New scientific opportunities for studies of matter at extreme conditions at the European XFEL

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ILP Forum 2021
September 30, 2021

Outline

- Introduction to X-ray Free Electron Lasers
- The European XFEL and first scientific results
- Status of the High Energy Density Instrument
- Outlook

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Different types of high brilliance lightsources

Storage rings (SR)

- High perf. x-ray source
- Very stable; highly efficient
- Many user installations for large variety of applications

→ **X-ray** scattering, microscopy, spectroscopy

X-ray FEL radiation

- Peak brightness x-ray source
- Single-pass; few sources
- So far only few user installations; applications u. study

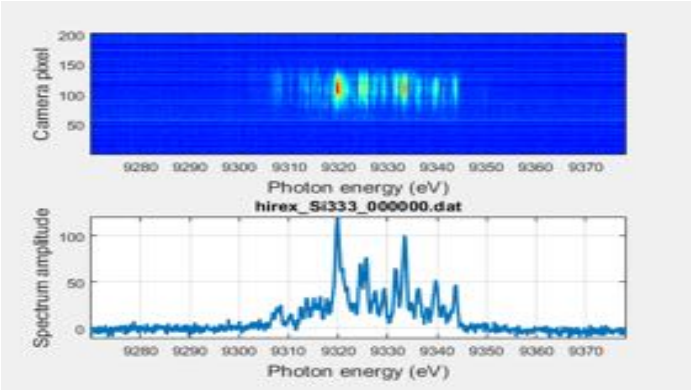
→ **X-ray** ultrafast methods using scattering, microscopy, spec-troscopy; non-linear methods

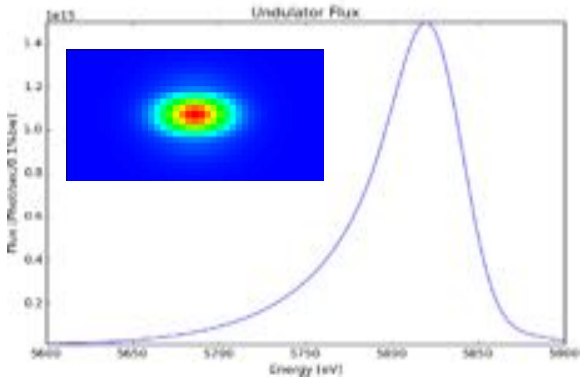
Visible Laser radiation

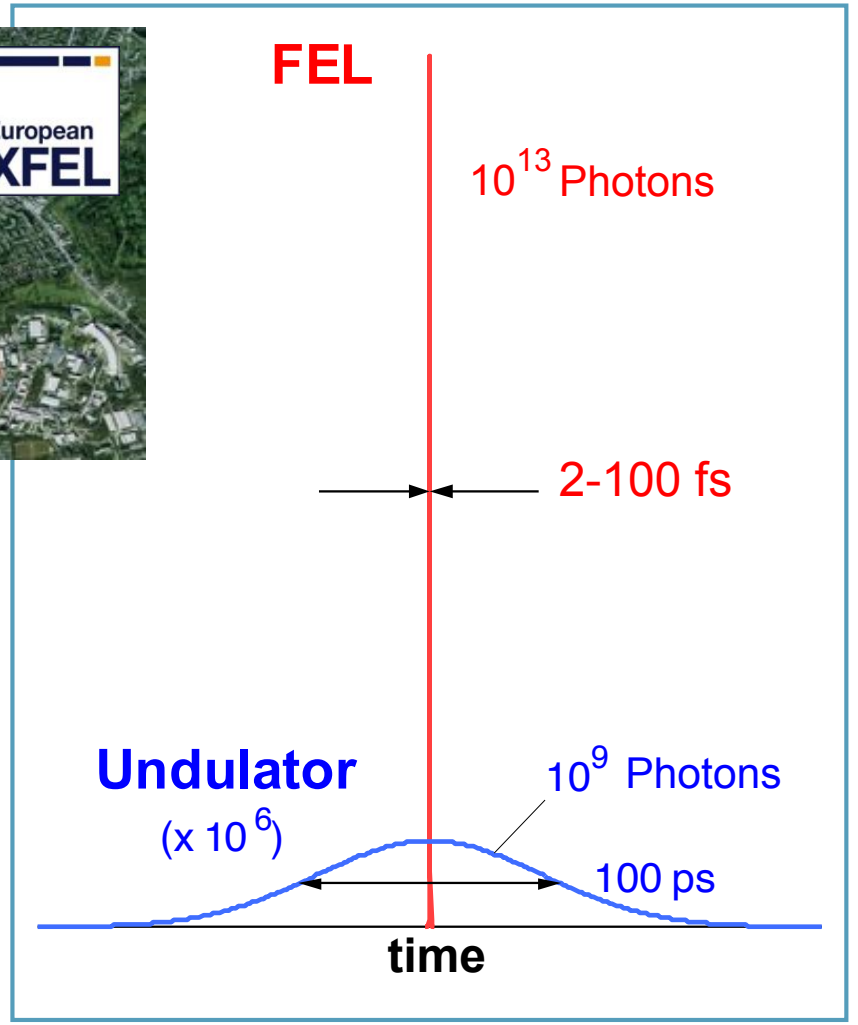
- Commercially or home-built, widely distributed, High power/energy
- Huge community
- Attosecond & non-linear techn.

→ **Light** ultrafast and non-linear methods using microscopy or spectroscopy

XFEL radiation is very different from synchrotron radiation







- fs pulse: a probe of atomic motion (100fs) ..
- hard X-rays: atomic positions, chemical selectivity, bulk sensitivity

Acoustic vibration

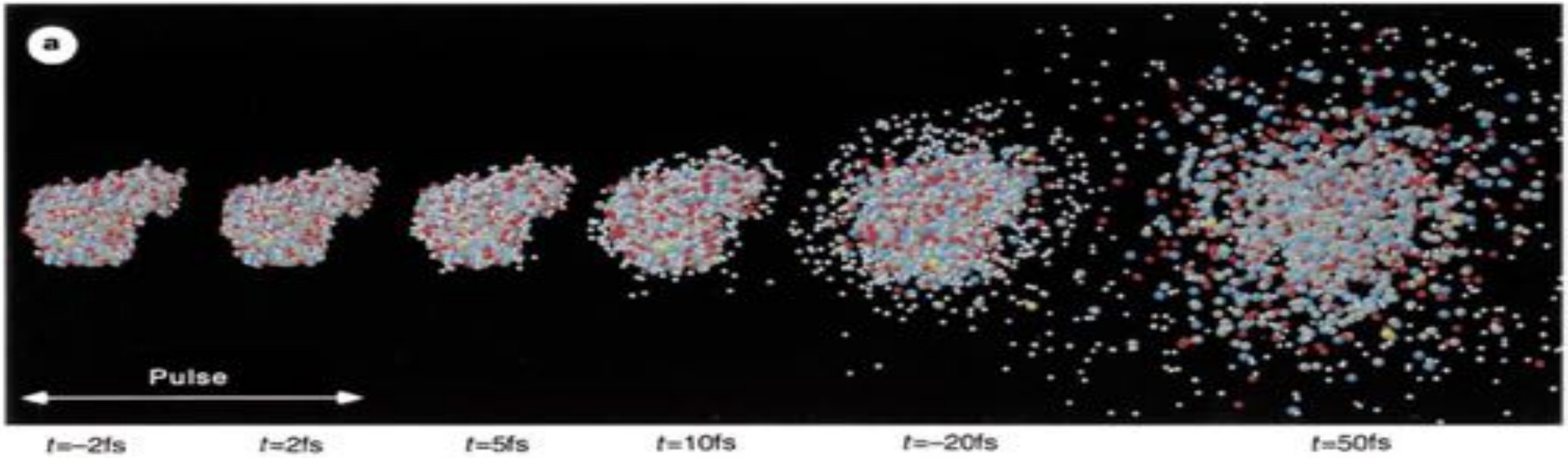
Speed of sound: $v = 3000\,m/s$, a 3 Å Yd $10^{-13}\,s$ 100 fs

- Can we measure phonon dynamics ?
- Can we see how charge migrates from one atom to another ?

Diffract before destruction: a totally new approach to structural determination with X-rays

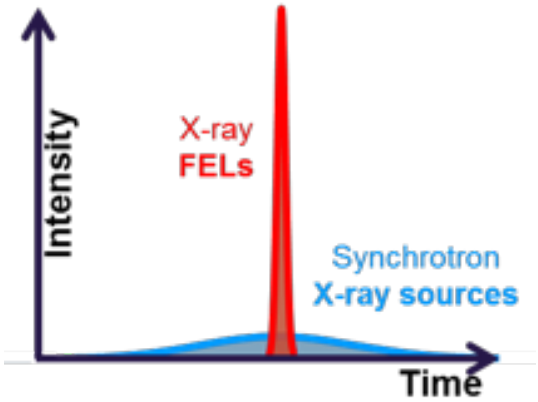
Free Electron Lasers : The exploding protein

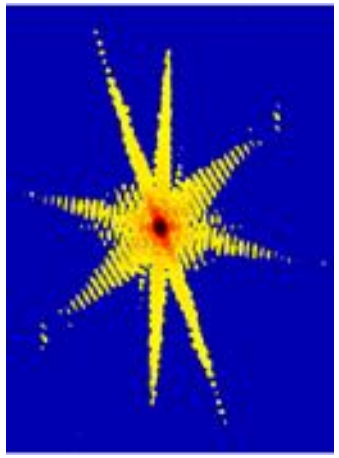
R. Neutze et al, Nature 406, 752 (2000)



- Can we beat radiation damage ?
- Can we measure at room temperature ?
- Can we make movies of proteins at work ?

New opportunities offered by X-ray FELs





Ultrashort pulses

1 100 fs

Coherence

Almost full transverse

Partially temporal

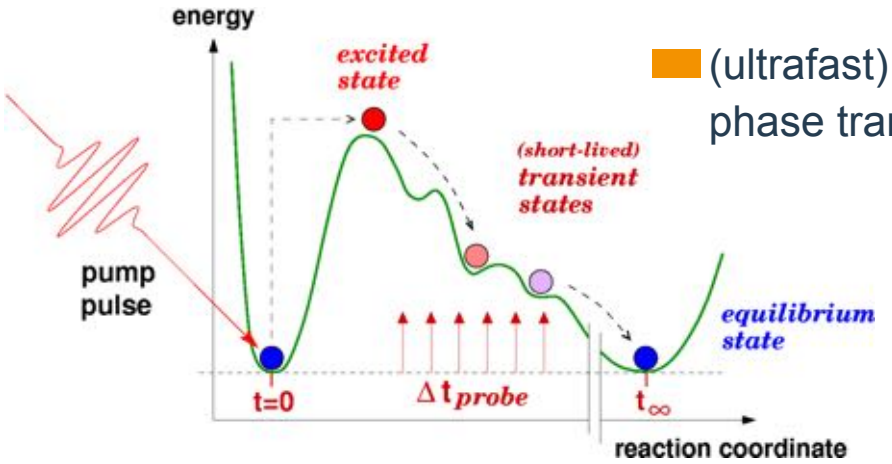
Intensity/power

up to few mJ

up to >10^{20} W/cm^2

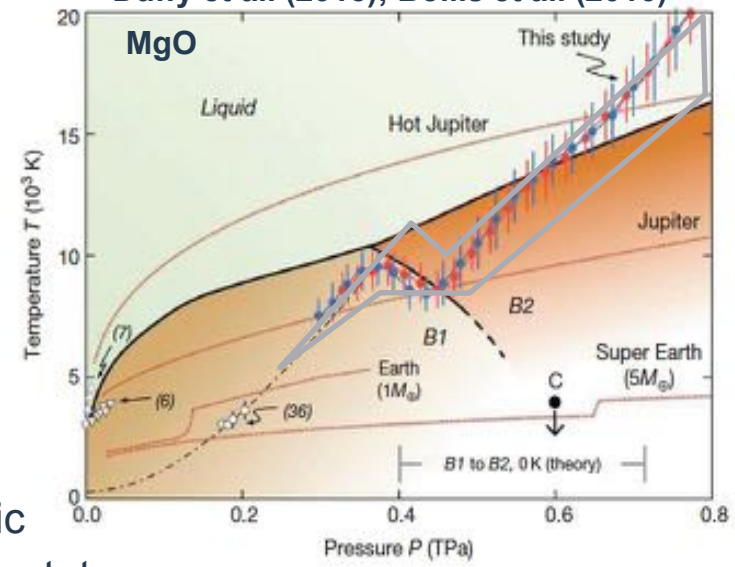
- Structural dynamics
  - **Measurement of atomic and electron dynamics with high spatial [0.1 nm] and temporal [10 fs] res.**
  - **physics, materials sciences, chemistry, life science**
- Imaging at the nanoscale
  - **Imaging experiments on confined and extended objects with atomic to mesoscale resolution [0.1 1000 nm]**
  - **physics, materials sciences, chemistry, life science**
- Non-linear x-ray science
  - **Start using non-linear techniques to obtain hidden information (off-diagonal elements in reaction matrices)**
  - **physics, chemistry**

Open science problems

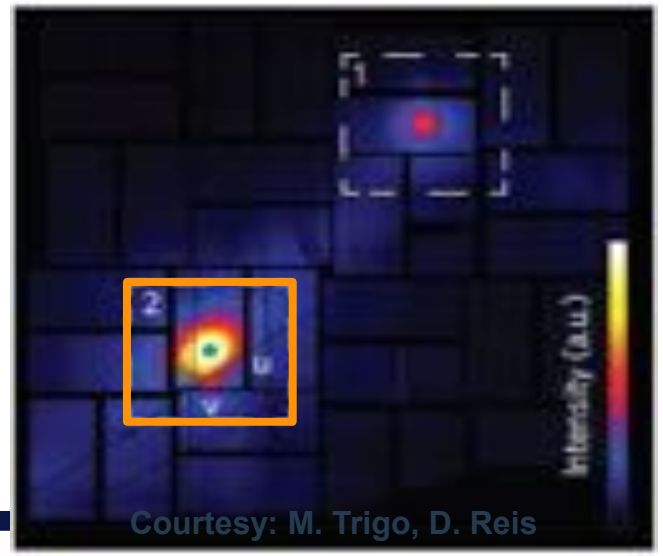


- (ultrafast) (bio-)chemical processes: reactions, phase transitions, bond breaking & forming

Duffy et al. (2015); Bollis et al. (2016)



- (ultrafast) structural and electronic transitions: phase transitions, new states



- systems , function ‘excited states, non-reversible processes

- complex (bio-)structures and their temporal evolution

Outline

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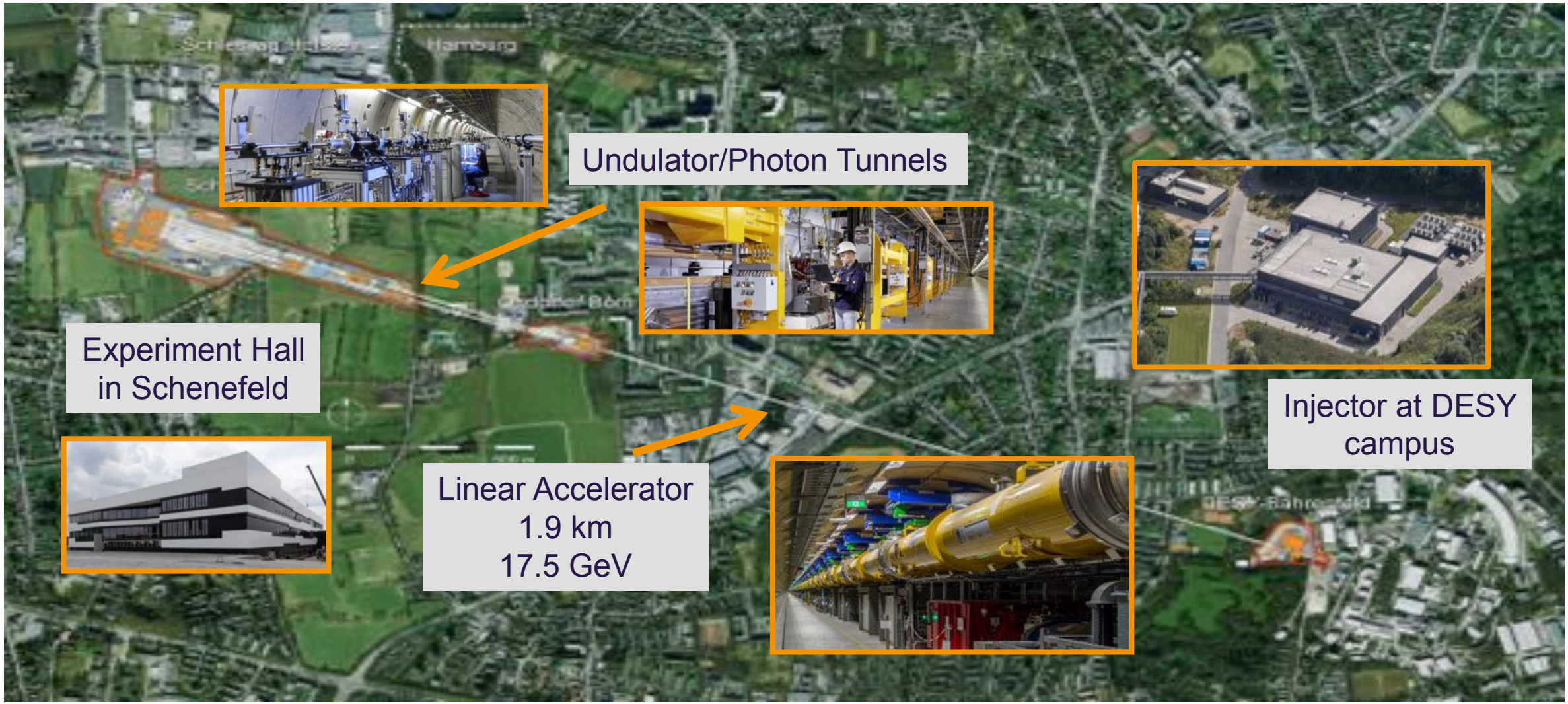
About the European XFEL

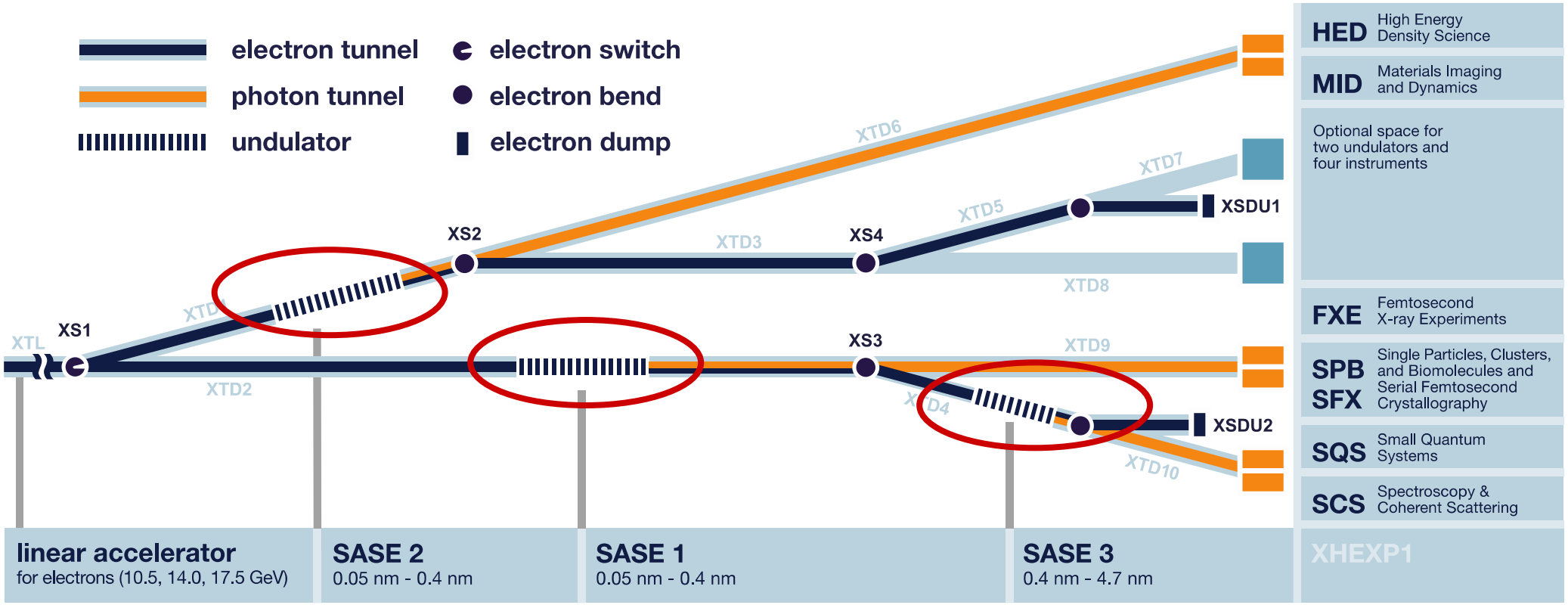
- International user facility for XFEL research
- Germany 58%, Russia 27 %, others 1 –3%
  - EuXFEL: Construction and operation of the X-ray Laser Facility
  - DESY: Construction and operation of the accelerator
  - Staff XFEL 650 (of which ~250 @ DESY)
    - Start construction 2009
    - Start of operation 1 July 2017
      - 1,54 B€ (2018 prices)
      - 50% cash, 50% in-kind
      - Yearly running costs 130 M€ (20
        - Soft & hard X-ray FEL radiation
        - Multi-disciplinary science community

Layout of the European XFEL



Beam distribution & instruments

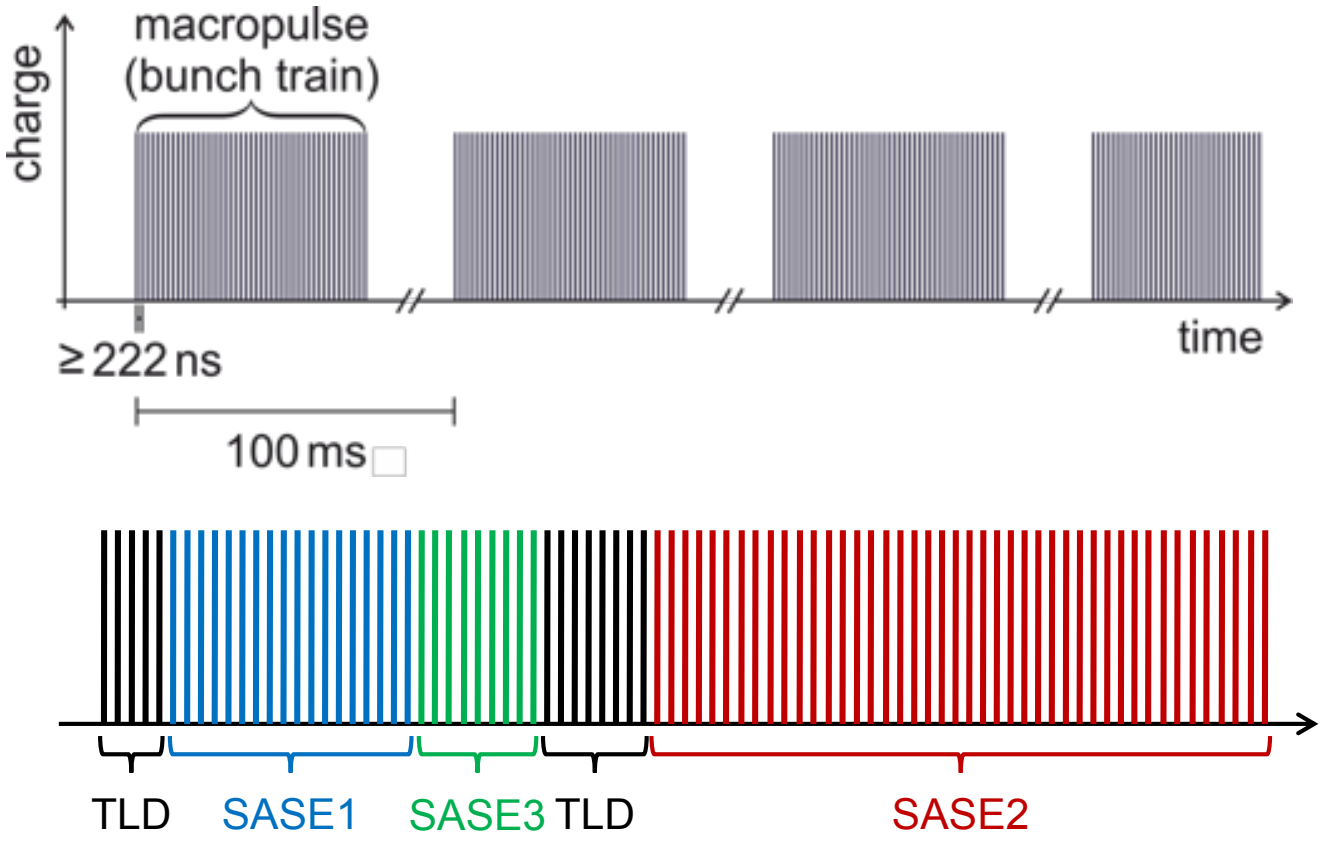
Undulator Segment	FEL radiation energy [keV]	Wavelength [nm]
SASE 1	3 - over 24	0.4 - 0.05
SASE 2	3 - over 24	0.4 - 0.05
SASE 3	0.27 –3	4.6 –0.4



Key parameters of EuXFEL

Parameter	Value
Electron Energy	8.5 –17.5 GeV
Photon energy	0.26 - 25 keV
Pulse duration	2 –100 fs
Seeding	Commissioning
# of pulses	27000 /s
# of FELs	3
# of instruments	6
Start of operation	2017

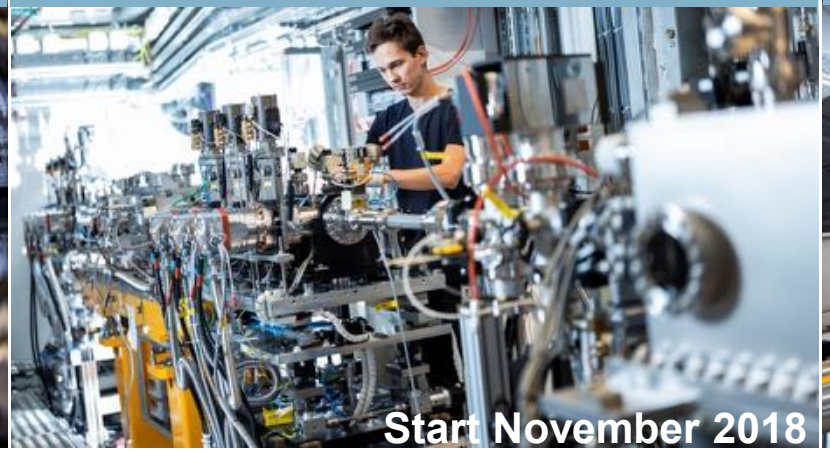
- Specific electron & x-ray beam delivery pattern
  - **RF repetition rate: 10 Hz**
  - **RF flat-top length: ~ 600 µs**
  - **Up to 2700 bunches/train**
  - **Bunch spacing: Up to 4.5 MHz**



All six Instruments in User Operation since 2019

SPB/SFX (Adrian Mancuso)

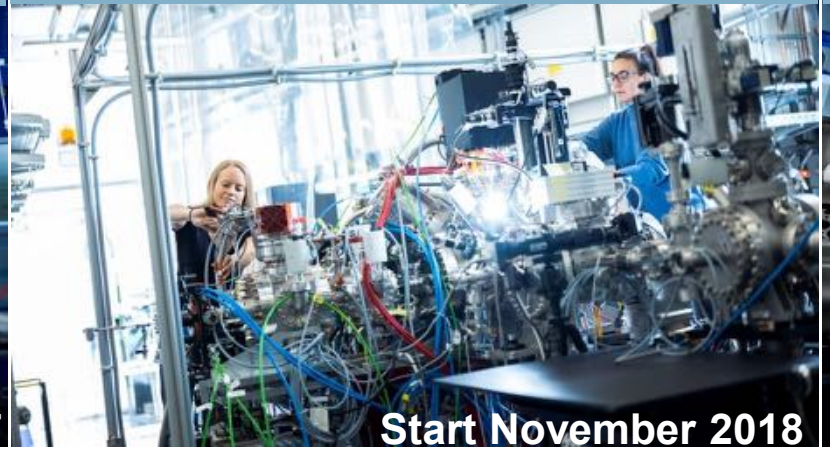
SCS (Andreas Scherz)



MID (Anders Madsen)

FXE (Chris Milne)

SQS (Michael Meyer)



HED (Ulf Zastrau)

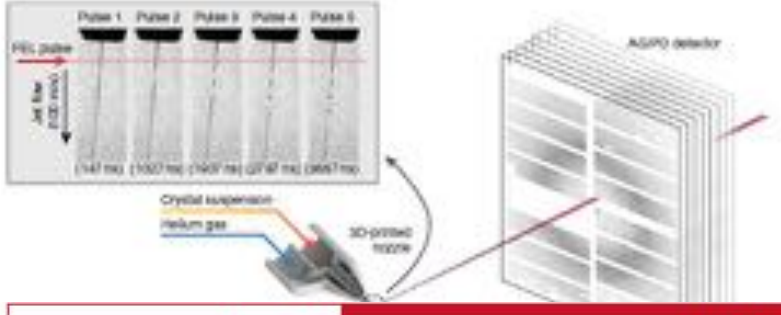
nature COMMUNICATIONS

ARTICLE

OPEN

Megahertz serial crystallography

Max O. Wiedorn et al.



nature methods ARTICLES

Time-resolved serial femtosecond crystallography at the European XFEL

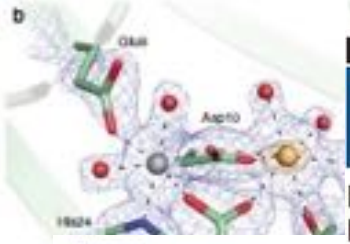
Suraj Pandey[1,14], Richard Bean[2,14], Tokushi Sato[2,14], Ishwor Poudyal[1], Johan Bielecki[2], Jorvani Cruz Villarreal[3], Oleksandr Yefanov[4], Valerio Mariani[4], Thomas A. White[4], Christopher Kupitz[5], Mark Hunter[5], Mohamed H. Abdellatif[4], Saša Bajt[6], Valerii Bondar[2], Austin Echelmeier[3], Diandra Doppler[3], Moritz Emons[2], Matthias Frank[7], Raimund Fromme, Yaroslav Gevorkov[4,8], Gabriele Giovanetti[2], Man Jiang[2], Daihyun Kim[3], Yoonhee Kim[2], Henry Kirkwood[2], Anna Klimovskaia[2], Juraj Knoska[4,9], Faisal H. M. Koua[4], Romain Letrun, Stella Lisova[10], Luis Maia[2], Victoria Mazalova[4], Domingo Meza[11], Thomas Michelat[2], Abbas Ourmazd[1], Guido Palmer[2], Marco Ramilli[2], Robin Schubert[11], Peter Schwander[1], Alessandro Silenzi[2], Jolanta Sztuk-Dambietz[2], Alexandra Tolstikova[4], Henry N. Chapman[4,9], Alexandra Ros[3], Anton Barty[4], Petra Fromme[3], Adrian P. Mancuso[2,13] and Marius Schmidt

European XFEL

ARTICLE

OPEN

Megahertz data collection from protein microcrystals at an X-ray free-electron laser



THE JOURNAL OF PHYSICAL CHEMISTRY Letters

Revealing Hot and Long-Lived Metastable Spin-States in the Photoinduced Switching of Solvated Metallogrid Complexes with Femtosecond Optical and X-ray Spectroscopies

Maria Naumova, Aleksandr Kalinko, Joanne W. L. Wong, Mohamed Abdellah, Huifang Geng, Edoardo Domenichini, Jie Meng, Sol Alvarez Gutierez, Pierre-Adrien Mante, Weihua Lin,

RESEARCH

Science

SPECTROSCOPY

Photon-recoil imaging: Expanding the view of nonlinear x-ray physics

U. Eichmann[1]*, H. Rottke[1], S. Meise[1], J.-E. Rubensson[2], J. Söderström[2], M. Agåker[2,3], C. Så M. Meyer[4], T. M. Baumann[4], R. Boll[4], A. De Fanis[4], P. Grychtol[4], M. Ilchen[4,5], T. Mazza[4], J. M V. Music[4,5], Y. Ovcharenko[4], D. E. Rivas[4], S. Serkez[4], R. Wagner[4], S. Eisebitt[1,6]

Letter Vol. 6, No. 9 / September 2019 / Optica 1106

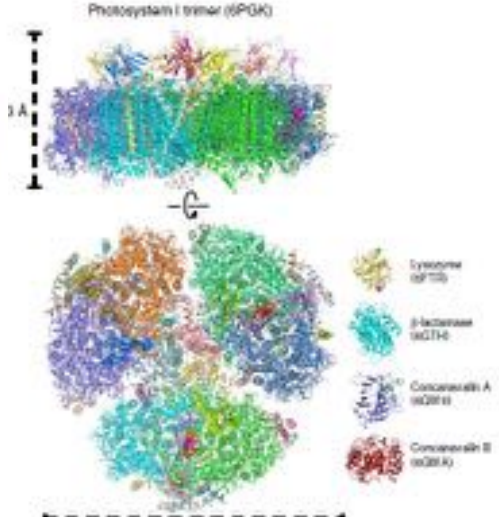
optica

Megahertz x-ray microscopy at x-ray free-electron laser and synchrotron sources

ARTICLE

OPEN

Membrane protein megahertz crystallography at the European XFEL



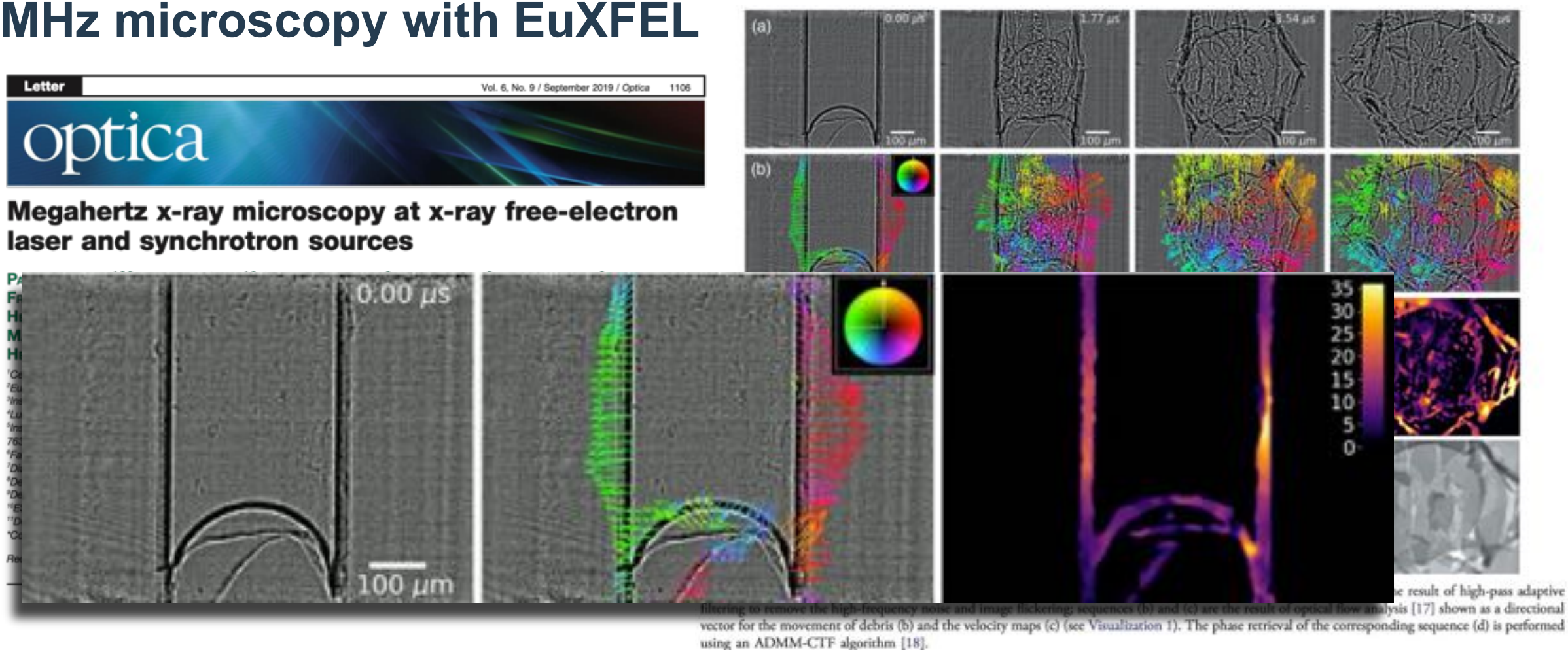
Structural Dynamics

Evaluation of serial crystallographic structure determination within megahertz pulse trains

Cite as: Struct. Dyn. 6, 064702 (2019); https://doi.org/10.1063/1.5124387
Submitted: 14 August 2019 . Accepted: 21 October 2019 . Published Online: 04 December 2019

Oleksandr Yefanov, Dominik Oberthür, Richard Bean, Max O. Wiedorn, Juraj Knoska, Gisel Pena, Salah Awel, Lars Gumprecht, Martin Domaracky, Iosifina Sarrou, P. Lourdu Xavier, Markus Metz, Saša Bajt, Valerio Mariani, Yaroslav Gevorkov, Thomas A. White, Aleksandra Tolstikova, Pablo Villanueva-Perez, Carolin Seuring, Steve Aplin, Armando D. Estillore, Jochen Küpper, Alexander Klyuev, Manuela Kuhn, Torsten Laurus, Heinz Graafsma, Diana C. F. Monteiro, Martin Trebbin, Filipe R. N. C. Maia, Francisco Cruz-Mazo, Alfonso M. Gañán-Calvo, Michael Heymann, Connie Darmanin, Brian Abbey, Marius Schmidt, Petra Fromme, Klaus Giewekemeyer, Marcin Sikorski, Rita Graceffa, Patrik Vagovic, Thomas Kluyver, Martin Bergemann, Hans Fangohr, Jolanta Sztuk-Dambietz, Steffen Hauf, Natascha Raab, Valerii Bondar, Adrian P. Mancuso, Henry Chapman, and Anton Barty

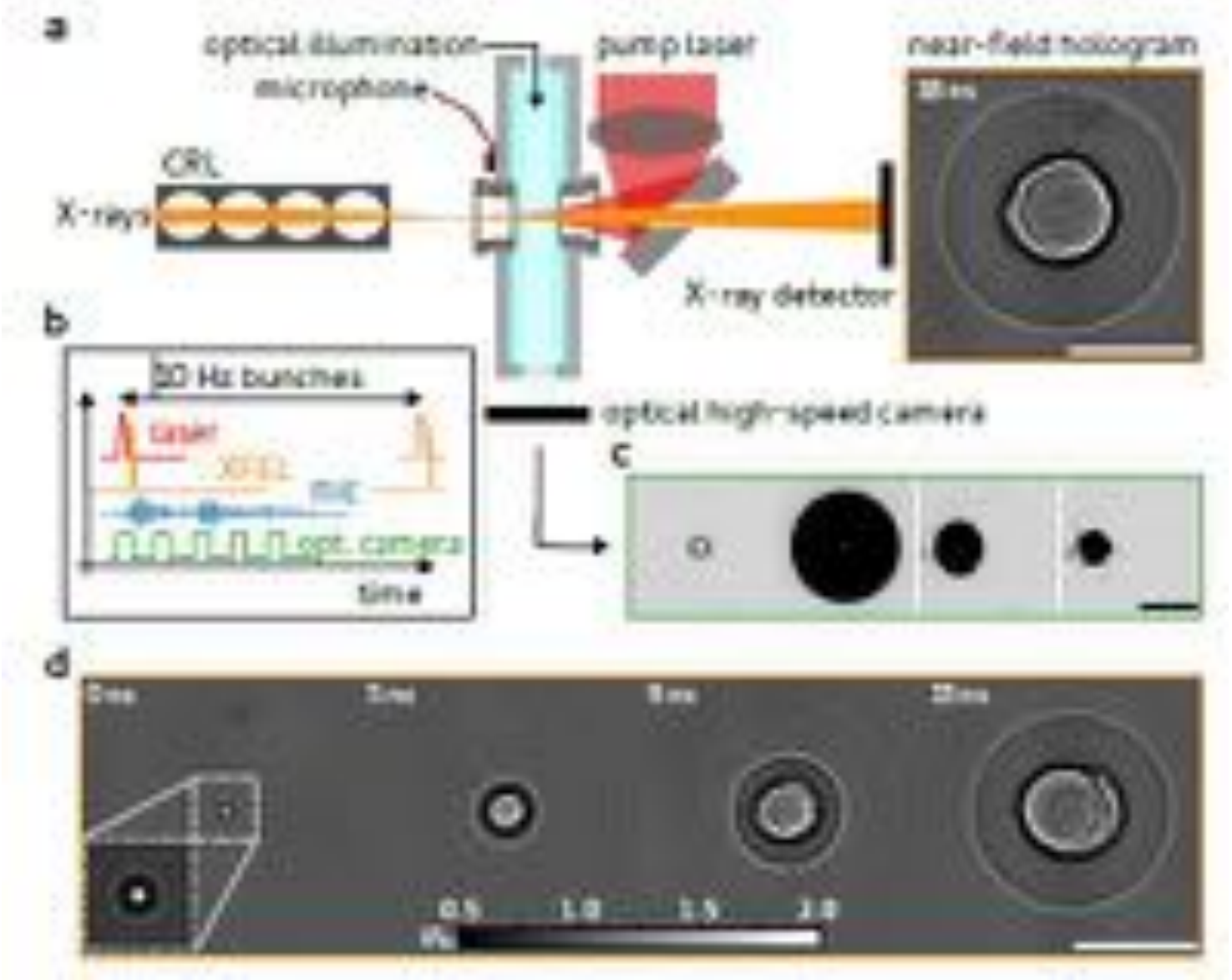
MHz microscopy with EuXFEL



Next step: MHz projection tomography, paving the way for 3D movies of fast phenomena with important potential industrial applications

Vagovic et al, Optica Vol. 6, pp. 1106-1109 | (2019)

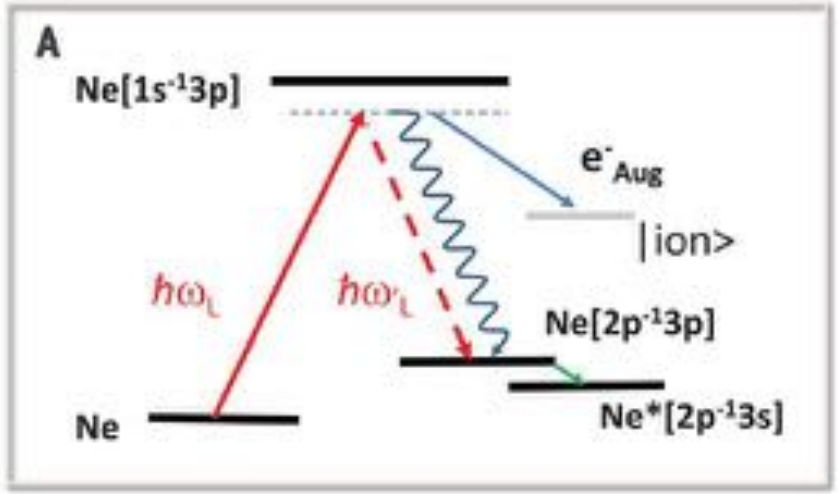
Ultrafast holographic imaging of cavitation bubbles

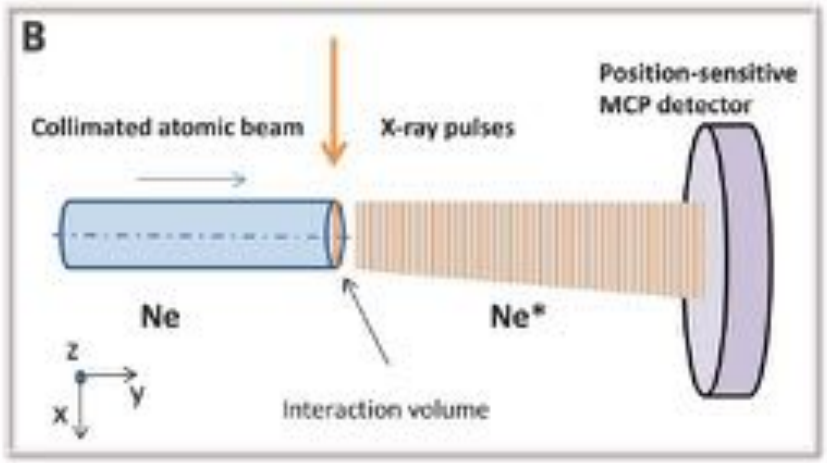


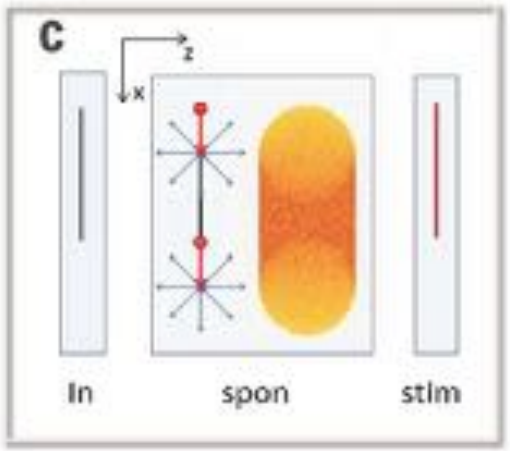
- non-equilibrium physics
- medical procedures
  - •emulsify tissue in cataract surgery
  - •bubble-mediated drug delivery
- sonochemistry
- ultrasonic cleaning
- corrosion prevention

Vassholz et al., Nat Commun 12, 3468 (2021)

Stimulated X-Ray Raman Scattering

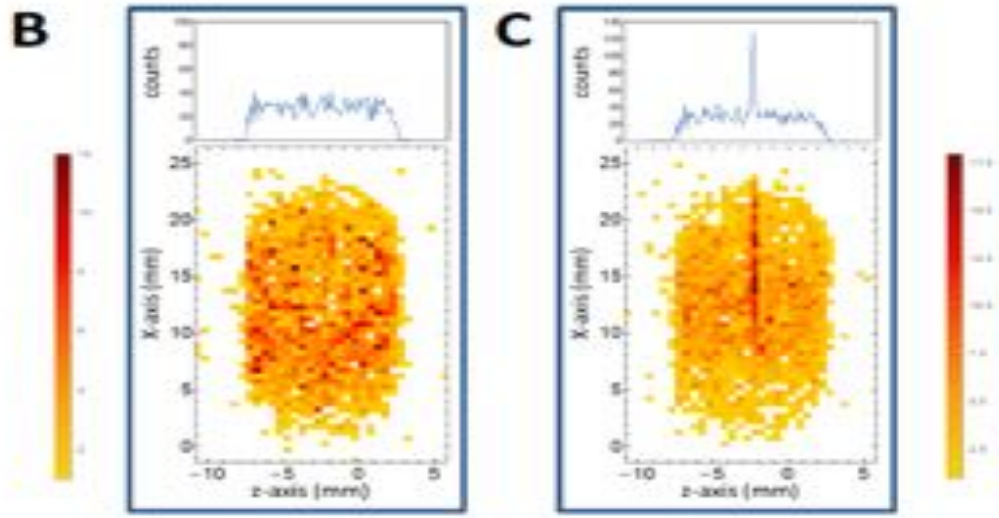






Science

Photon-Recoil Imaging: expanding the view of nonlinear X-ray physics



860 eV
Spontaneous emission
- momentum in all directions

855 eV
Stimulated emission
- no momentum transfer

Eichmann et al., Science 369, 1630 –1633 | (2020)

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European XFEL

HiBEF User Consortium

HED High-Energy Density science

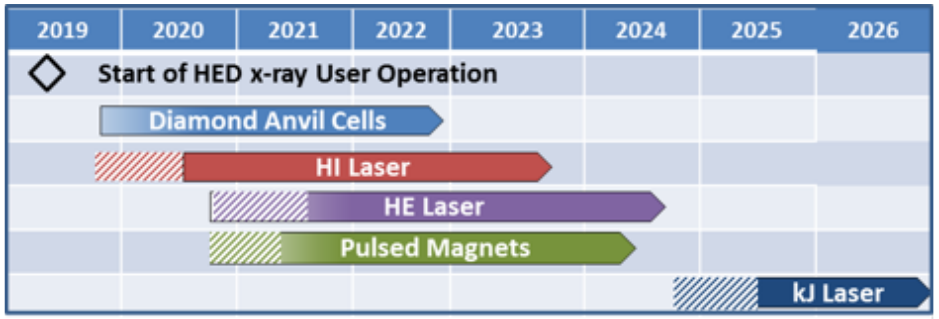
HZDR

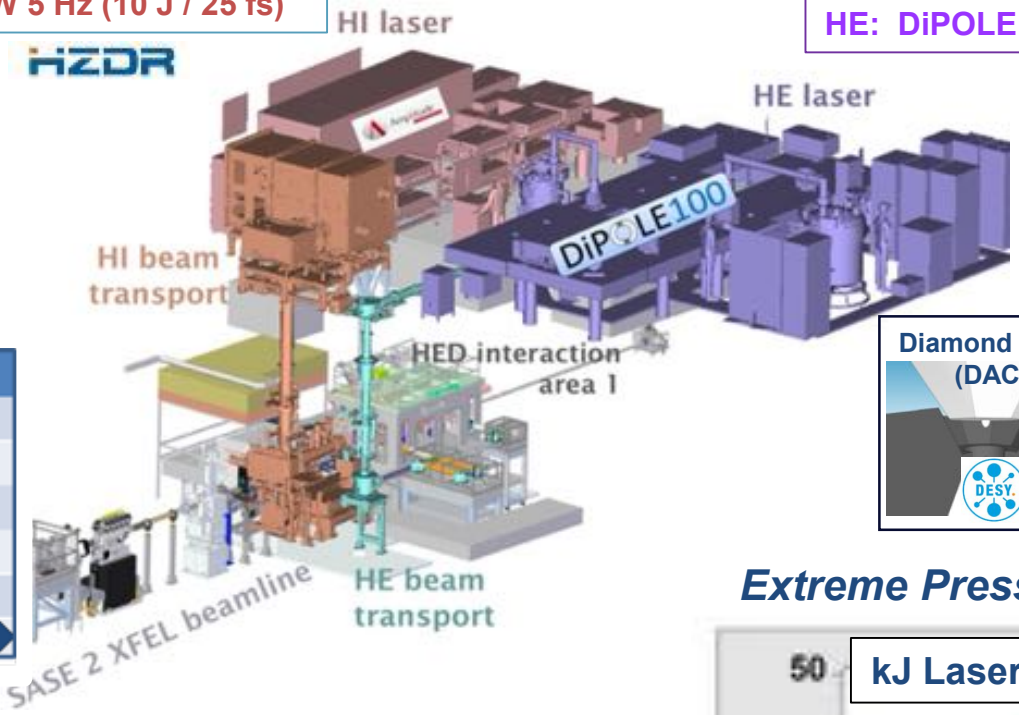
DESY.

Science & Technology Facilities Council

HI JENA HELMHOLTZ Helmholtz Institute Jena

HI: Amplitude 300 TW 5 Hz (10 J / 25 fs)

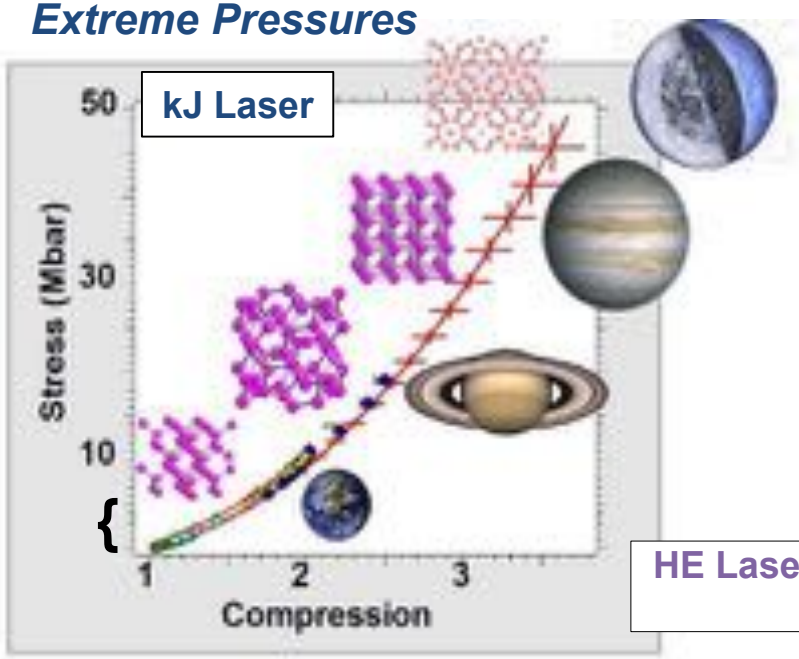




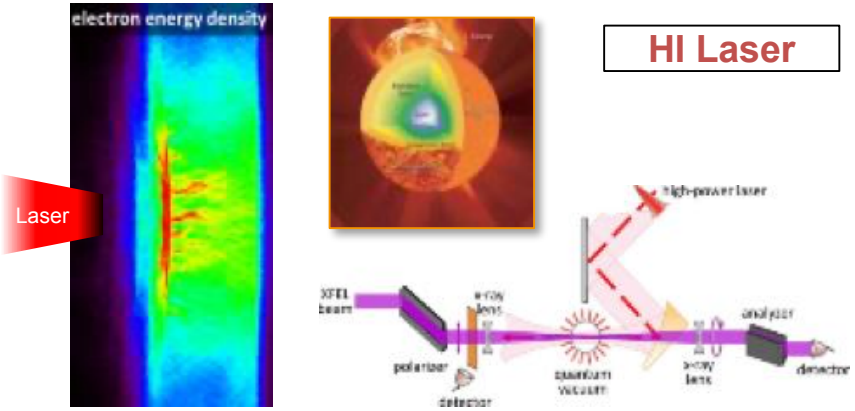
HE: DiPOLE 100-X: 100 J, 10 ns, 10 Hz

Science & Technology Facilities Council

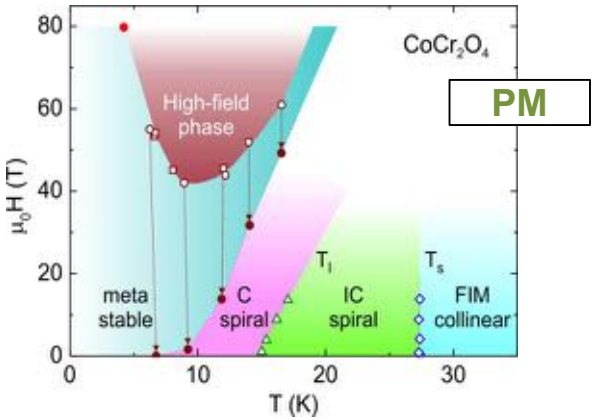
Extreme Pressures



Relativistic Plasmas & Extreme Fields



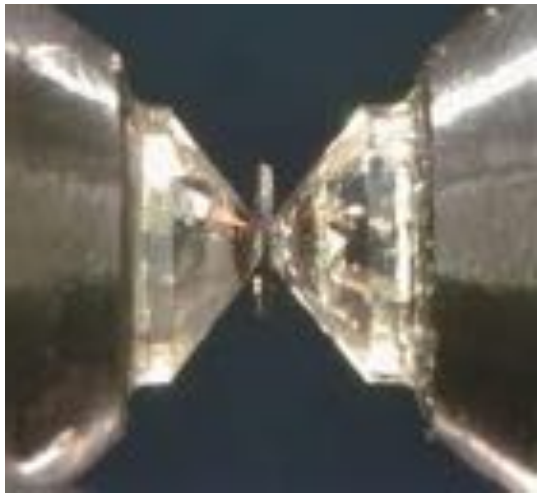
Magneto-structural transitions

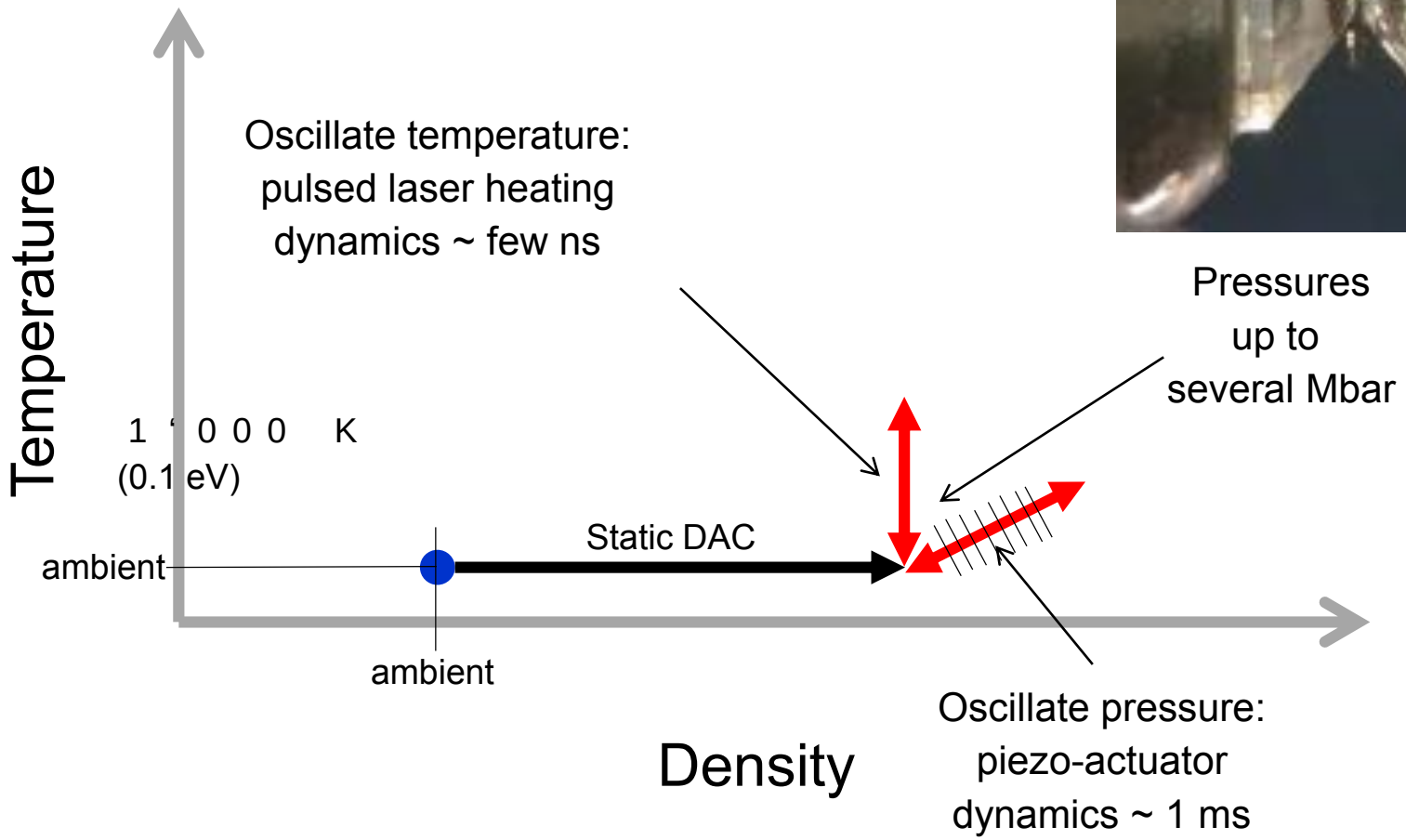


European XFEL

Preparation of extreme conditions at HED

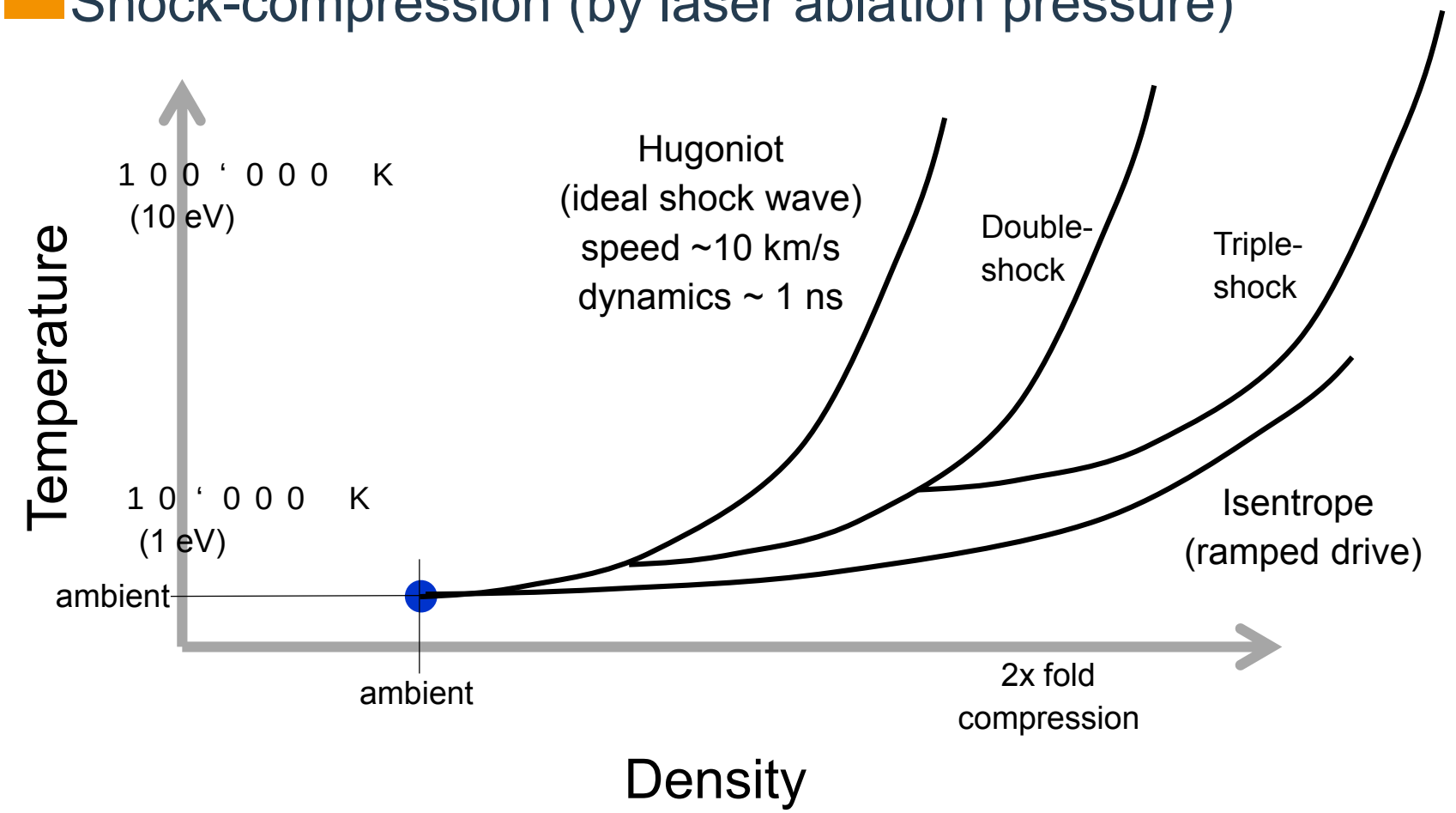
Diamond Anvil Cells (DAC)





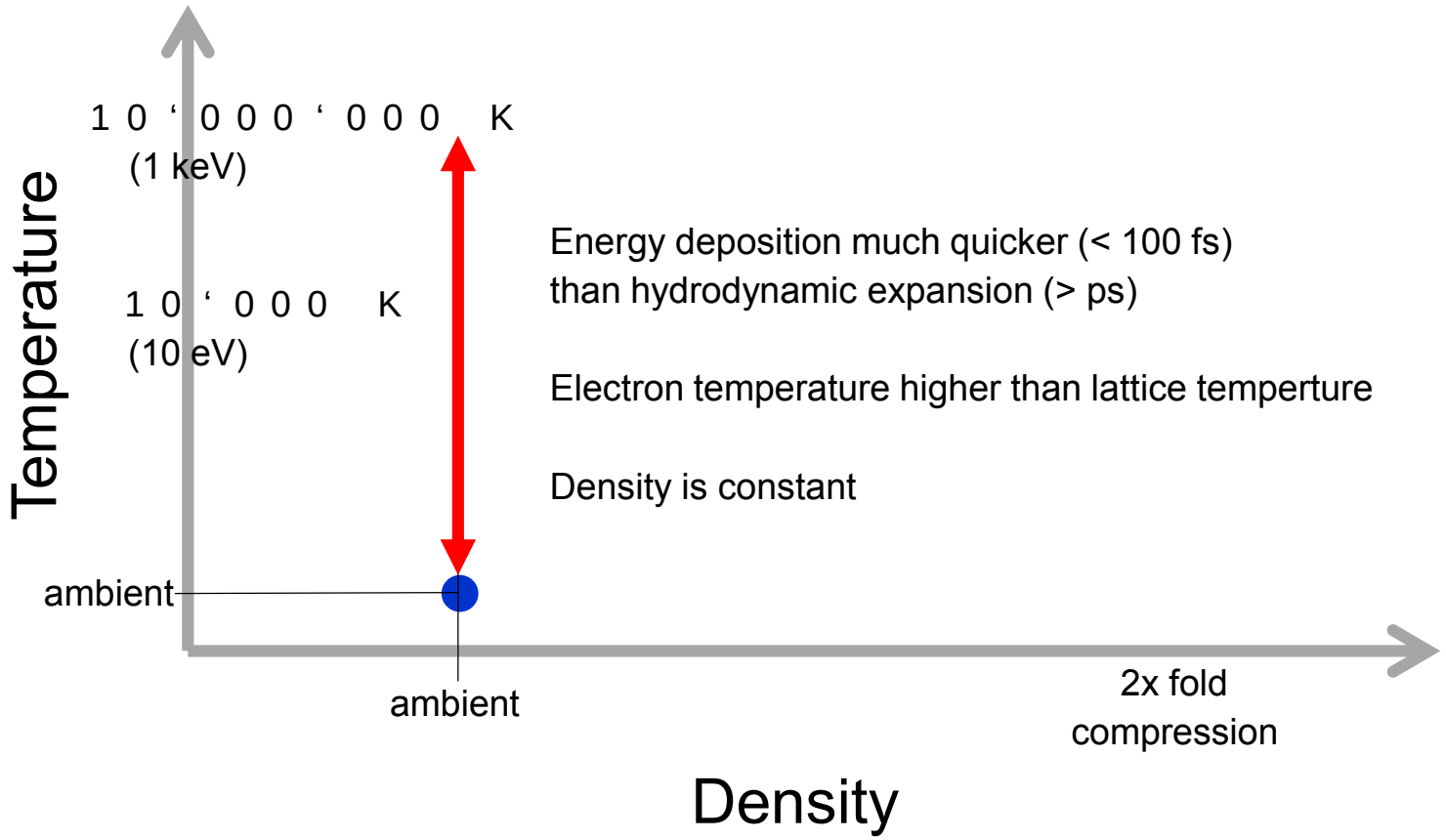
Preparation of extreme conditions at HED

Shock-compression (by laser ablation pressure)



Preparation of extreme conditions at HED

Isochoric heating (energy transfer by ultrafast pulse)



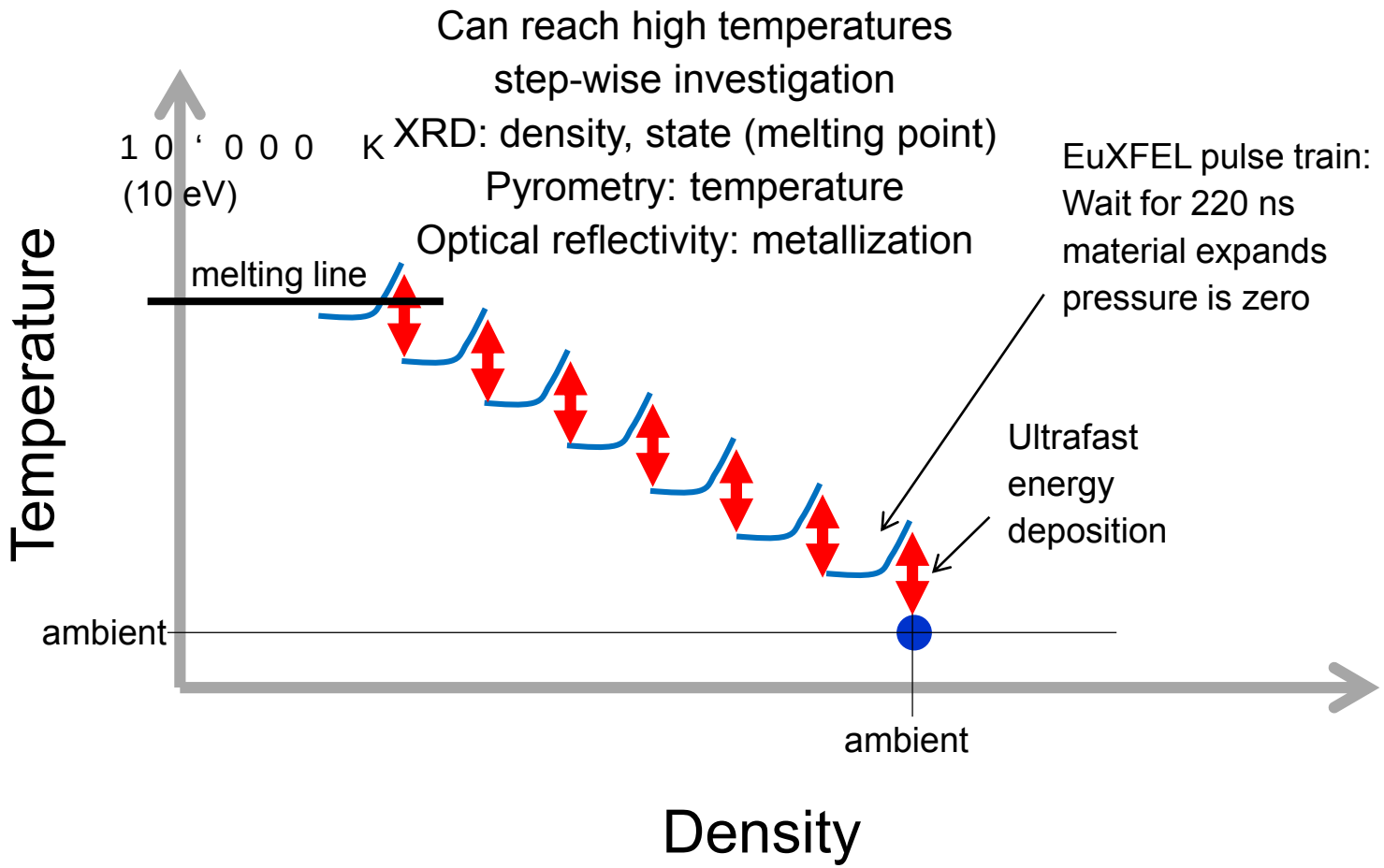
Energy deposition much quicker (< 100 fs)
than hydrodynamic expansion (> ps)

Electron temperature higher than lattice temperture

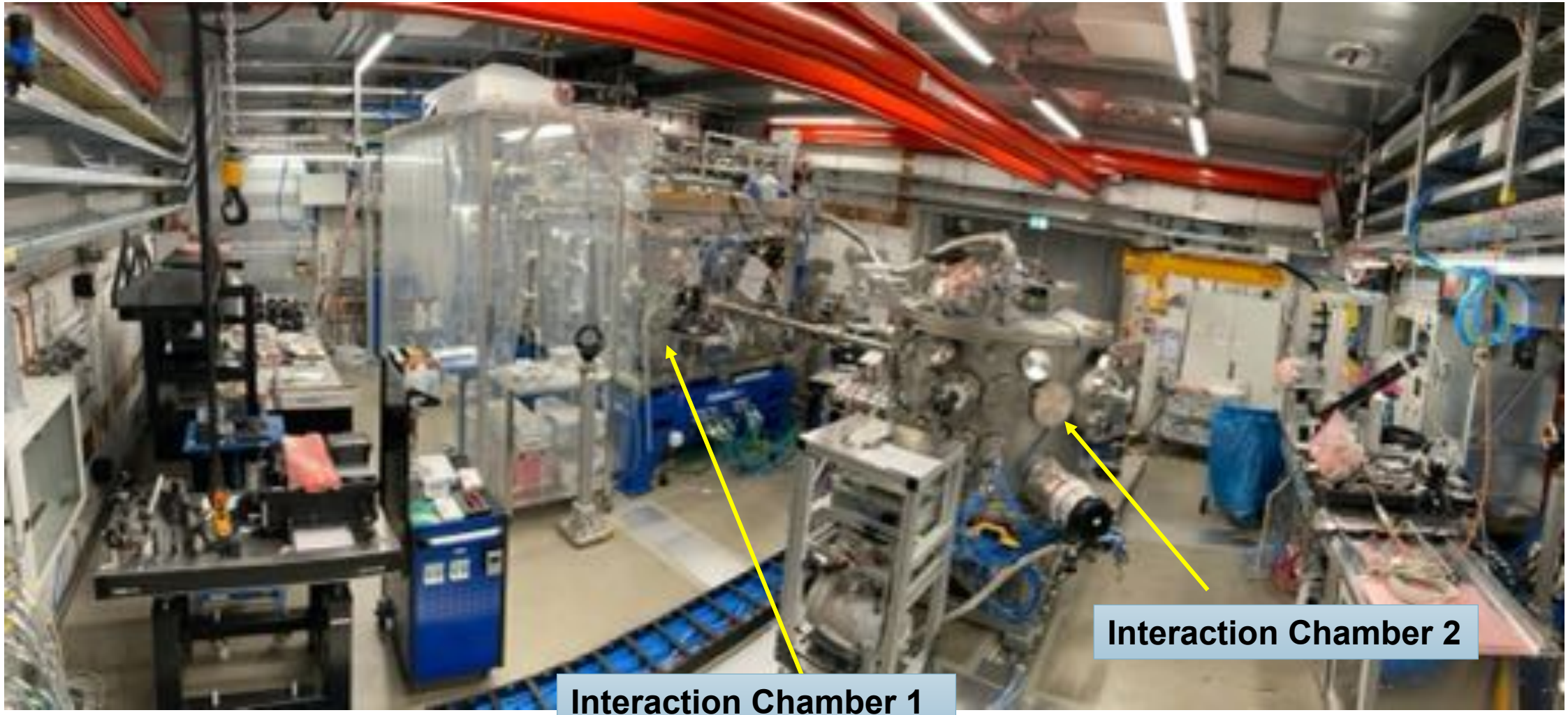
Density is constant

Preparation of extreme conditions at HED

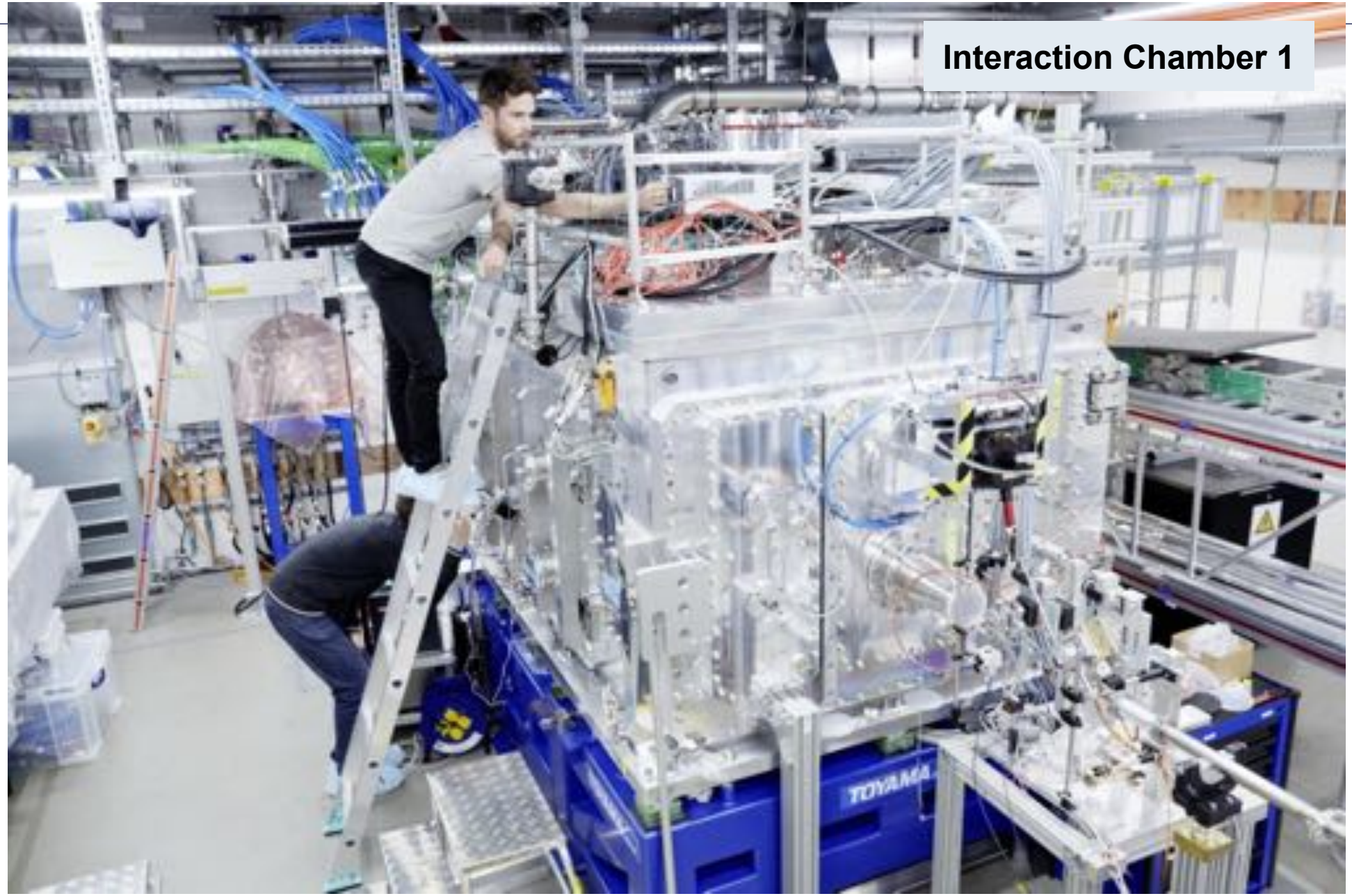
Isobaric heating (energy transfer by ultrafast pulse)

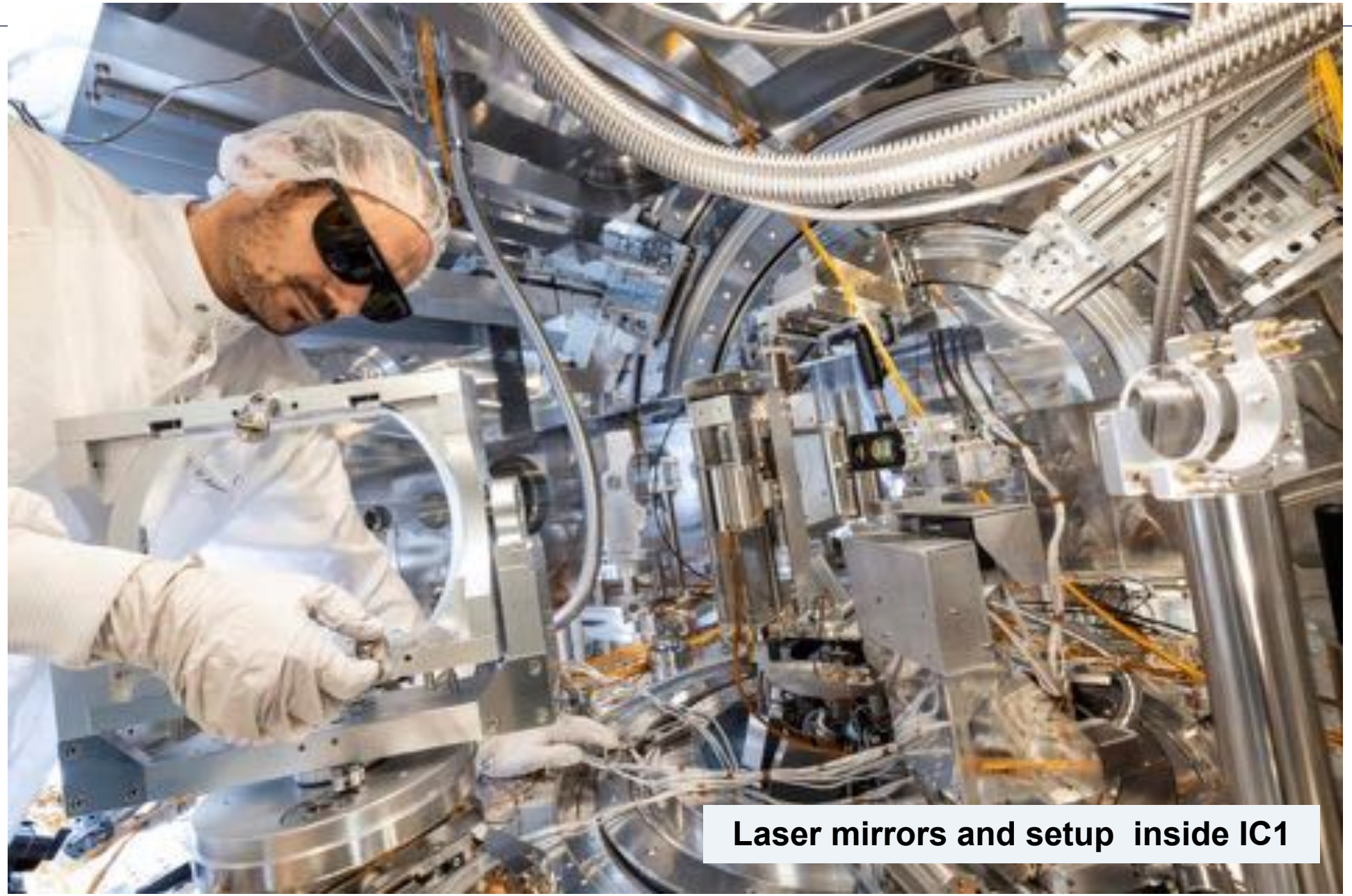


HED experimental hutch



Interaction Chamber 1

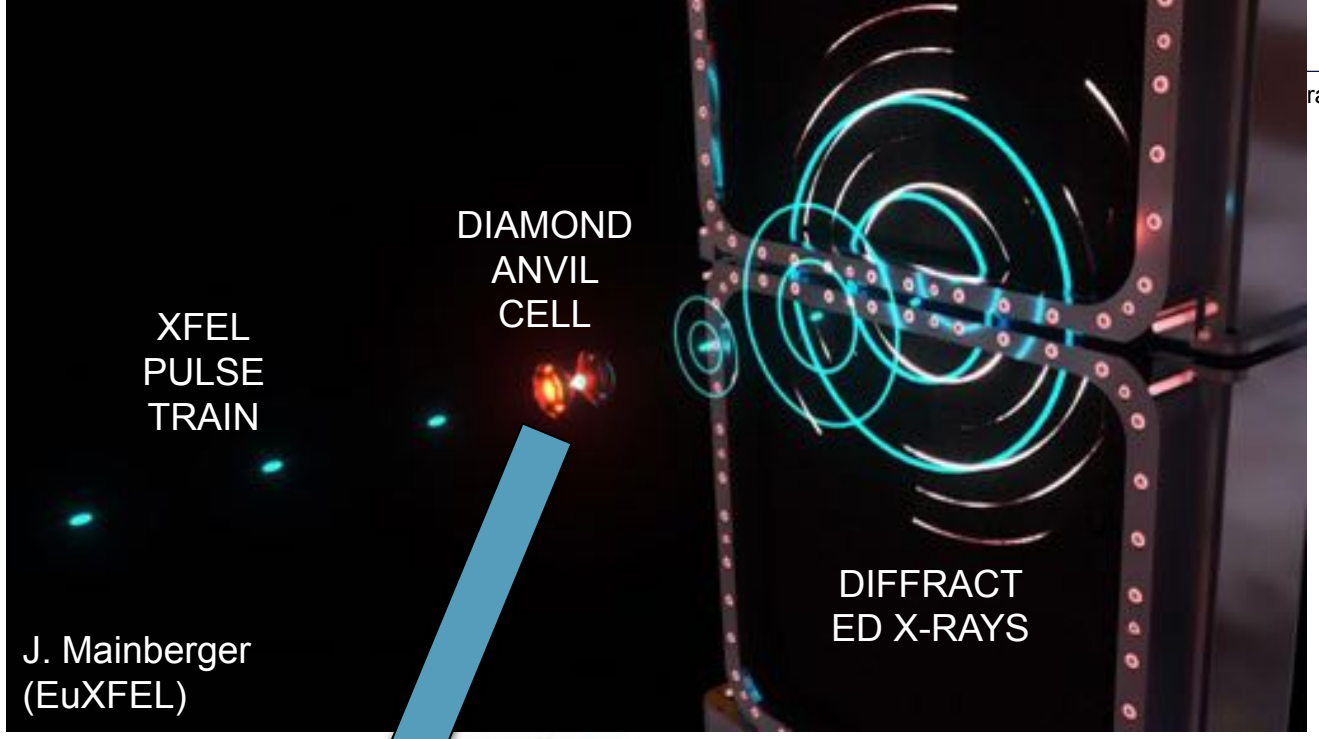


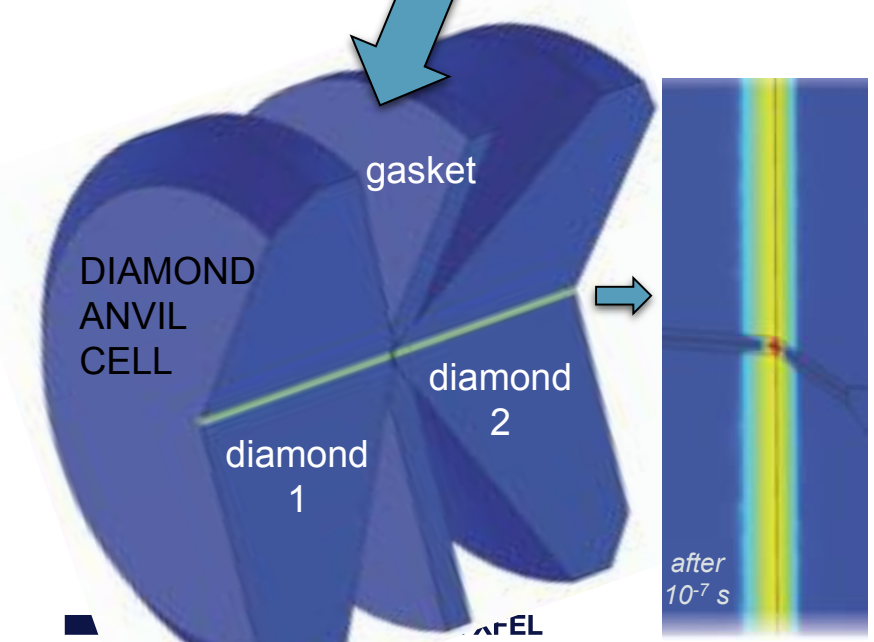


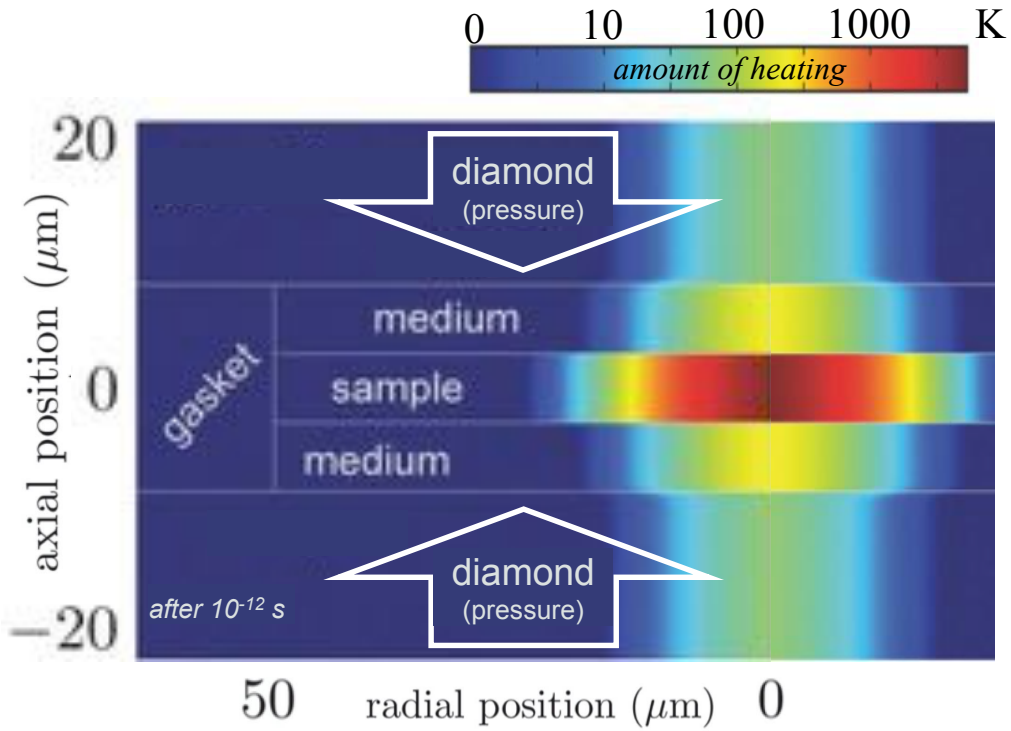
Laser mirrors and setup inside IC1

Coupling EuXFEL to Diamond Anvil Cells

Exp # 2292, October 2019
Community Beamtime (70 participants)

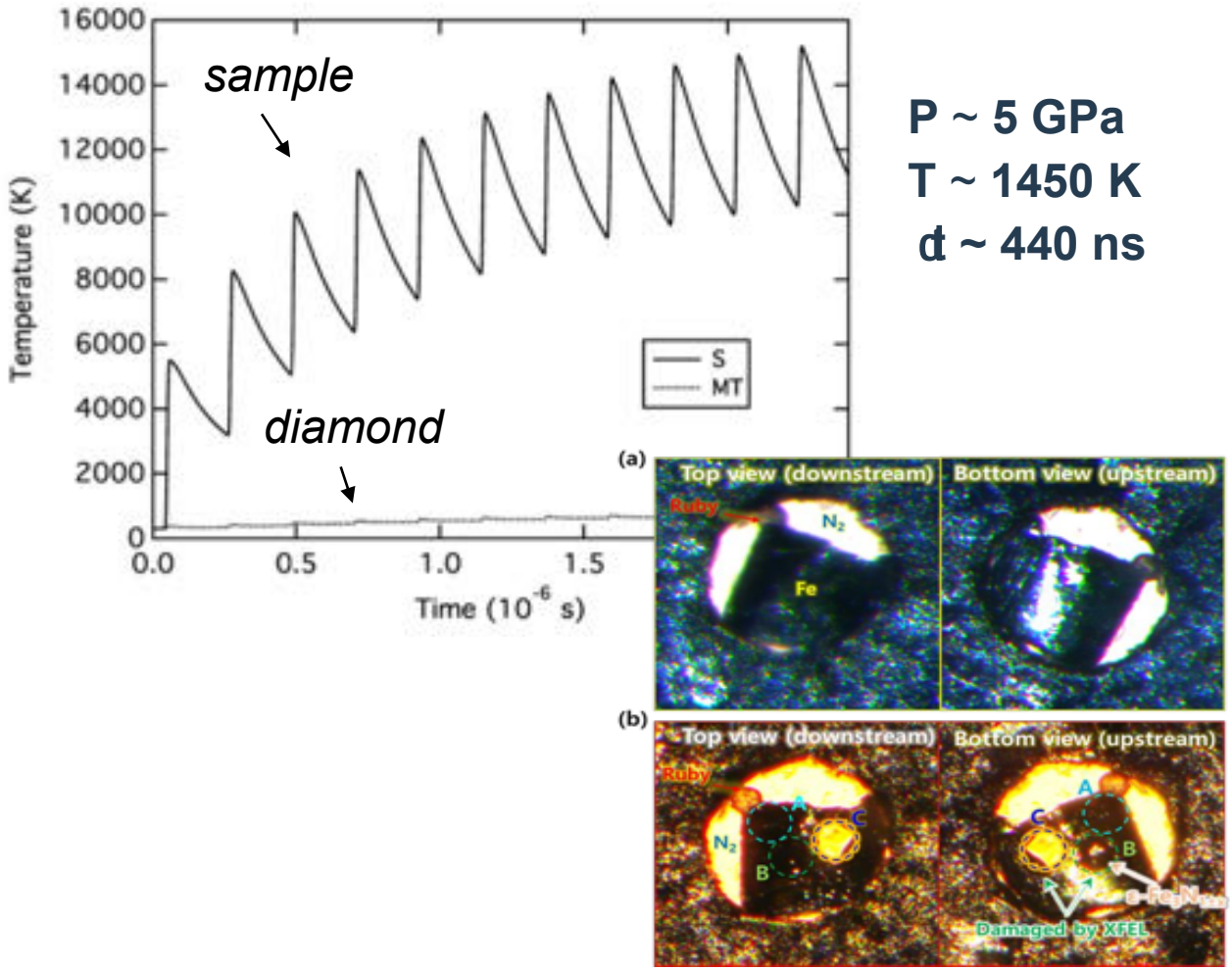




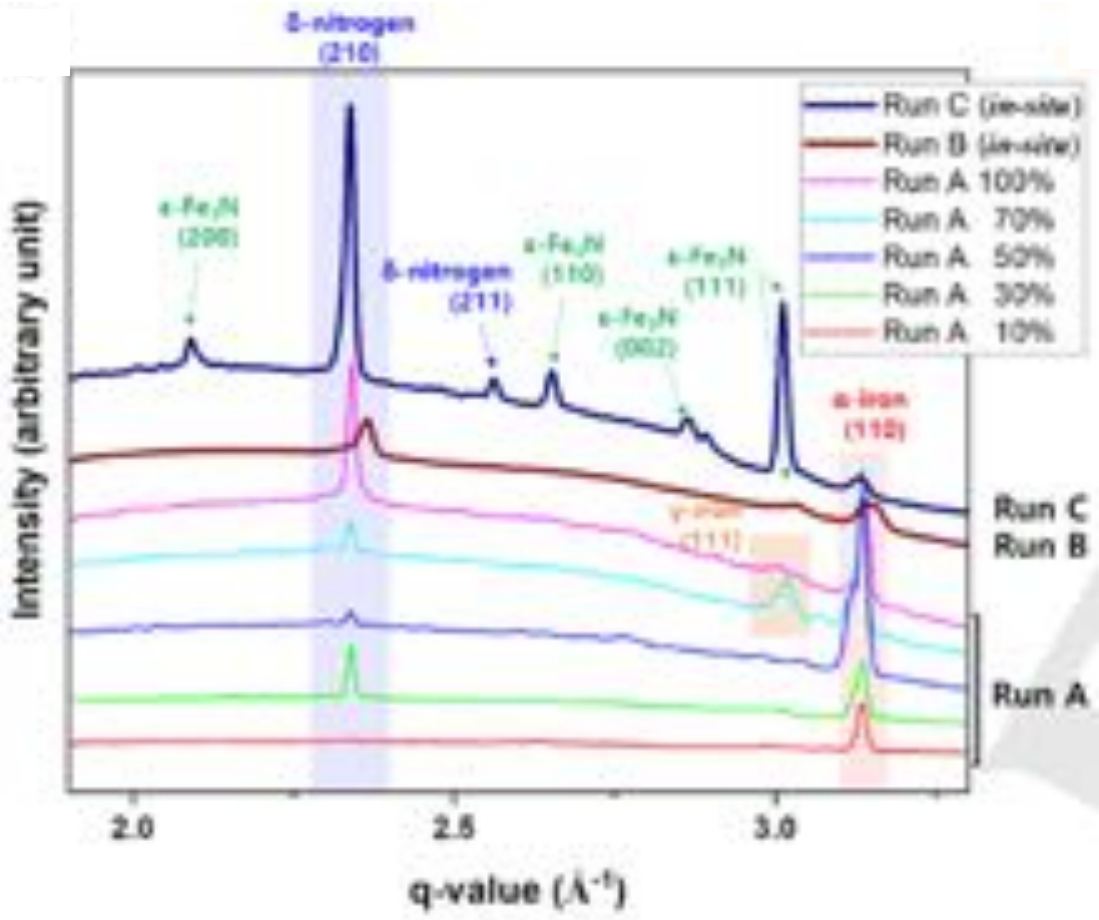


Meza-Galvez et al., *J. App. Phys.*, 2020

Synthesis of -Iron Nitride -$Fe_3N_{1.33}$ at High P and T



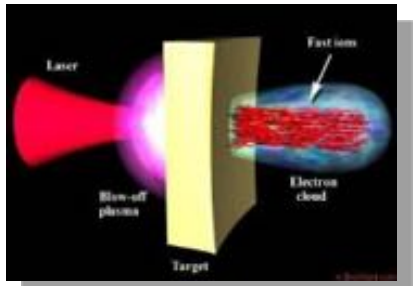
P ~ 5 GPa
T ~ 1450 K
ɗt ~ 440 ns



Hwang, H. et al. 2020 JPCL

First synchronized XFEL and RELAX shots on target

- Develop a predictive understanding of intense laser-matter interactions and relativistic solid density plasma physics
- New physics opportunities e.g., probing structure of QED Vacuum in strong external fields



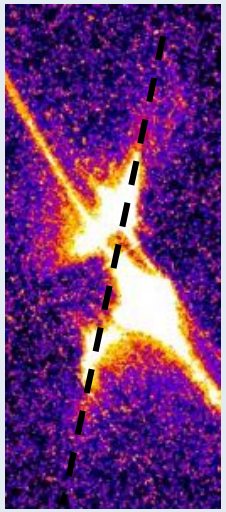
Challenges of ultra-relativist short pulse laser:

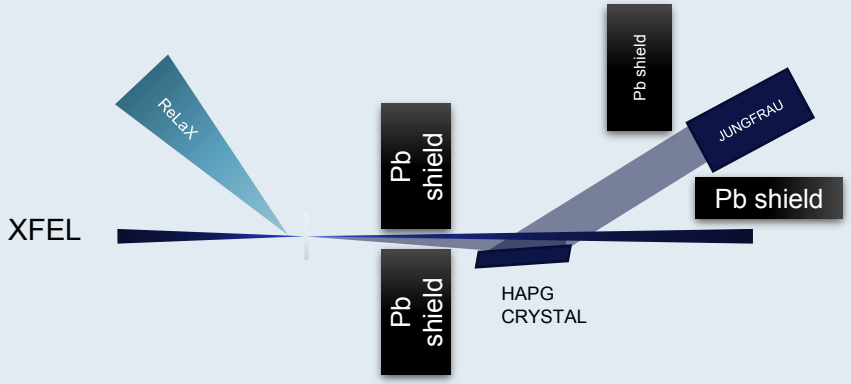
- Relativistic electron generation (~MeV).
- High energy bremsstrahlung generation (~MeV).

August 2020

XFEL : 8.15 keV, 2 mJ
ReLaX : 3 J, 30 fs. ~10^{20} W/cm^2

X-Ray 750fs after RELAX
W wire, Φ = 15 µm
SAXS signal





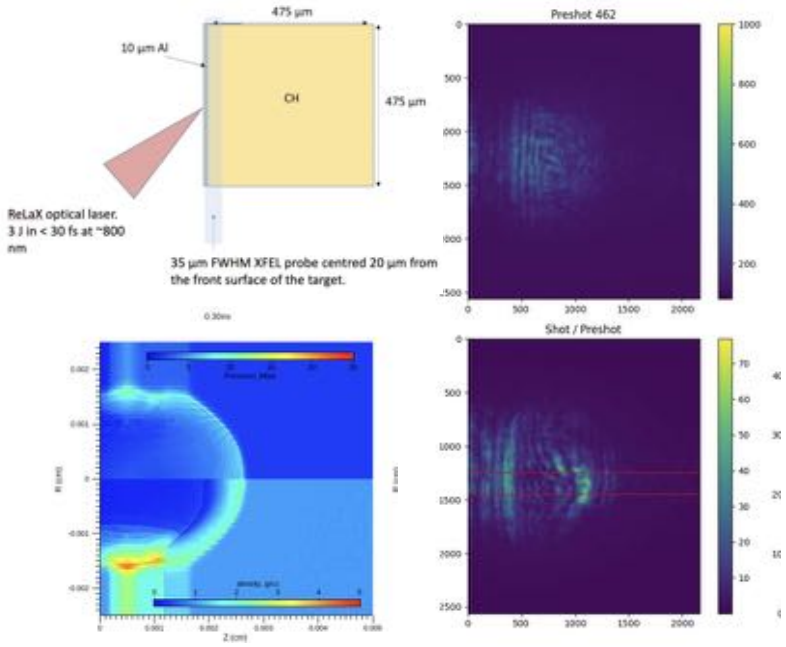
Alejandro L. Garcia

Smid et al. Rev. Sci. Instrum. 91, 123501 (2020)

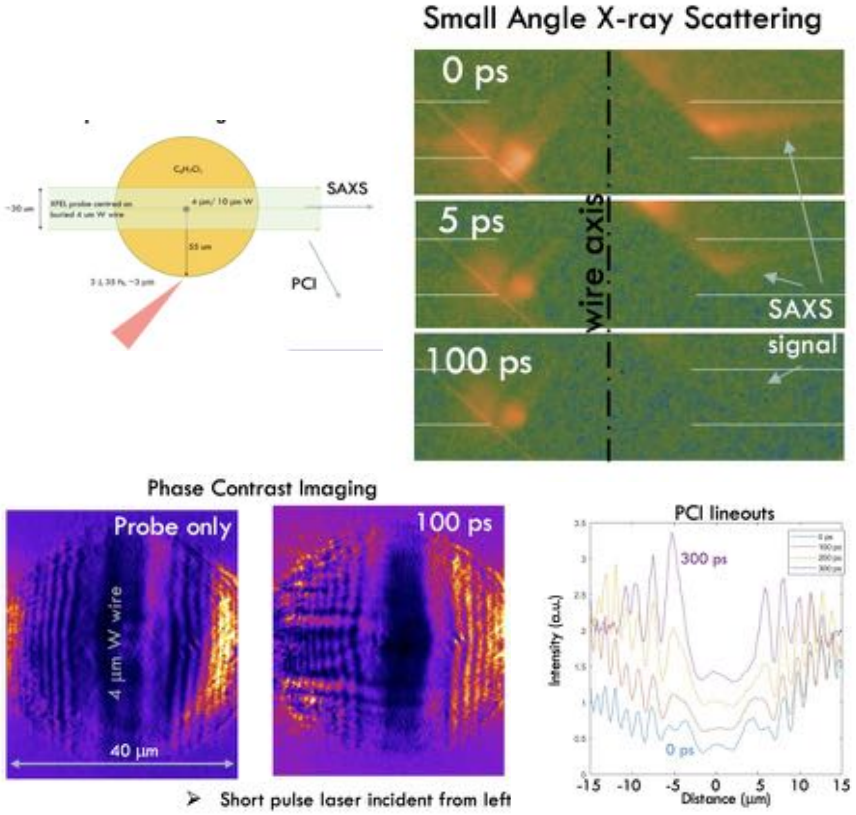
HED & HIBEF

First User experiments with RELAX

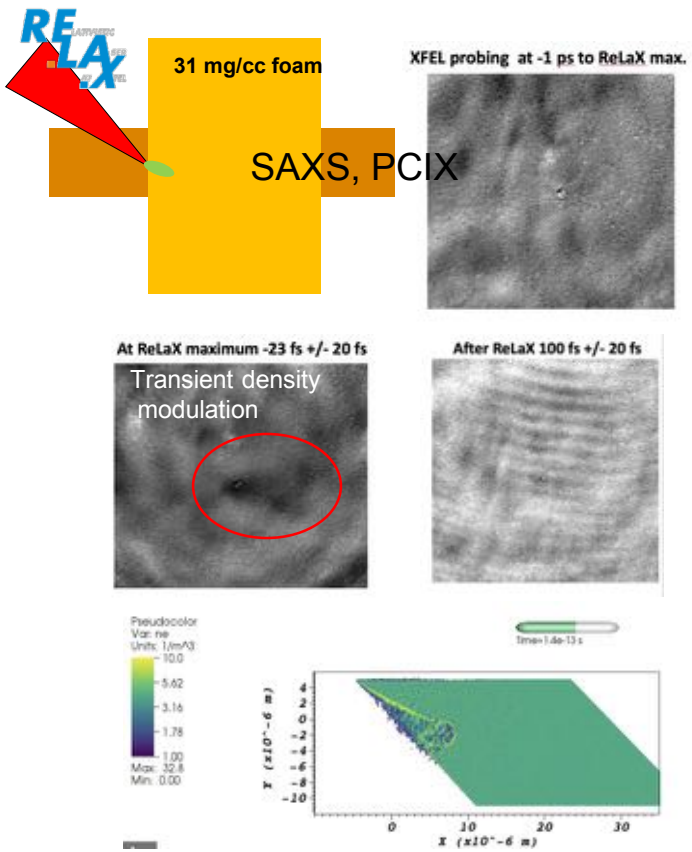
Shock wave propagation in polymers



Metal wires embedded in polymer



Relativistic transparency from foam targets



HiBEF European XFEL

HED High-Energy Density science

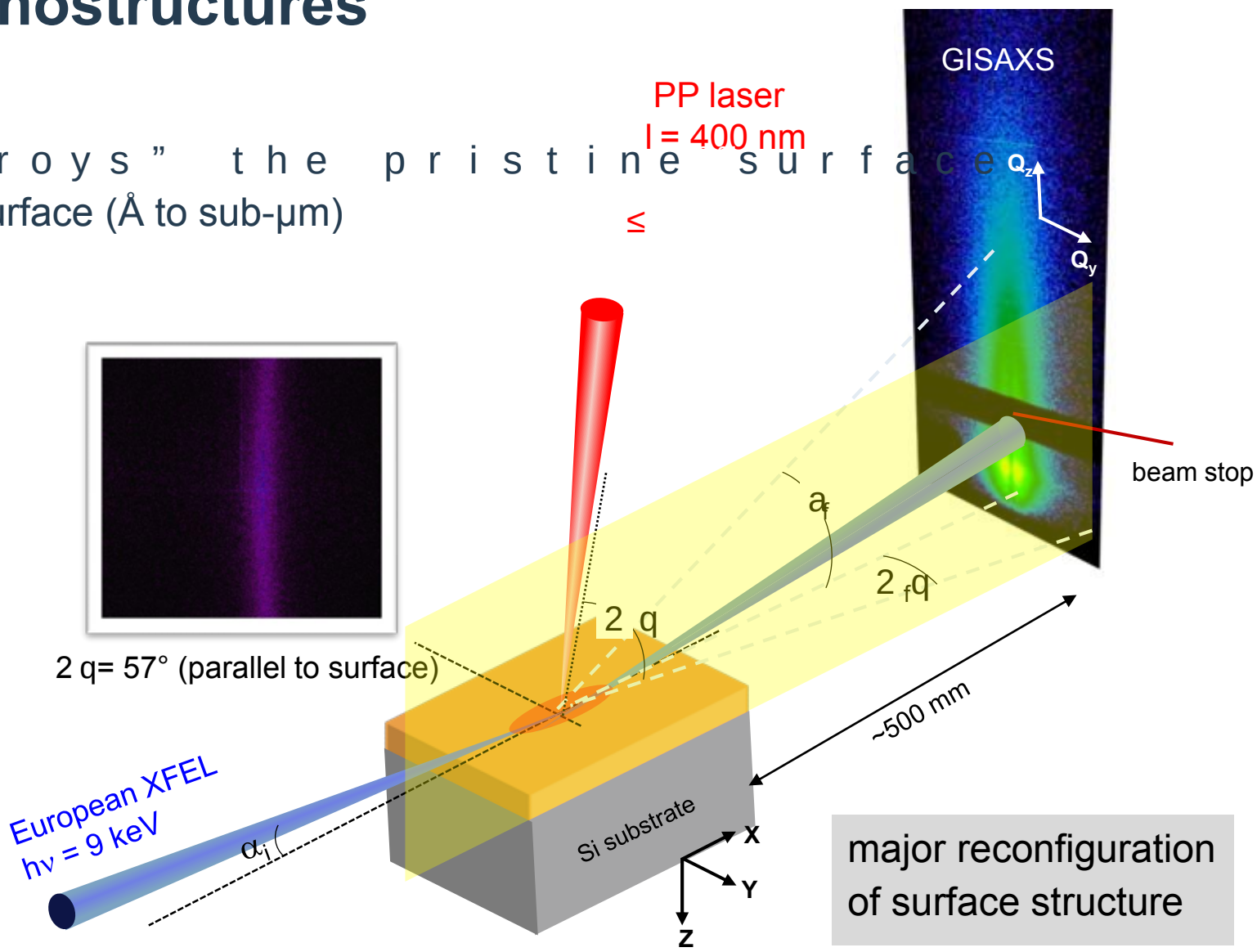
Surface dynamics and nanostructures

- Preparation of TW experiments
- Mimic how pre-pulse "destroys" the pristine surface
  → in situ visualization of surface&subsurface (Å to sub-µm)
  with fs –ps precision

10 100 nm depth from the surface

~fs	1. Laser is absorbed by electrons
fs –ps	2. Phase transition, plasma creation
> ps	3. Thermalization with lattice and ions
ps –ns	4. Surface ablation, expansion
ns - > µs	5. Re-solidification

PI J-P. Schwinkendorf
MP: M Nakatsutsumi
LC: M. Makita
with main contributions from U. Siegen, SLAC



major reconfiguration of surface structure

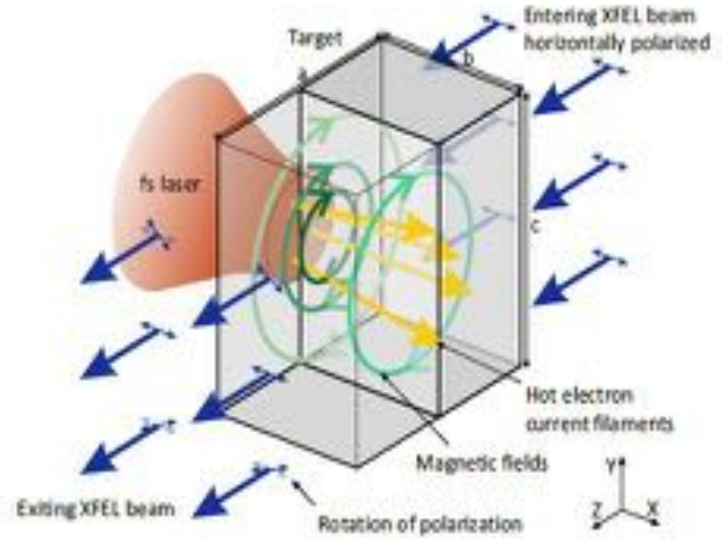
Courtesy M Nakatsutsumi

Outline

- Introduction to X-ray Free Electron Lasers
- The European XFEL and first scientific results
- Status of the High Energy Density Instrument
- Outlook

Goals for the upcoming years at HED

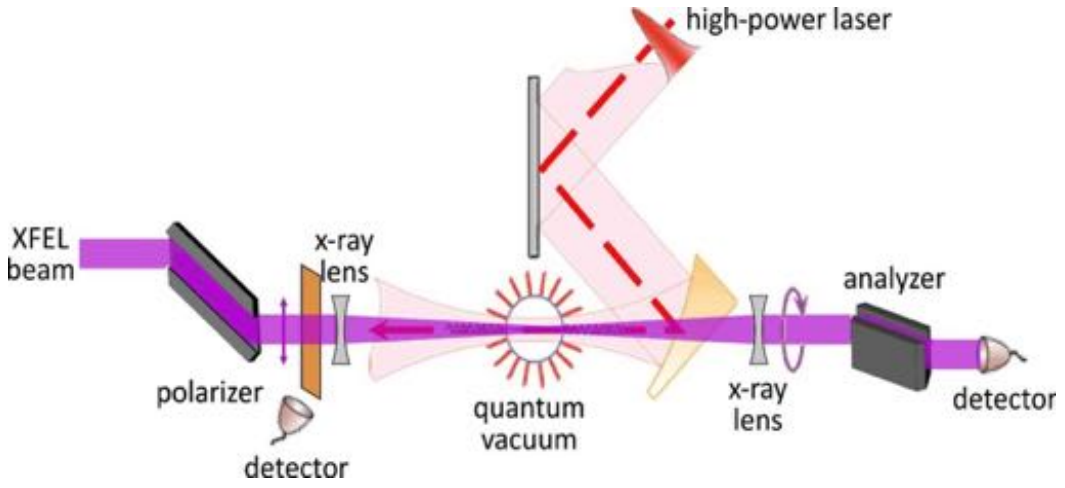
Measurement of **magnetic fields** in solid-density plasma via Faraday rotation



rotation of ~0.1 mrad and fields of ~10^3 T expected

LG. Huang, *et al.*, Phys. of Plasmas 24 (2017)
T. Wang, *et al.*, Phys. of Plasmas 26 (2019)

Detection of vacuum birefringence induced by a strong EM field as predicted by QED



ellipticity of 10^{-13}… 1 10^{-2} expected @ 300 TW

T. Heinzl, *et al.*, Opt. Comm. 267 (2006)
F. Karbstein, *et al.*, Phys. Rev. D 92 (2015)
H.-P. Schlenvoigt, *et al.*, Phys. Scrip. 91 (2016)

Widening and diversifying our User Community

- Increase diversity (geographical and scientific) in usage of facility
  - **Offer standard (user friendly) configurations**
  - **Focus on training/support for new users**
- Promote/encourage scientific collaborations with
  - **EuXFEL staff (shared PhD students)**
  - **Super Users (Community proposals)**
- New access schemes
  - **Long Term Proposals**
  - **Screening**

A look into the future..

- EuXFEL is still a "young" facility
- Hard X-rays coupled to MHz repetition rate opening new perspectives
- Much of its potential still to be exploited
  - Instrument completion
  - Non-linear phenomena, wavemixing, etc..
  - Coupling to ultrafast sources: XUV to MIR, TH
  - Special modes: self-seeding, 2-color, fs pulse, ...
  - Harder X-rays

Workshops in 2021-2022

- Cavity-based X-ray FEL (24-26 March 2021)
- Superconducting Undulators for Advanced Light Sources (19-21 April 2021)
- Attosecond to Few-Femtosecond Ultrafast Science at Future FELs (28-30 June 2021)
- Non-linear science & relaxation phenomena
- **Scientific opportunities with hard XFEL radiation (Spring 2022)**
- Femto-chemistry & catalysis (Spring 2022)
- Structural biology

Thank you for your attention !