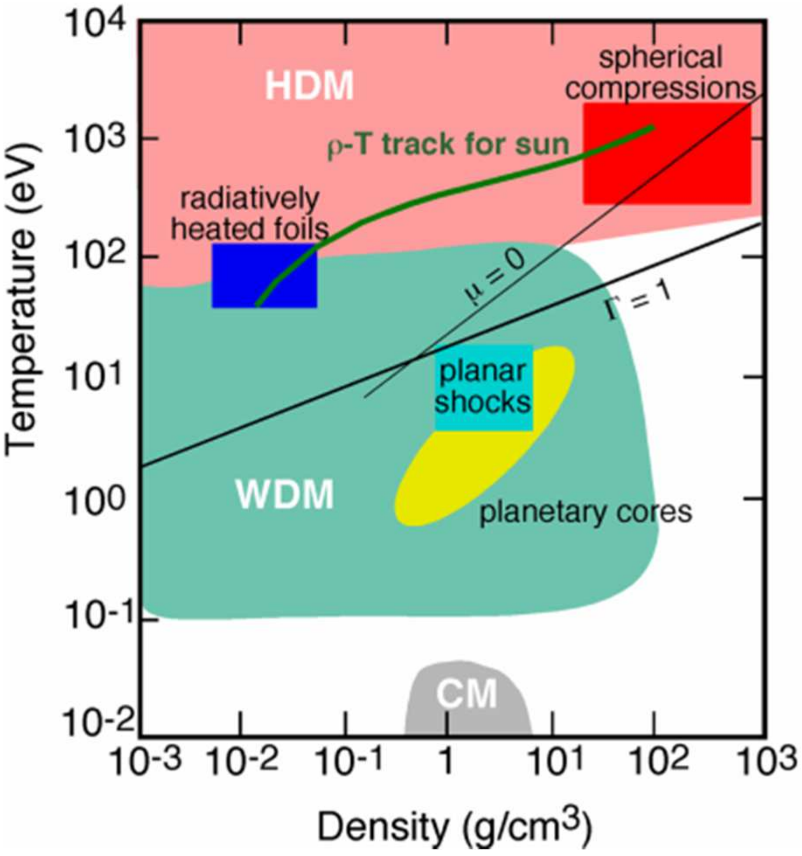
$$\Gamma = \frac{E_c}{kT_e}$$

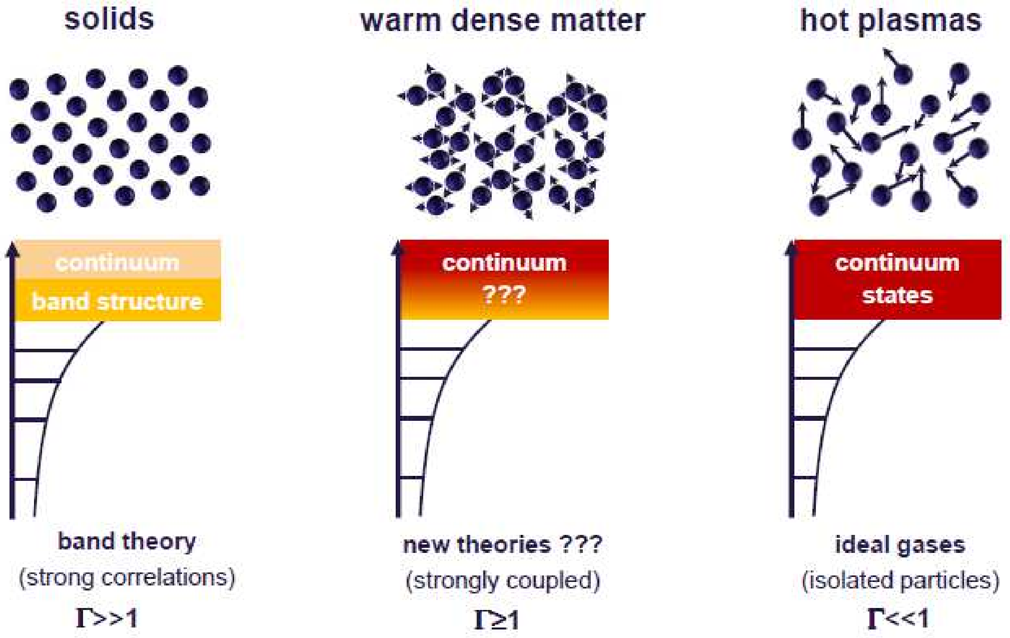
Non-ideal plasmas

- ‘Strong-coupling’
- Collisions and correlations
- high density & low temperature $\Gamma \sim 1$

The plasma phase diagram

Transition from ‘cold’ solids to ‘hot’ plasmas





Γ = coupling parameter = ratio of potential to thermal energy

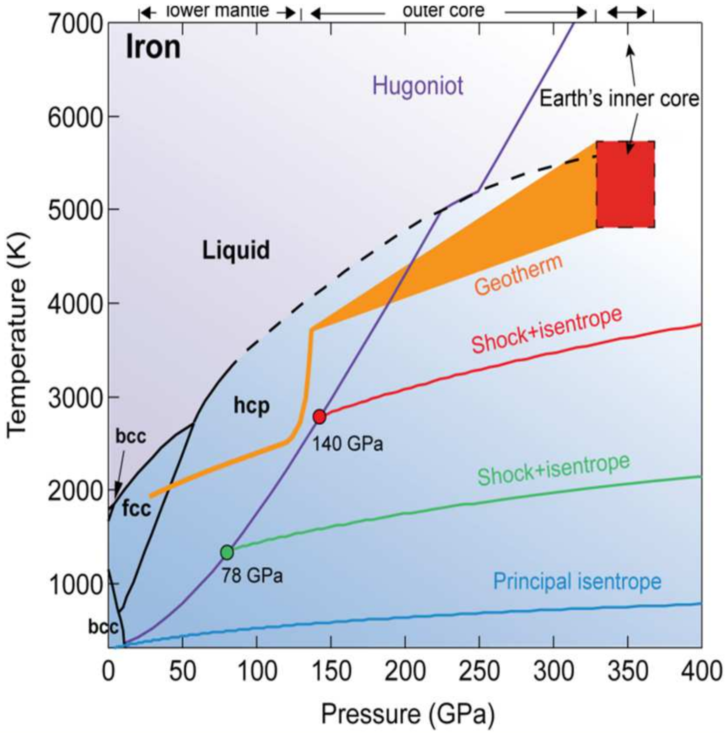
How to study matter at these extreme states

(Quasi-)static compression

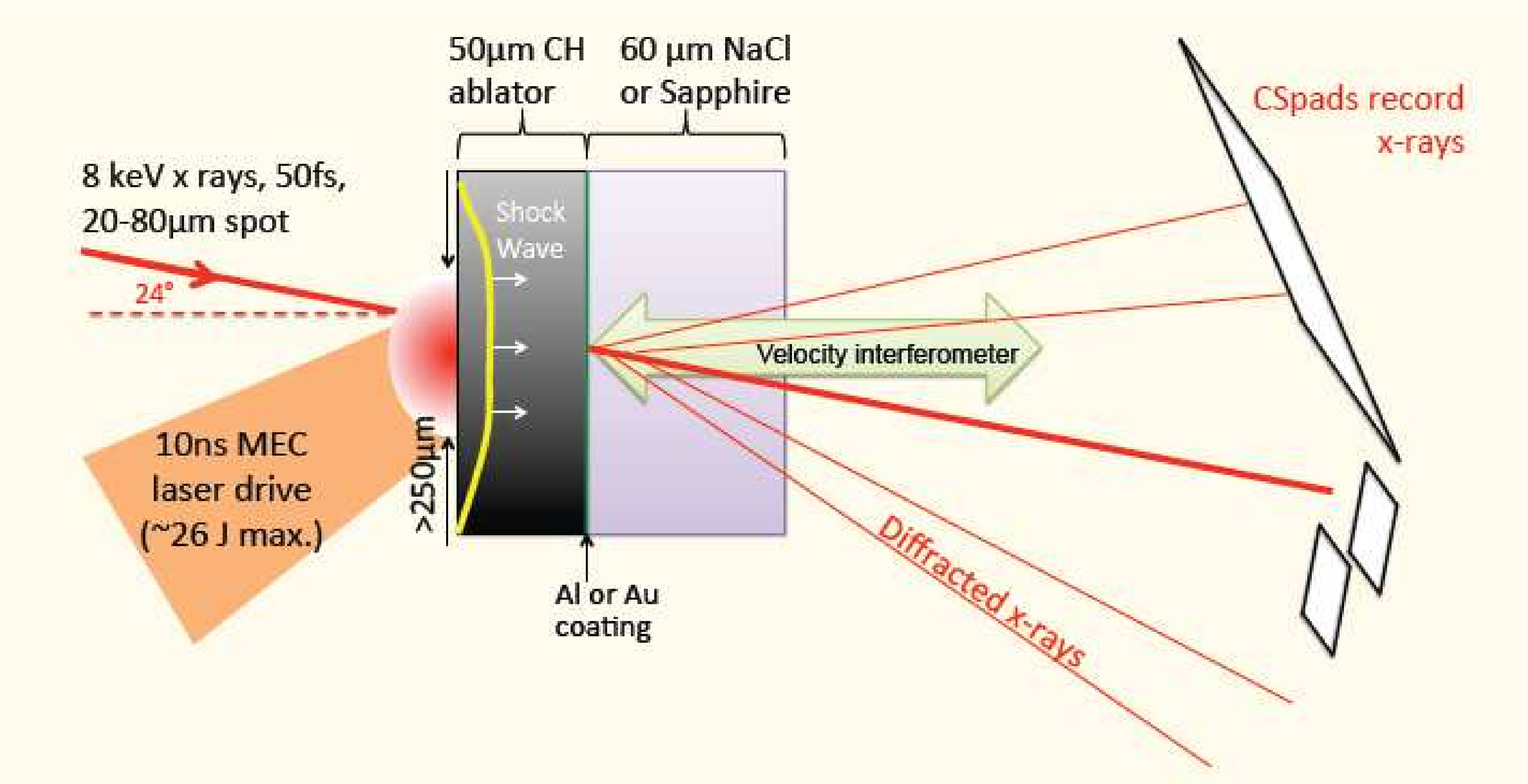
- Use diamond-anvil-cells (DAC)
- Pressures → P <400 GPa
- Laser-heating → T~few 1000 deg C
- Confinement

Dynamic compression

- Use lasers (or matter) to drive ‘shock’
- Ablation of matter creates shockwave
- Specially shaped laser pulses can compress matter quasi-isentropic (‘shockless’)
- Can reach higher pressures, temperatures
- Dynamic: strain rate can be varied
- Short-lived (10s of ns)



Dynamic compression principle



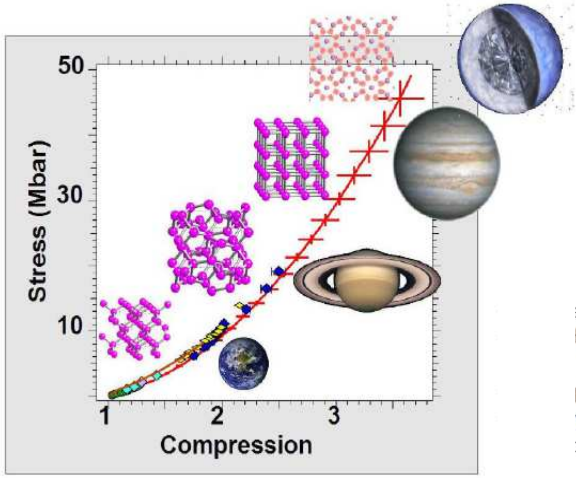
courtesy J. K. Wicks

Excite solid matter to states of high P, T, rho

Dynamic compression

- Material properties at extreme P and T
- Structural & electronic properties
- Existance and properties of new materials

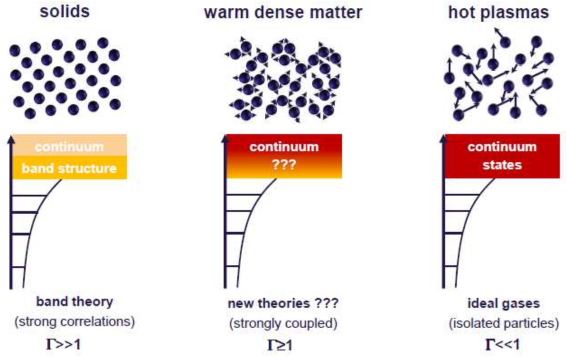
⇒ Application to planetary models



Isochoric generation of plasmas

- Measure properties of electron & ion systems
- Study effect of correlations

⇒ Understand/describe solid to plasma transition



Γ = coupling parameter = ratio of potential to thermal energy

Experimentally needed

- Strong drivers (lasers of various type)
- X-ray probe techniques → access to microscopic structure & prop.

Complex solids in high magnetic fields

Motivation

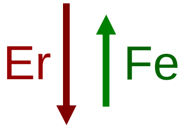
Magnetic field strength as add. variable

- New structures & properties
- Phase transitions
- Mostly complex solids

Need high fields of >30 T

$Er_3Fe_5O_{15}$ –
A ferrimagnet

2-sublattice ferrimagnet



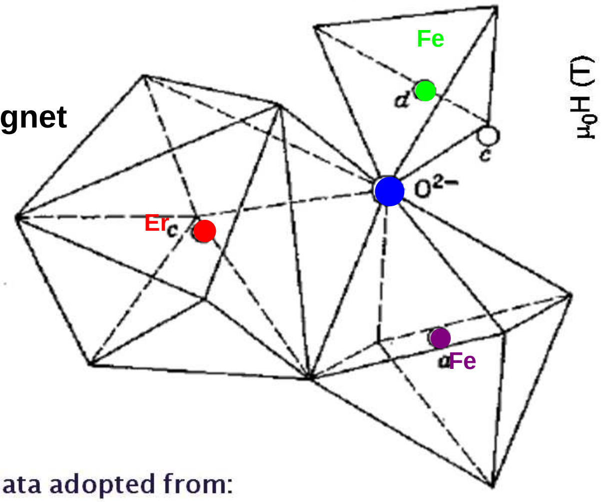
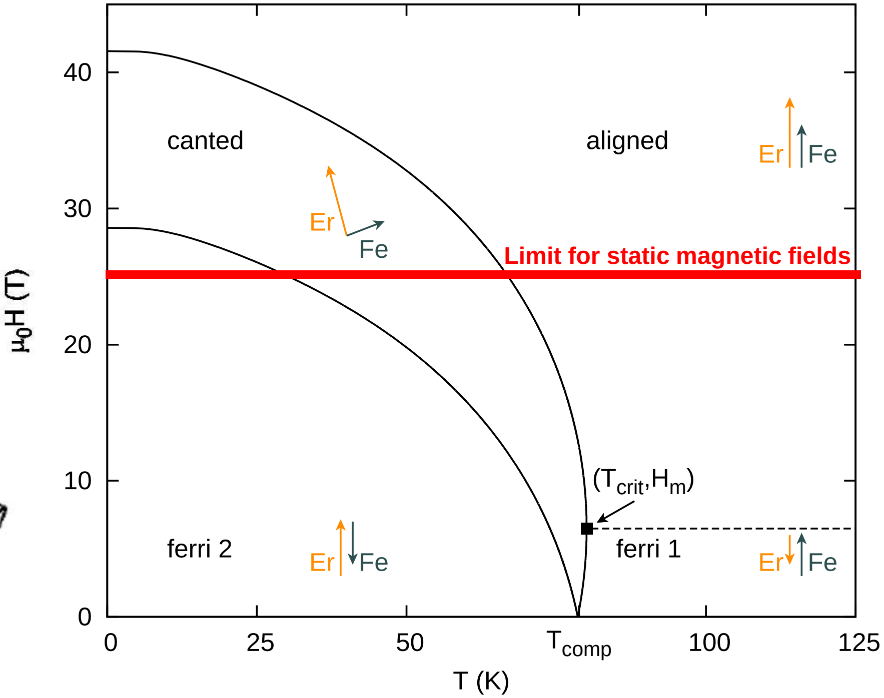


Figure and data adopted from:
A. H. Morrish. The Physical principles of Magnetism.

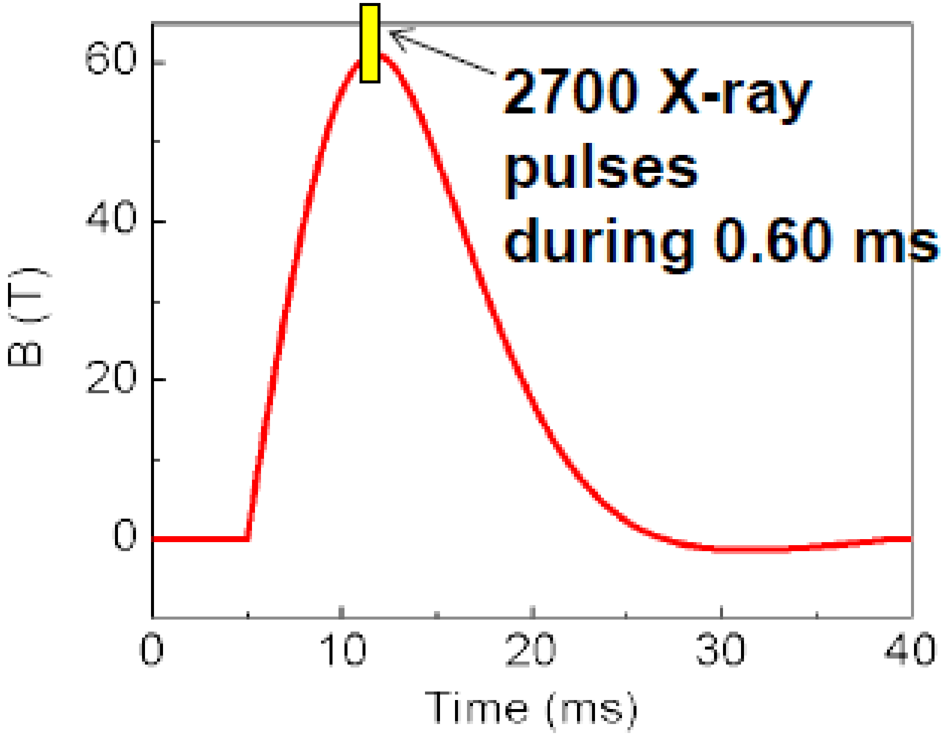


C. Strohm et al., PRB 86, 214421 (2012)

Pulsed magnet technology (I)

Large volume magnets

- Fields of 30 up to 100 T
- ~1 MJ stored energy
- X-ray geometry needed



HZDR

1 MJ, 100 kE, 1 GW

ESRF-LNCMI

30 T, 2 K, split-coil

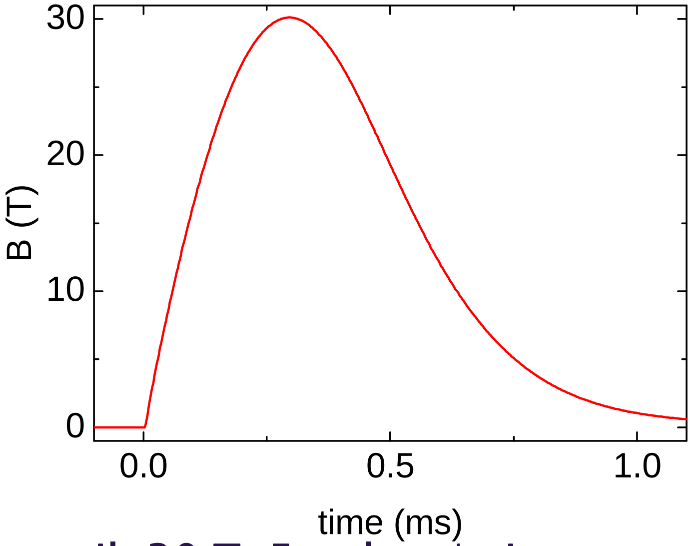
Development goals

- >50 T fields
- Separate sample cryostat
- Split-coil geometry
- Optimized pulse duration/rate

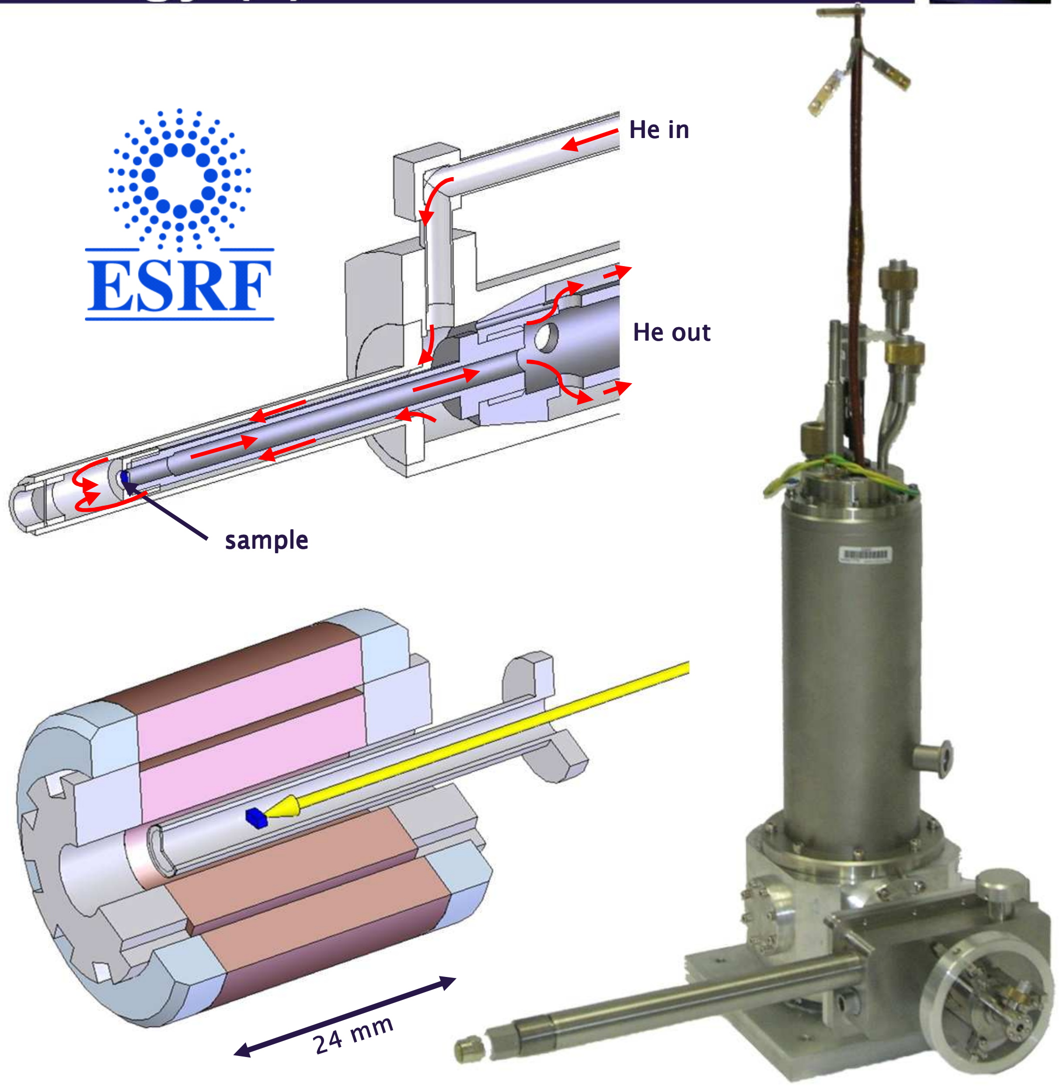
Pulsed magnet technology (II)

Mini-coils

- Smaller sample volume
- Shorter pulses
- Less stored energy
- Higher repetition rate
- Ready to use



- coil: 30 T, 5 pulses/minute
- sample cryo 5 K → 300 K



P. van der Linden, et al. *Rev. Sci. Inst.* 79, 075104 (2008)

Interaction of intense x-rays with matter

Powerful x-ray pulses

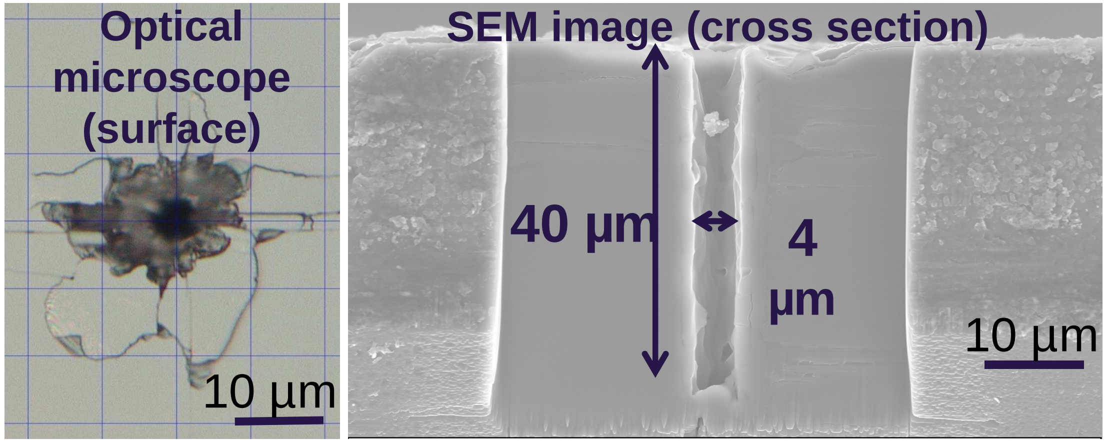
X-ray FEL pulses can significantly alter matter

Si

single pulse exposure

10 keV, 1 µm focus, 70 µJ

K. Yamauchi et al.

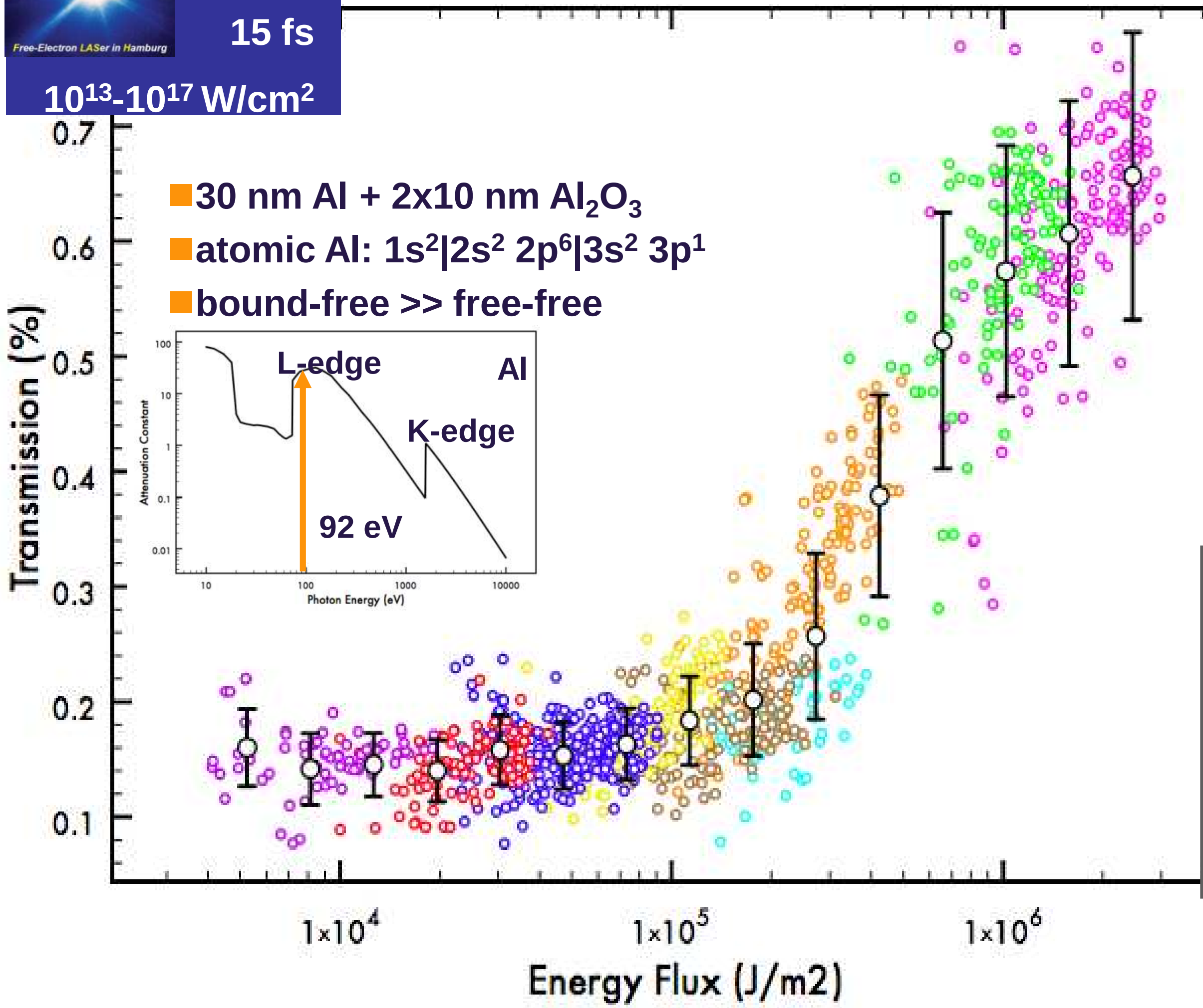


Observation of saturable absorption

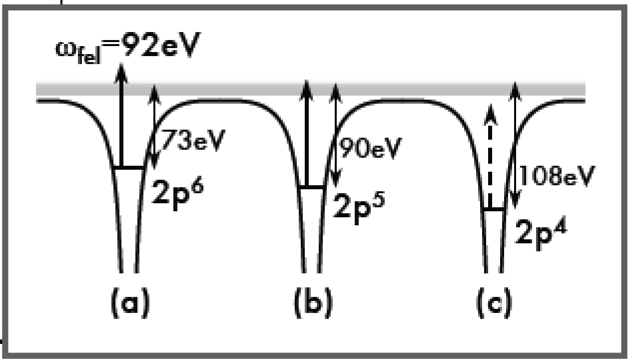
92 eV

15 fs

10^{13}-10^{17} W/cm^2



- 30 nm Al + 2x10 nm Al_2O_3
- atomic Al: $1s^2|2s^2\ 2p^6|3s^2\ 3p^1$
- bound-free >> free-free



- recombination takes longer than pulse duration
- depletion of L_2-shell
- process stops when energy levels shift

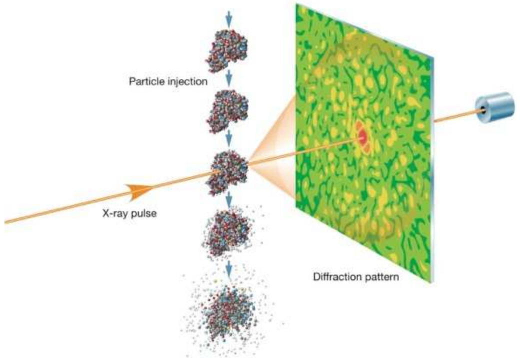
B. Nagler, U. Zastrau, R. Fäustlin et al., Nat. Phys. 5, 693(2009)

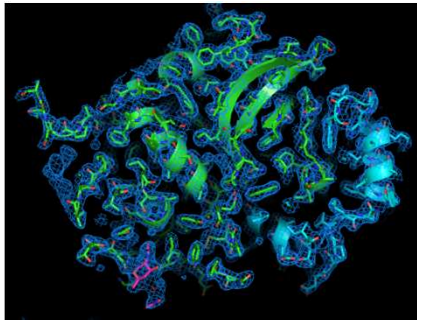
Interacting x-ray probe

In x-ray science it is typically assumed that the x-rays do not affect the probed system (non-invasive probe).

- For FELs this needs to be verified case-by-case
- Cross-section for photo-ionization significantly larger than for scattering

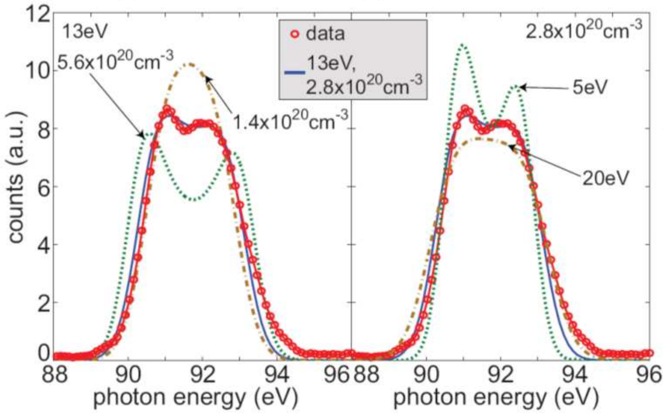
X-ray diffraction





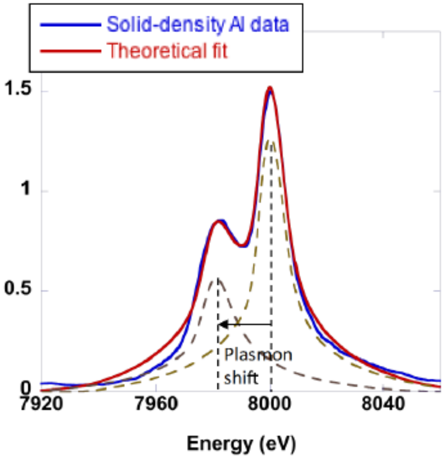
Cathepsin B,
2.1 A,
L. Redecke et al.,
Science Express,
29 Nov 2012

X-ray scattering



Liquid H (n~2 × 10^{22} cm^{-3})
XUV (90 eV)
R.R. Fäustlin et al.,
PRL104, 125002 (2010)

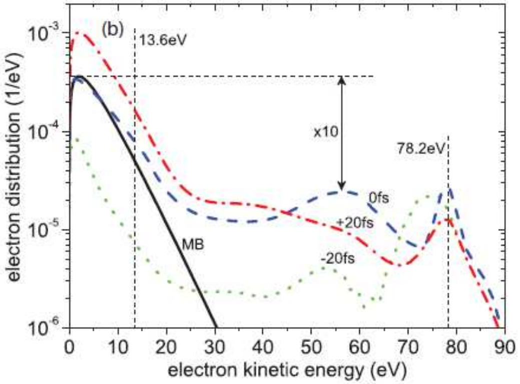
Solid Al (n~1.8 × 10^{23} cm^{-3})
X-ray (8 keV)
L.B. Fletcher et al.,
JINST8, C11014 (2013)



Use x-rays as a pump

X-ray energy is entirely absorbed in electronic system

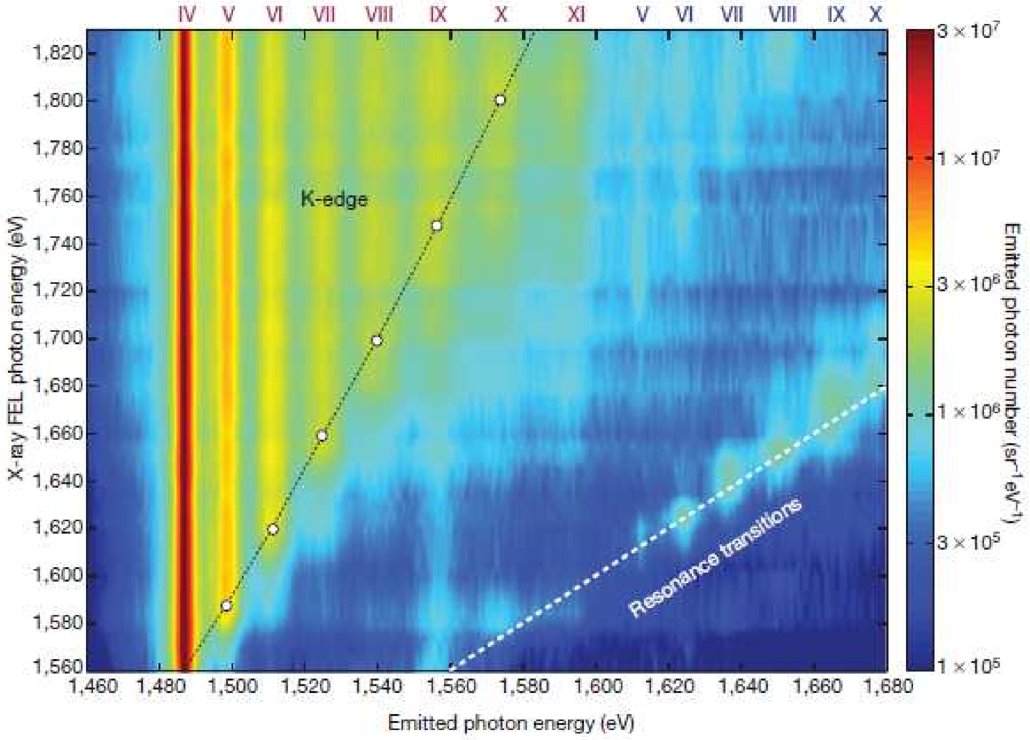
- Photo-ionization
- Auger-processes
- Electron scattering



R.R. Fäustlin, B. Ziaja et al., PRL104, 125002 (2010)

Features

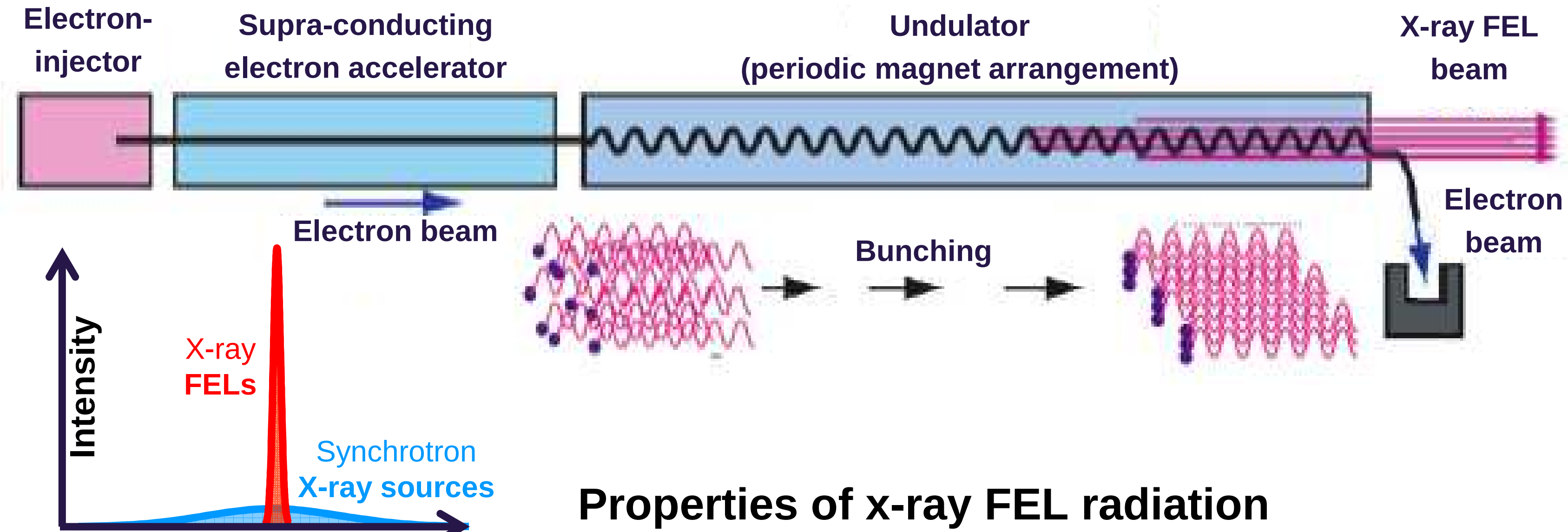
- Isochoric heating
- Single-photon & sequential multi-photon ionization
  - ➔ **High ionization states**
- 2-temperature plasma
  - ➔ **Hot (warm) electrons**
  - ➔ **Cold ions**
- Transients

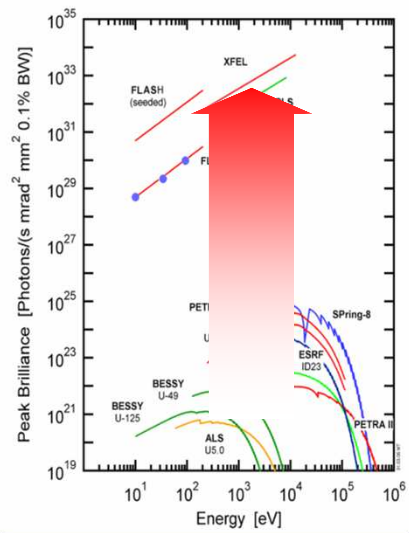


1.5 – 1.8 keV, Al, S. Vinko et al., Nature 482, 59 (2012)

Why use x-ray FELs ?

X-ray FEL radiation - general





Properties of x-ray FEL radiation

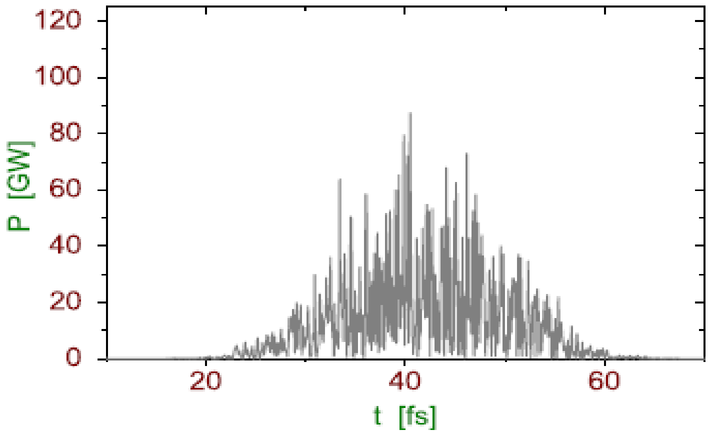
- Photon energy: ~30 – 20.000 eV
- Pulse duration: 1 – 200 fs
  - ➔ 10^3-10^4 × shorter than conventional sources
- Peak brightness: ~10^{30} – 10^{33}
  - ➔ 10^9 × higher than conventional sources
  - ➔ 10^{12} photons / 100 fs / 100 eV @ 10 keV diff.-lim.
- Full transverse / high temporal coherence

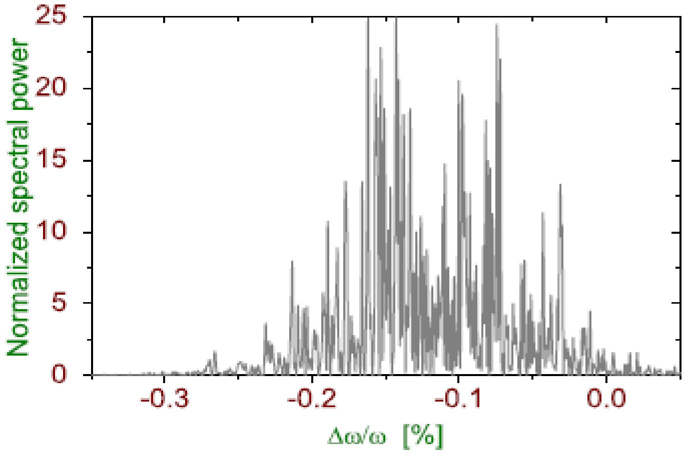
SASE vs. seeded FEL radiation

SASE

(self-amplified spontaneous emission)

- time & spectrum; 12 keV, 250 pC

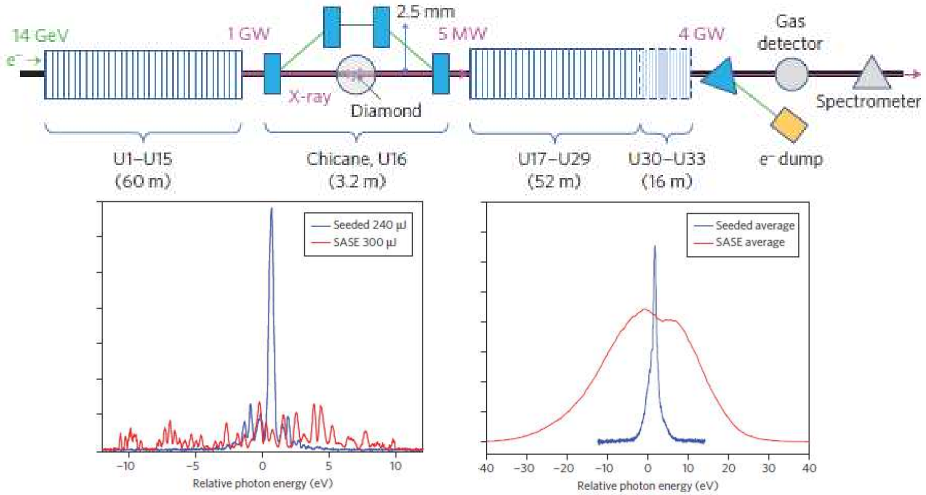




Seeded FEL

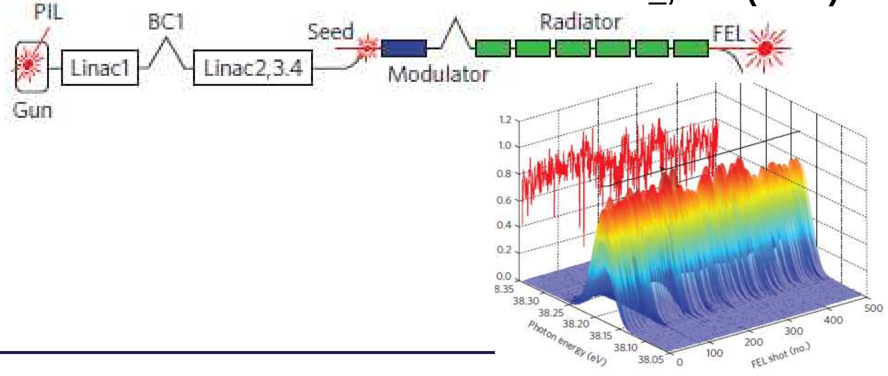
- **Self-seeding**

J. Amann et al., Nat. Phot. 6, 693 (2012)



- **External seeding**

E. Allaria et al., Nat. Phot. 6, 699 (2012)



How can x-ray FELs contribute to HED science

Very high definition of x-ray beam

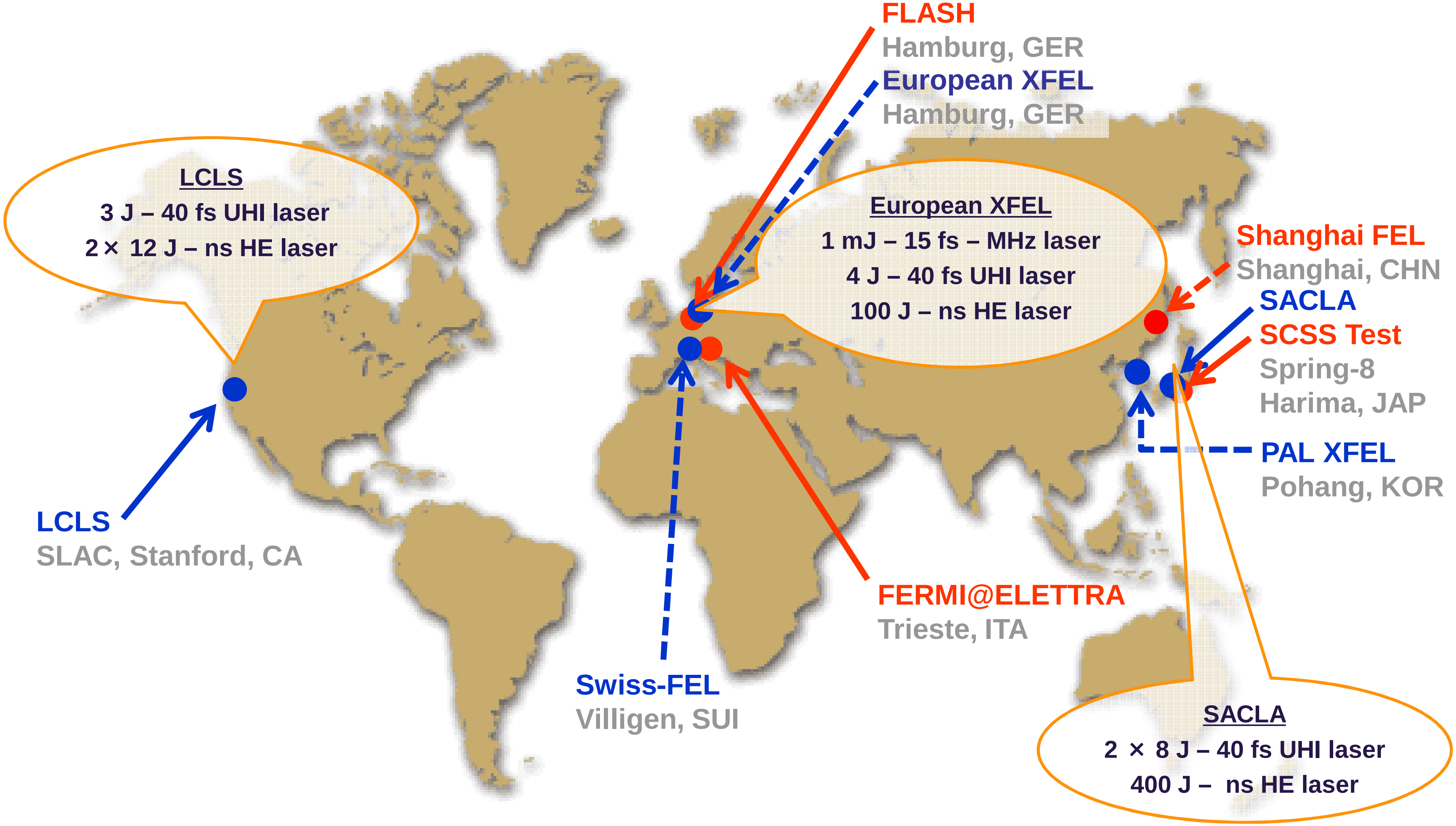
- Spatial resolution
  - → **x & y – few µm; z – sample thickness / O(100 µm) possible**
- Temporal resolution
  - → **1 – 100 fs pulse duration; synchronization to OL ~10 fs shown**
  - → **No pre-pulse issues**
- Spectral resolution
  - → **Natural bw ~10^{-2} – <10^{-3}; seeded ~10^{-4}; monochromatization 10^{-4} – 10^{-6}**
  - → **Bandwidth broadening to O(100 eV) under development**

High intensity of pulses & high number of pulses (10 Hz)

- Single shot data collection
- Complex and flux-limited x-ray techniques can be applied
- Use x-ray pulse for driving samples (employing split & delay also probe)

Coherence → Imaging

Soft/Hard X-ray FELs worldwide with big OLs



FLASH
Hamburg, GER
European XFEL
Hamburg, GER

LCLS
3 J – 40 fs UHI laser
2 × 12 J – ns HE laser

European XFEL
1 mJ – 15 fs – MHz laser
4 J – 40 fs UHI laser
100 J – ns HE laser

Shanghai FEL
Shanghai, CHN
SACLA
SCSS Test
Spring-8
Harima, JAP

PAL XFEL
Pohang, KOR

LCLS
SLAC, Stanford, CA

FERMI@ELETTRA
Trieste, ITA

Swiss-FEL
Villigen, SUI

SACLA
2 × 8 J – 40 fs UHI laser
400 J – ns HE laser

Content

- Introduction to HED science with FELs
- The HED instrument at European XFEL
- Instrumentation challenges

Overview HED instrument

X-ray properties

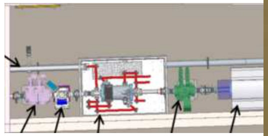
- 5(3) – 25 keV
- 10^{13} – 10^{11} pths/pulse
- 1 – 200 µm spots
- 10^{-6} – 10^{-2} bw

Optical lasers

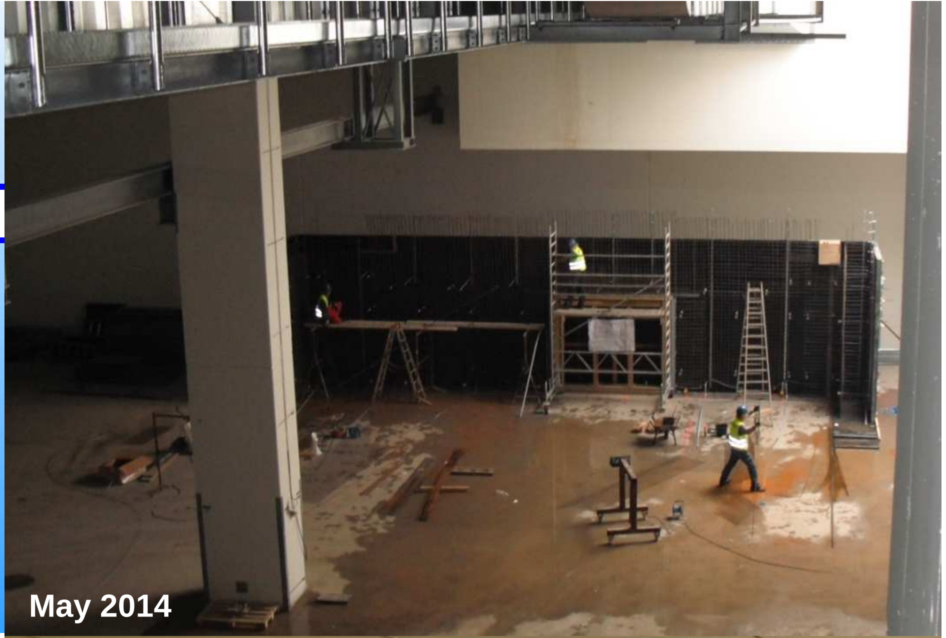
- MHz – mJ – 15 fs
- 10 Hz – 100 J – ns (shaped)*
- 10 Hz – 100 TW – 40 fs*

* HIBEF contributions

Setups & techniques



- 1 multi-purpose
- 2 dedicated
- XRD, SAXS, XAS, IXS, imaging

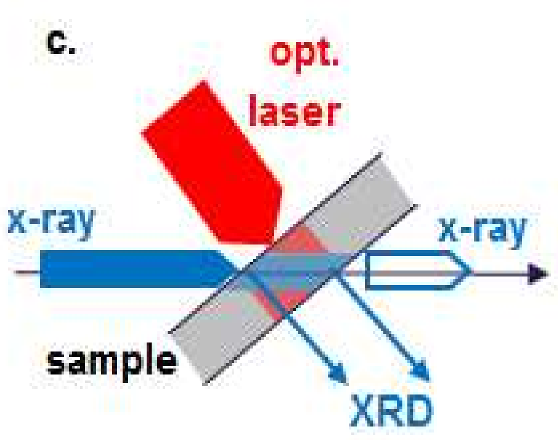

May 2014


Aug 2014

The HED instrument

Enable the use of x-ray excitation, scattering, diffraction, spectroscopy, and imaging techniques

- Large flexibility in setups
- Use of various pump sources to excite samples (OL, XL, ext. fields)



Integrate strong excitation sources in instrument design

- High energy/power optical lasers
- Pulsed magnetic fields
- Pulsed electric fields

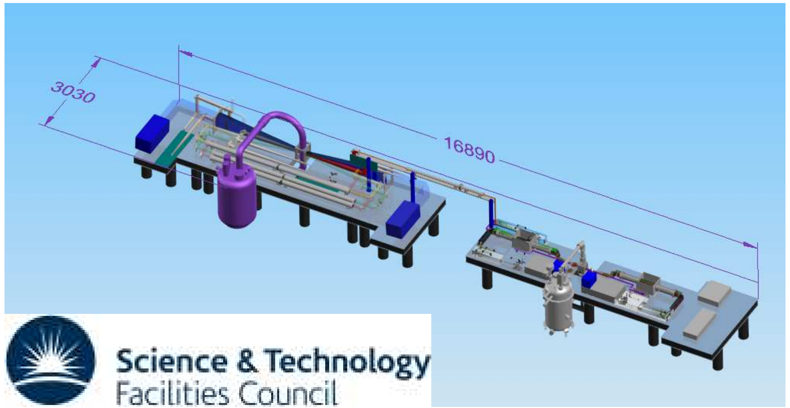
	X-ray techniques								OL techniques			
	XRD	IXS	XAS	XMCD	X-ray imaging	XPA	SAXS	ESP	Interferometry	Microscopy	FDI	VISAR
X-ray pumping	●	●	●		●			●	●	●	●	
OL pumping	●	●	●			●	●	●	●		●	●
Pulsed B-field	●		●	●								

„Laser plan“ for the HED instrument

Start of operation

- PP laser system (mJ; MHz; 15–100 fs & 10 mJ, 100 KHz, ~1 ps)
- 100 TW ultrashort pulse laser (few J; 10 Hz; 40 fs) [contributed by HIBEF UC]
- 100 J nanosecond laser (100 J; 1–10 Hz; 1–20 ns) [contributed by HIBEF UC]
- Small systems (VISAR, etc.)

→ high excitation



→ shocks, dynamic compression

→ rel. laser-plasma IA

HIBEF: Helmholtz International Beamline for Extreme Fields

Spokesman: *T.E. Cowan (HZDR)*
Co-PI's: *U. Schramm (HZDR), E. Weckert (DESY), T. Stoehlker (HIJ)*

HIBEF User Consortium: HZDR, DESY, HIJ, CFEL, DLR, FZJ, GFZ, GSI, HZB, MBI, MPIC, MPIK, MPI-S, MPQ, MPSD, U Bayreuth, HU Berlin, TU Darmstadt, TU Dresden, U Duisburg, U Frankfurt, U Freiburg, U Hamburg, FSU-Jena, LMU-Munich, TU Munchen, U Rostock, U Siegen, U Graz, TU Wien, PSI, EP-Lausanne, IOP-ASCR, CTU-Prague, CLPU-Salamanca, UPM-Madrid, IRAMIS-CEA, CEA-Arpajon, CELIA-Bordeaux, ESRF, Jussieu, LULI, UPMC, LNCMI, U Toulouse, U Pecs, U Szeged, Weizmann, U Roma, MUT-Warsaw, NCBJ-Swierk, U Wroclaw, IST-Lisbon, JIHT-RAS, Stockholm, Umea, Uppsala, Cambridge, Edinburgh, Imperial, QUB, UCL, Oxford, Plymouth, STFC-RAL, SUPA, Strathclyde, Warwick, York, Eu-XFEL, ELI-DC, EMFL, IOP-CAS, Peking Univ, SIOM, SJTU, Tata IFR, RRCAT, GSE-Osaka, ILE-Osaka, KPSI-JAEA, U Kyoto, Alberta, BNL, UC Berkeley, Carnegie Inst. Wash., General Atomics, LANL, LBL, LLNL, U. Michigan, ORNL, OSU, U. Penn, Rockefeller U, SLAC, UCSD, UNR, U Texas, WSU

High energy lasers

- **initially 100 TW/10 Hz & 100 J/10 Hz**
- **Future upgrades**

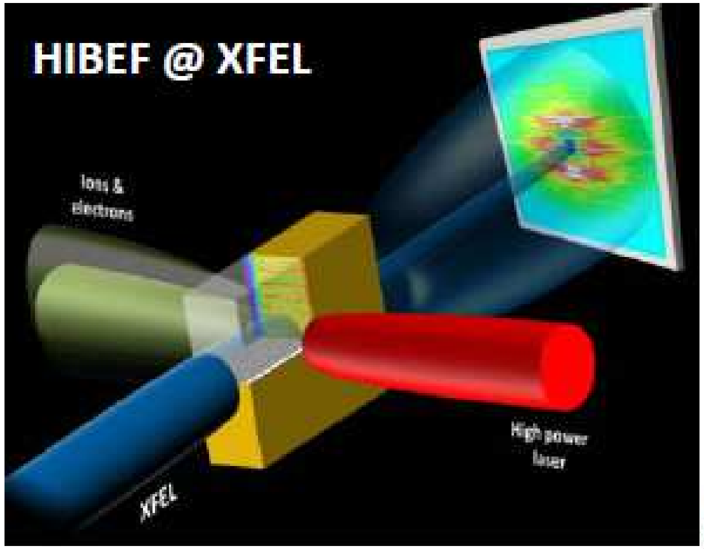
Pulsed magnetic field setup

Diagnostics, spectrometer, etc.

Man-power

Operation

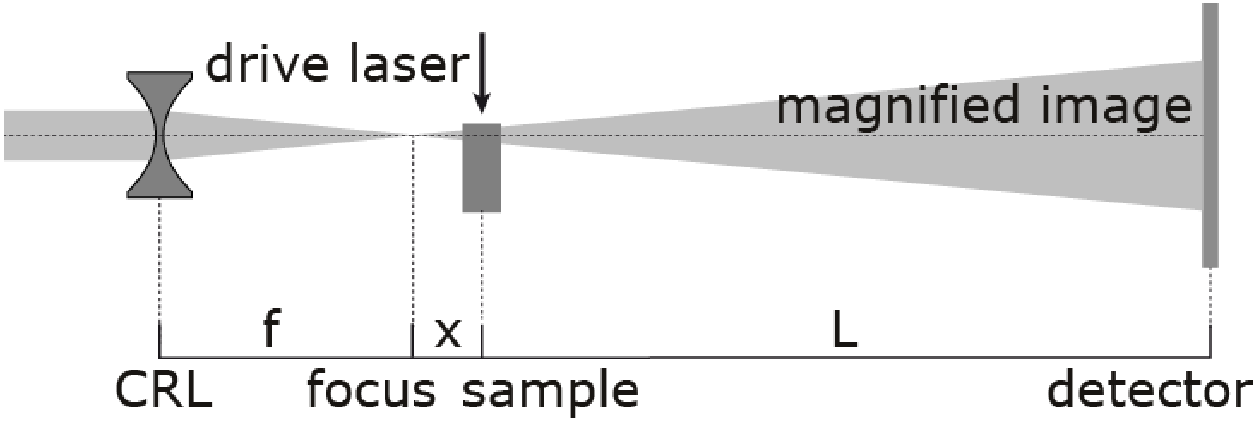
UK:	8 M€
HGF-FIS:	20.5 M€
Others:	12 M€



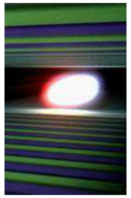
X-ray FEL shock front imaging

Imaging experiment performed at LCLS in May 2012 (A. Schropp et al.)

- Focussing/imaging technique : **Schropp et al., Sci. Rep.3, DOI: 10.1038/srep01633(2013)**
- 7.0 & 8.2 keV
- Phase-contrast imaging mode
- Using diverging beam projection



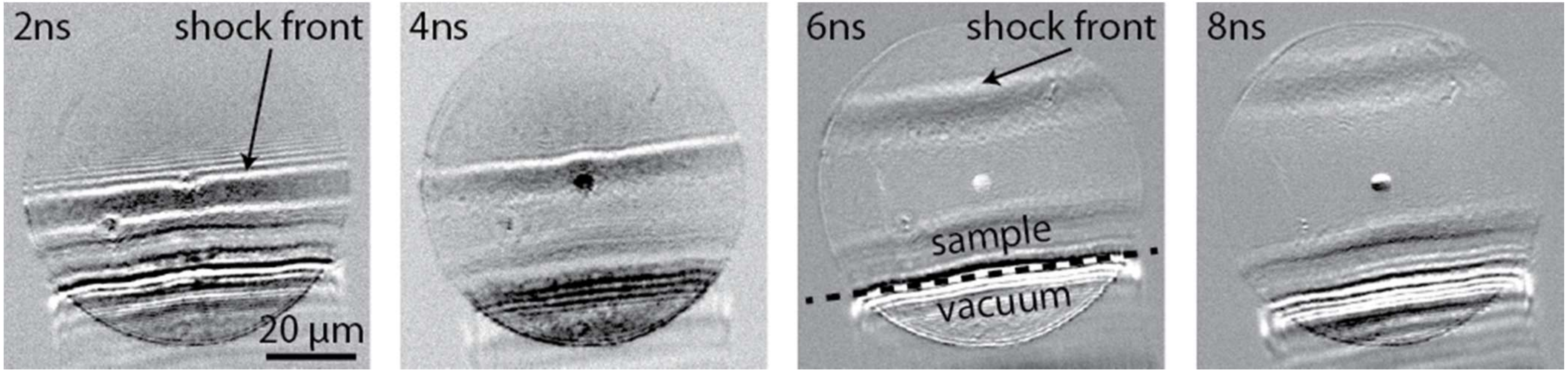
- Focal spot size ~120 nm (mono); beam divergence ~1mrad; f.o.v. ~100 µm



X-ray FEL shock front imaging

Test sample: glass **(all data: A. Schropp et al.)**

- 8.2 keV
- Phase-contrast imaging mode
- Using diverging beam projection



True sample: iron

- 7.0 keV
- ns movie

Accessible parameters

→ Shock velocity, density change, deformation length & time scale, viscosity

TECHNISCHE UNIVERSITÄT DRESDEN VolkswagenStiftung SLAC NATIONAL ACCELERATOR LABORATORY LCLS

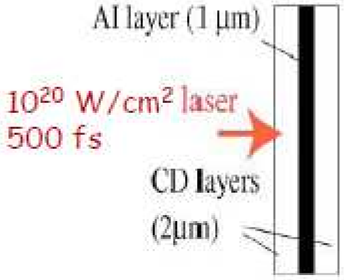
Coherent imaging of density fluctuations

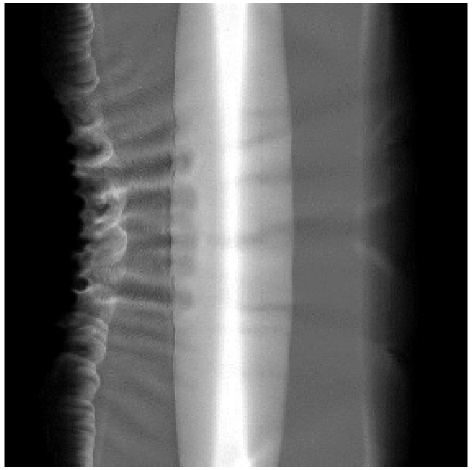
Relativistic laser-matter interaction

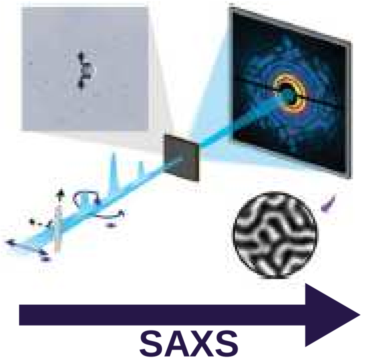
- Needed:
  - → **Ultrafast probing (space- & time-resolved) of B, Z*, j_e, T_e inside solid matter**
- Employ advanced x-ray techniques
  - → **XCDI, holography, SAXS, XRD, WAXS, XPCS, XANES, IXS, …**

Buried layers

(Courtesy: T. Cowan, T. Kluge)

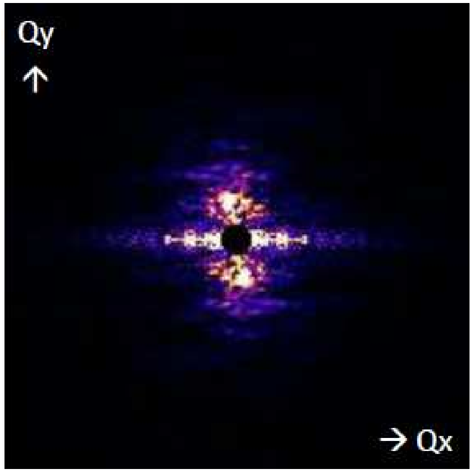




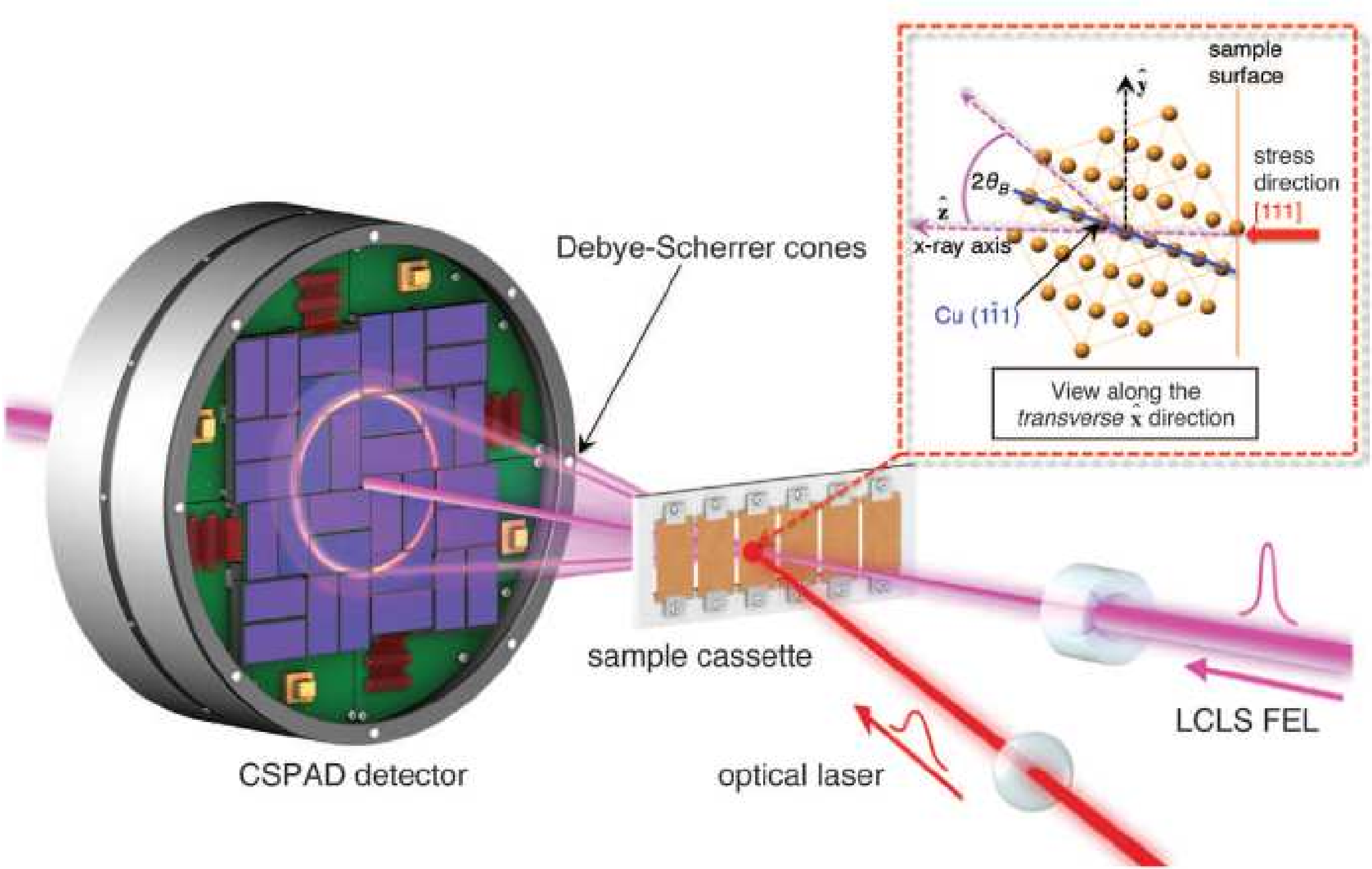


SAXS

(Simulation: C. Gutt)

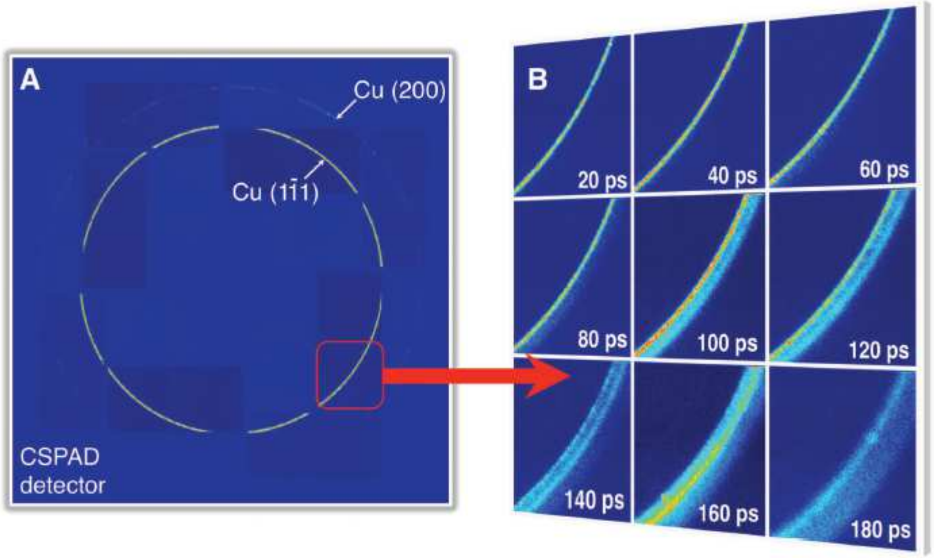


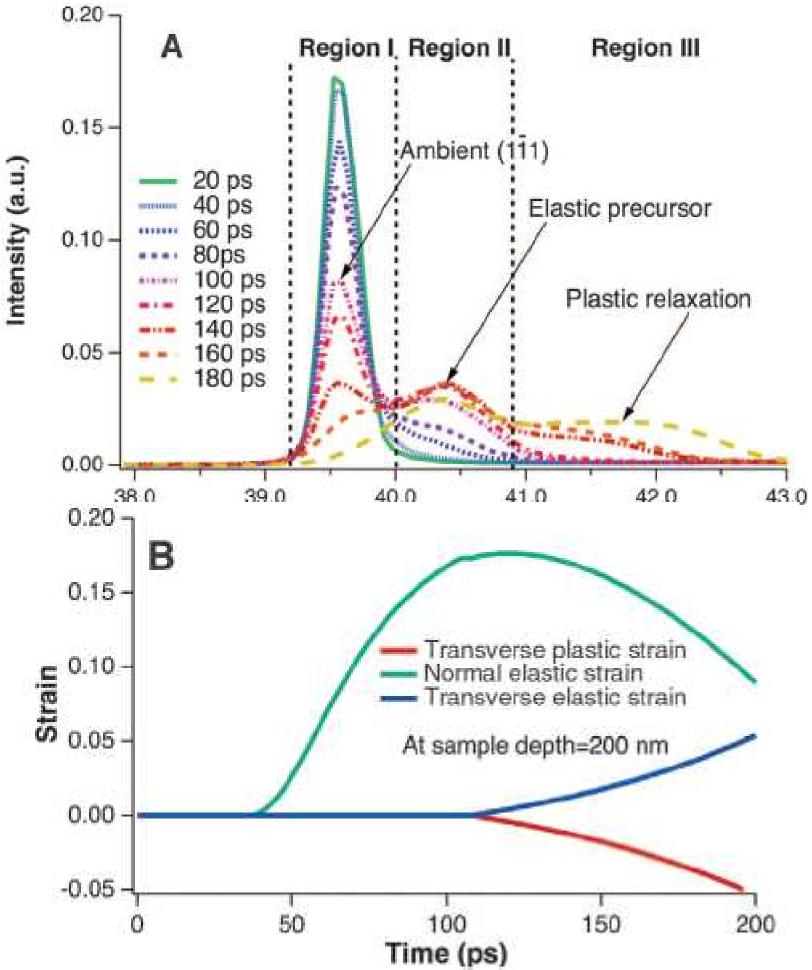
X-ray diffraction of shocked copper



D. Milathianaki et al., Science 342, 220 (2013)

X-ray diffraction of shocked copper



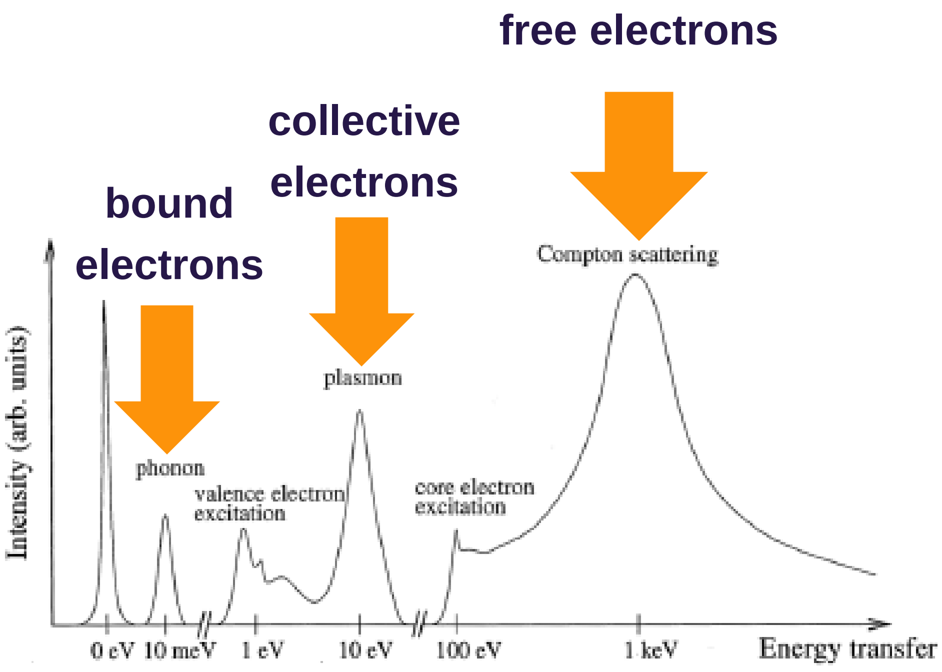


Observables

- Phase transitions
- Melting
- Elastic stress 73 Gpa
- Strain rate 10^9 s^{-1}

D. Milathianaki et al., Science 342, 220 (2013)

X-ray (inelastic) scattering



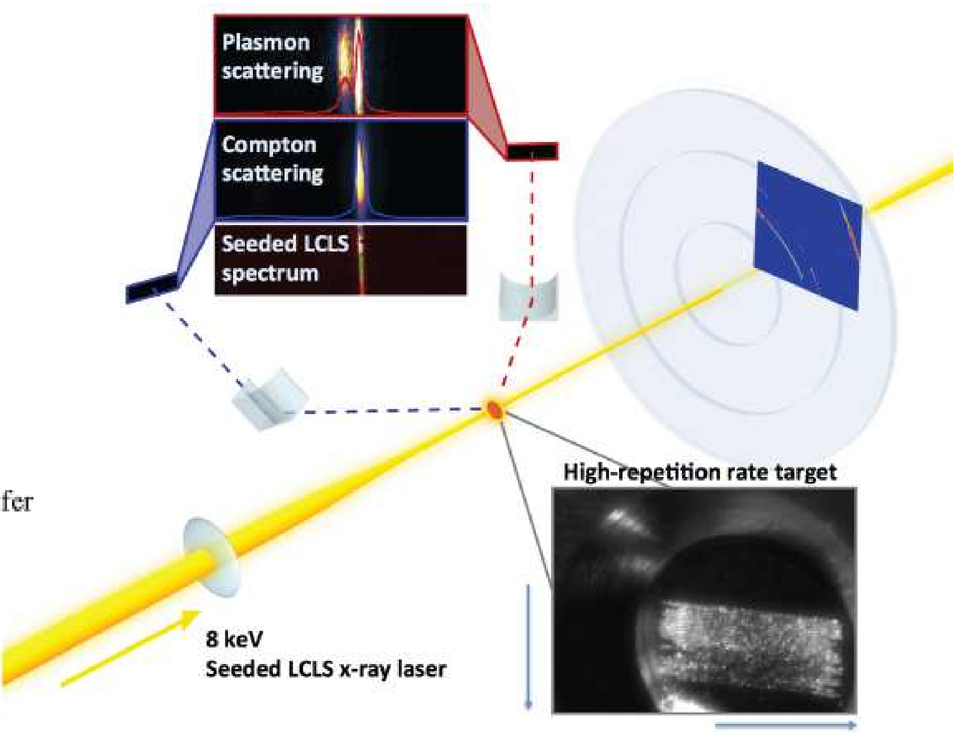
free electrons

collective electrons

bound electrons

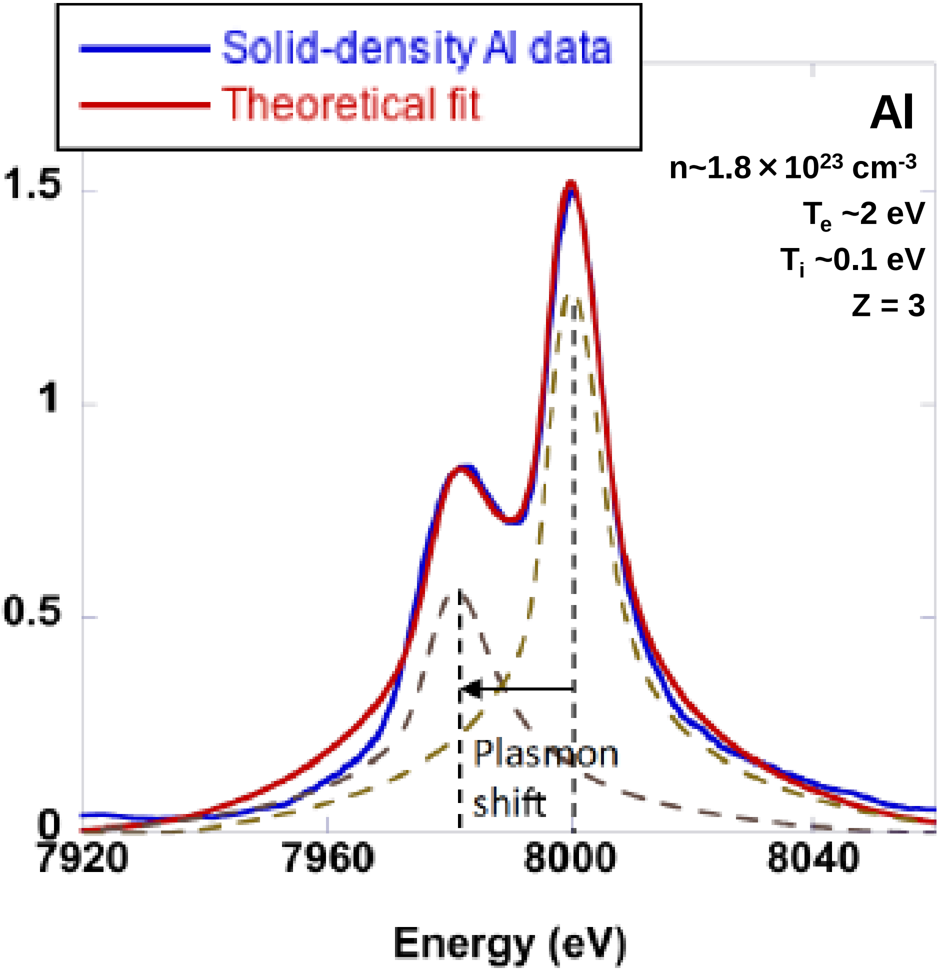
Observables

- Electron excitations
- Electron temperature
- Ionization
- Ion properties



L.B. Fletcher et al., JINST 8, C11014 (2013)

Self scattering at hard x-rays & solid Al



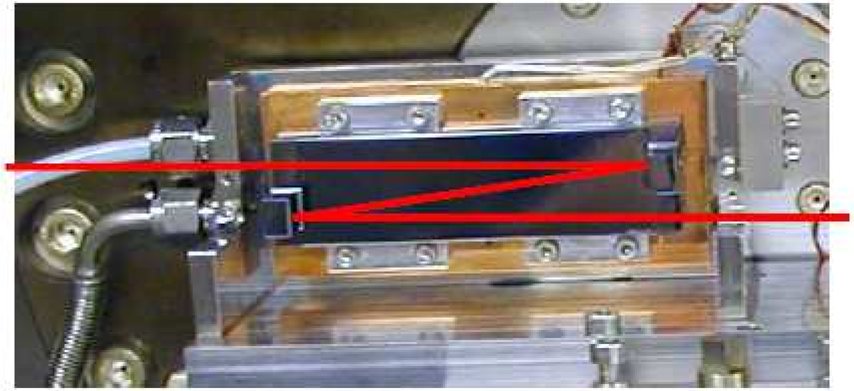
$n \sim 1.8 \times 10^{23}$ cm^{-3}
T_e ~2 eV
T_i ~0.1 eV
Z = 3

LCLS

~8 keV, 20-50 fs,
10^{17} W/cm^2

L.B. Fletcher et al., JINST 8, C11014 (2013)

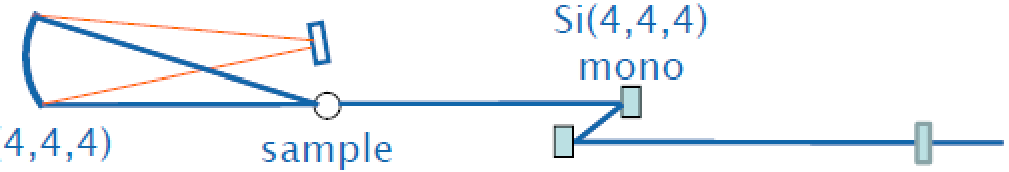
High resolution inelastic x-ray scattering



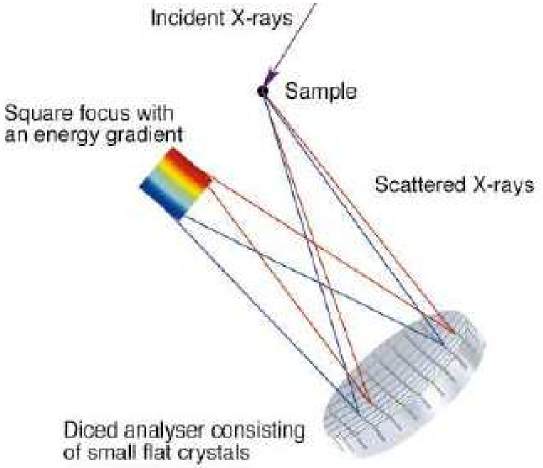
Si(4,4,4): $\Delta E/E = 5 \cdot 10^{-6}$

Working conditions:
Bragg angle @ $\vartheta_{PM} = 87°$
$E_{PM} = 7919.1$ eV
$\Delta E_{PM} \sim 100$ meV

Sensitive to the seed crystal angle at the level of 0.001°



- ~10.000 cubes of 0.7x0.7x2.3 mm³
- perfect crystal properties
- collection of sufficient solid angle



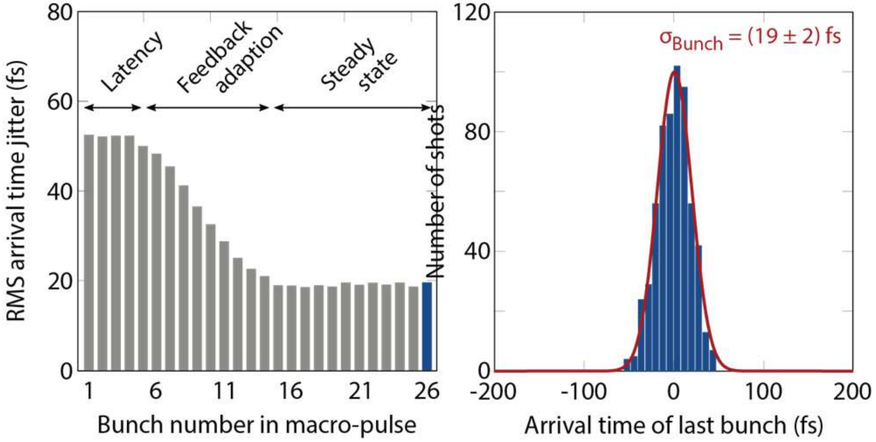
@ MEC: CSPAD (110 µm pixel size) & diced Si(444) crystal with R=1 m & $\theta = 87°$ ⇒ ~100 meV @ 7919 eV

Courtesy: G. Monaco et al.; to be published

Synchronization

Distribution of clock by optical laser

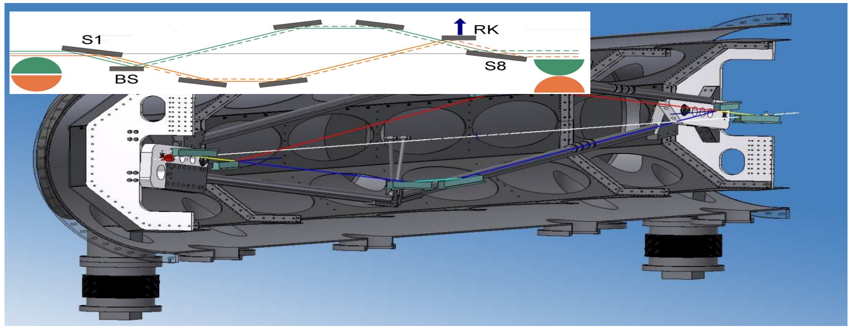
- Very accurate & length corrected
- Measure arrival time of e-
- Feedback to accelerator RF
- X-ray-to-OL within 10s of fs



FLASH results: A. Cavalieri et al., under publication

X-ray split & delay units

- Crystal-based (MID)
- Multilayer-based (HED)
- fs to few ps
- Stability ~fs, limited by mech. stability



S. Roling, H. Zacharias, et al.,
SPIE conf 8504, 850407 (2012)
BMBF project s 05K10PM2
& 05K13PM1

Content

- Introduction to HED science with FELs
- The HED instrument at European XFEL
- Instrumentation challenges

Instrumentation challenges

Deliver x-ray beam of varying spot size

- Spot sizes of <1 µm to 200 µm
- Full flux & full flexibility

10 Hz repetition rate experiments on solids

- Replace samples accurately
- Sample debris
- High power laser operation

Identifying flexible & efficient exp. configuration

- Vacuum interfaces
- Detectors

High field environments

- Optical lasers & pulsed magnets

Integration of all sub-systems

- Complex standalone systems
- Enabling operation by users

Acknowledgements

HED team at European XFEL

- K. Appel, M. Nakatsutsumi, I. Thorpe, B. Müller (guest), G. Priebe (OL)

Other European XFEL

- L. Batchelor, H. Sinn, G. Palmer, C. Deiter, A. Madsen, T. Roth, T. Haas, G. Wellenreuther, B. Becker-de Mos, S. Kozielski. W. Tscheu, A. Lalechos, V. Lamayaev, J. Schulz, M. Lederer, and many more

HIBEF User Consortium

- T. Cowan, A. Pelka, A. Ferrari (HZDR), E. McBride, H.-P. Liermann, J. Strempfer, M.v. Zimmermann (DESY), U. Zastrau (U Jena),

HED ART

- P. Audebert, A. Higginbotham, Hae-Ja Lee, R.W. Lee, H.-P. Liermann, D. Neely, P. Neumeier, K. Sokolowski-Tinten, S. Toleikis

plus

- F. Dorchies, J. Hastings, G. Monaco, A. Schropp

Summary

HED science applications at X-ray FEL facilities

- employ new x-ray pulse properties : fs duration – high power – coherence
- science applications appearing

New platform for studying matter in extreme states

- Instruments operating at LCLS and under construction at SACLA and European XFEL
- Coupling to high energy optical lasers for matter compression
- Develop and exploit various x-ray techniques for probing → in progress
- Possibility to use x-rays for excitation → requires further study

Start-up of European XFEL in full swing

- Civil construction completed; Installation of accelerator starts now
- First light by end of 2016; Early user runs in 2017
- HED instrument take first beam early 2017; high energy lasers should be available 4th Q 2017 for user experiments