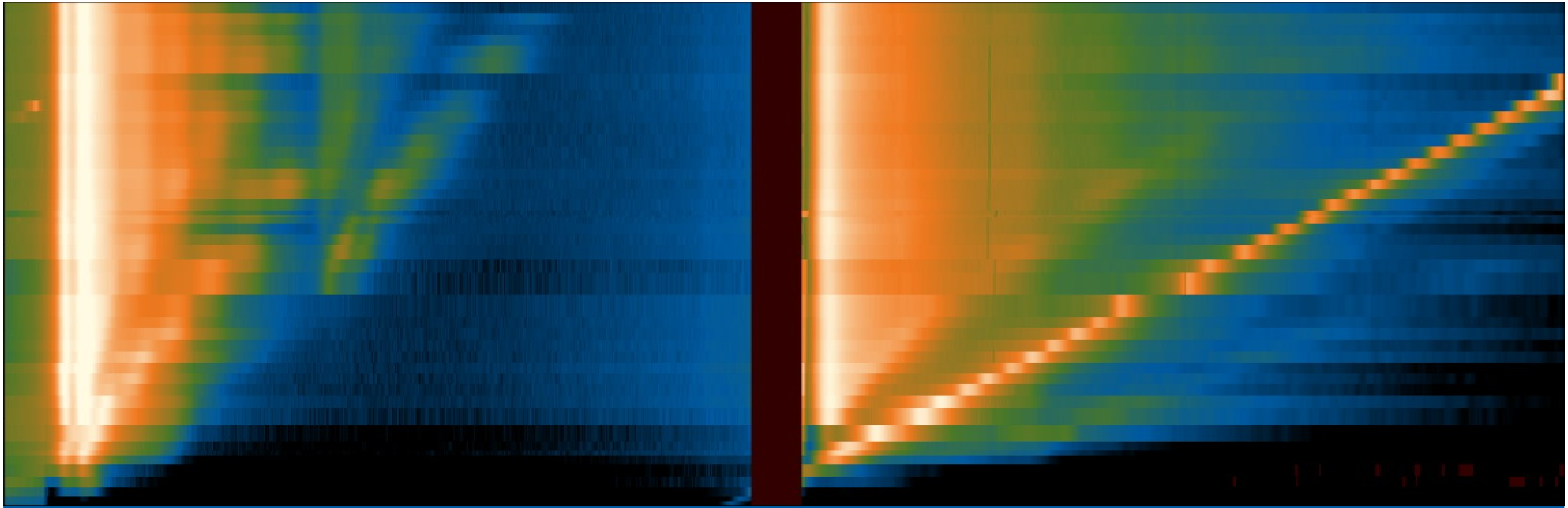


Spectroscopy of XFEL heated Cu

and x-ray absorption in laser-produced Warm Dense Cu

a pár dalších témat

Michal Šmíd · m.smid@hzdr.de· www.hzdr.de

Outline of the talk

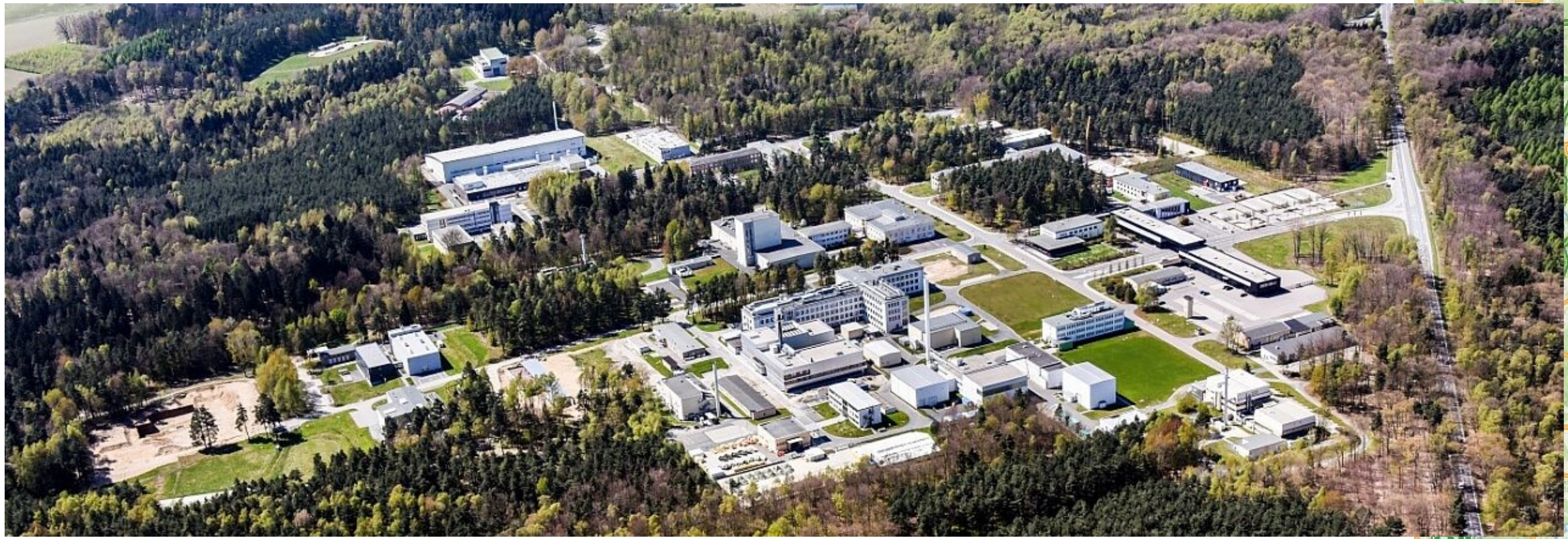
Úvod: HZDR, WDM, atomové přechody

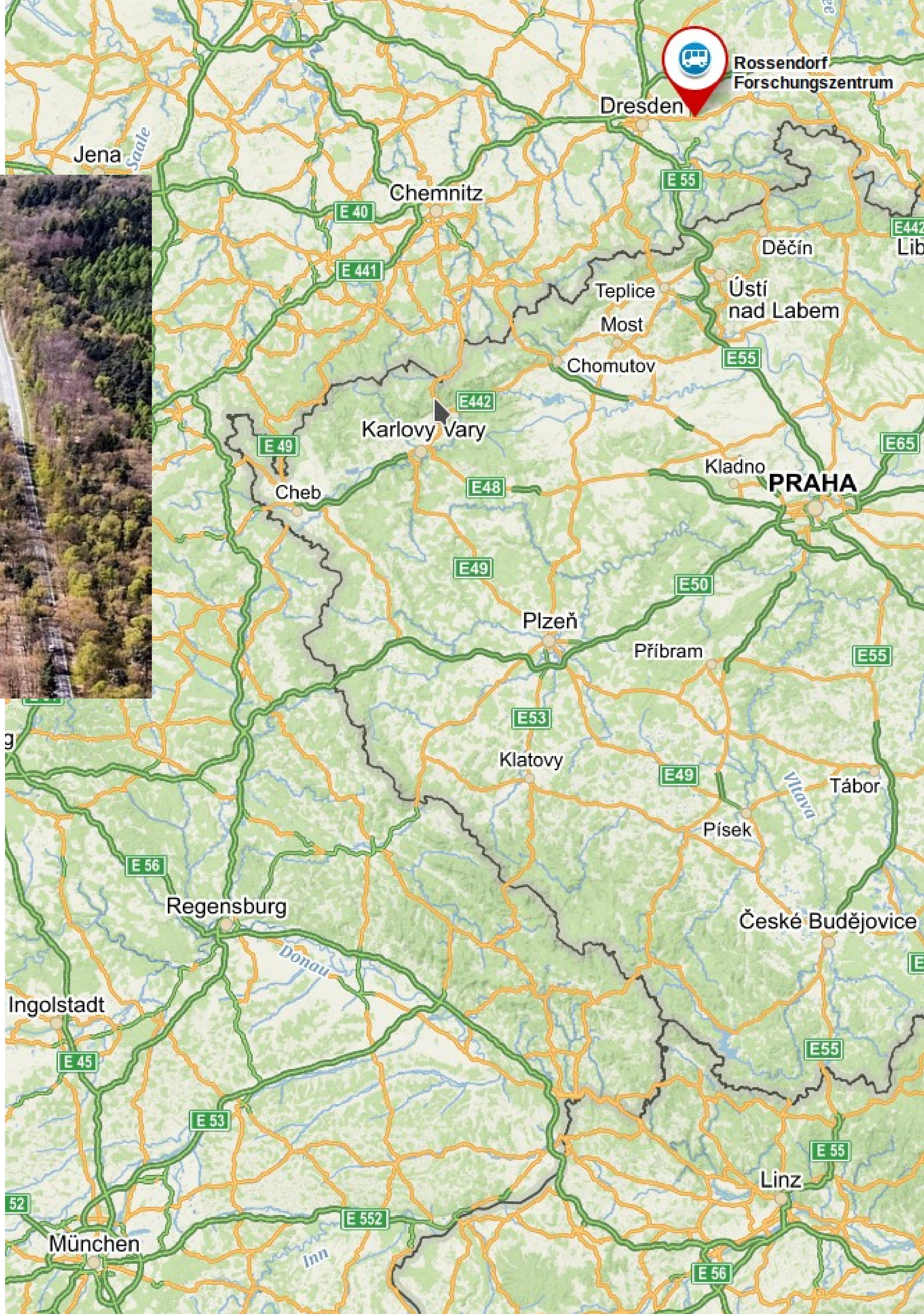
XFEL-only experiment

Draco experiment

něco inženýřského: HAPG mirror

HZDR





1400 zaměstnanců, z toho as i 670 vědců

180 hektarů

10 ústavů

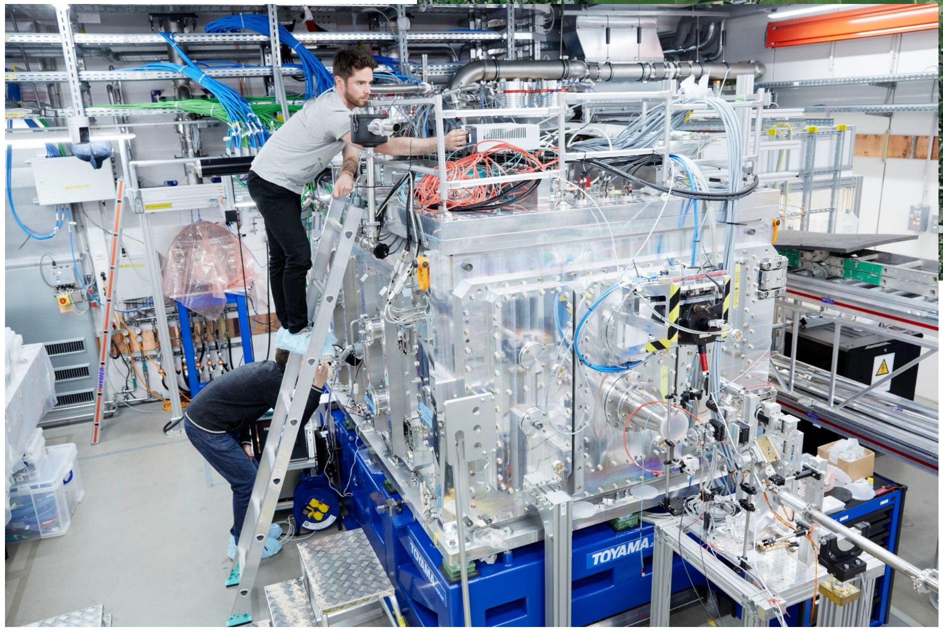
roční rozpočet 150M€

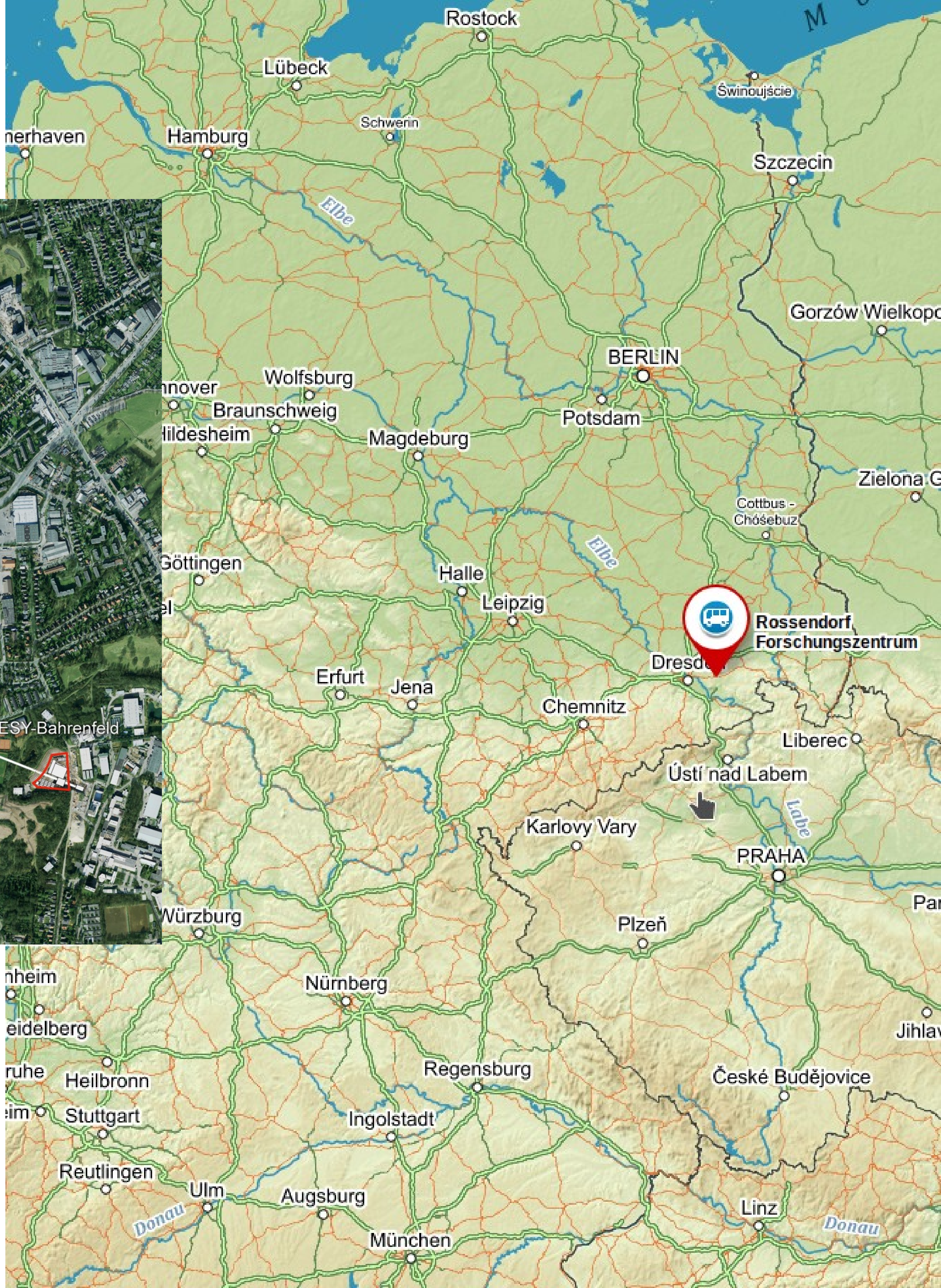
založeno 1956, největší výzkumný reaktor DDR

<u>Ústav radiační fyziky:</u>

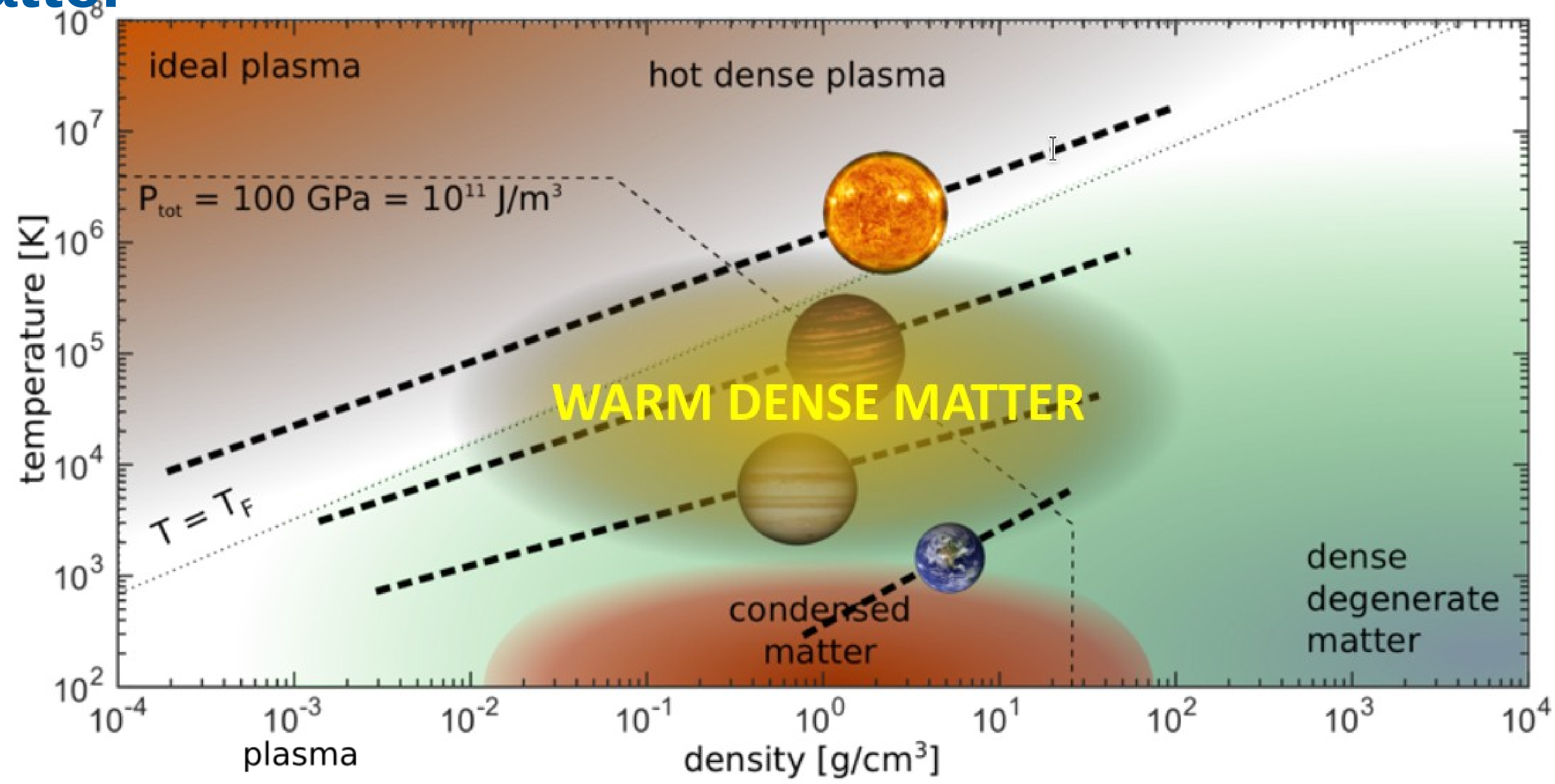
*Basic research in **accelerator**, nuclear, hadron and **laser** physics is this institute's top-priority. The Institute of Radiation Physics is also engaged in new ways of producing radiation and particle beams, and new detectors and measurement techniques for application to **cancer research**, nuclear safety and advanced materials.*

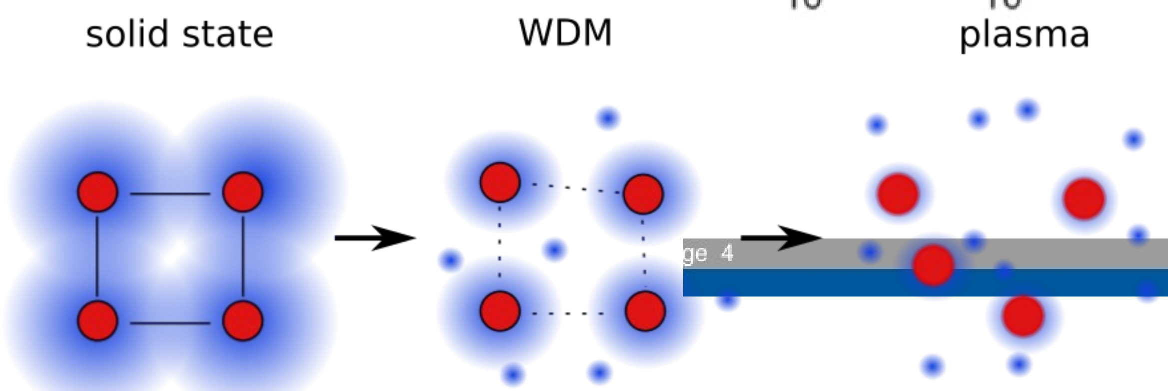
HZDR a XFEL: Hibef





Warm Dense Matter





*R. Neutze et al., Nature (2000)

Warm Dense Matter

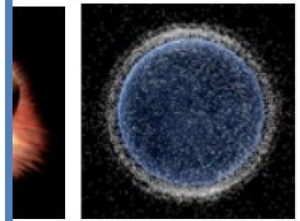
transition regime
solid state ⟺ hot dense plasma

properties:
- 0.1 – 10 time
- temperature
- pressure: ~1
- partially ioni
- partially deg
- strongly coupled ions
- $k_B T \sim \frac{e^2}{4\pi\varepsilon_0}\frac{1}{\langle d\rangle} \sim E_F \sim E_{bond} \sim$ eV

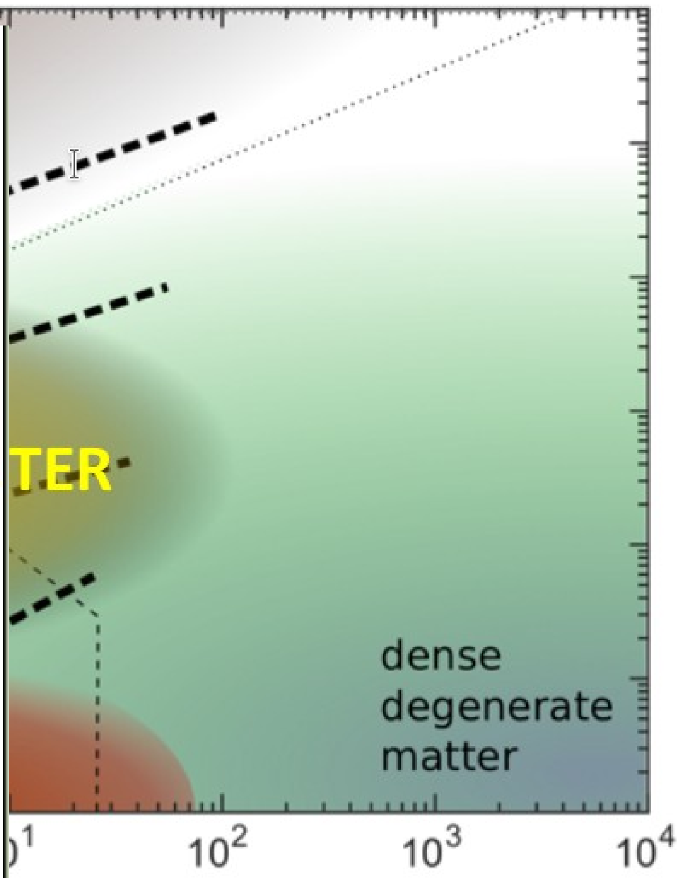
If you can compute it,
it is not warm dense matter.

If you can measure it,
it is not warm dense matter.

Planets / Brown Dwarfs / Stars



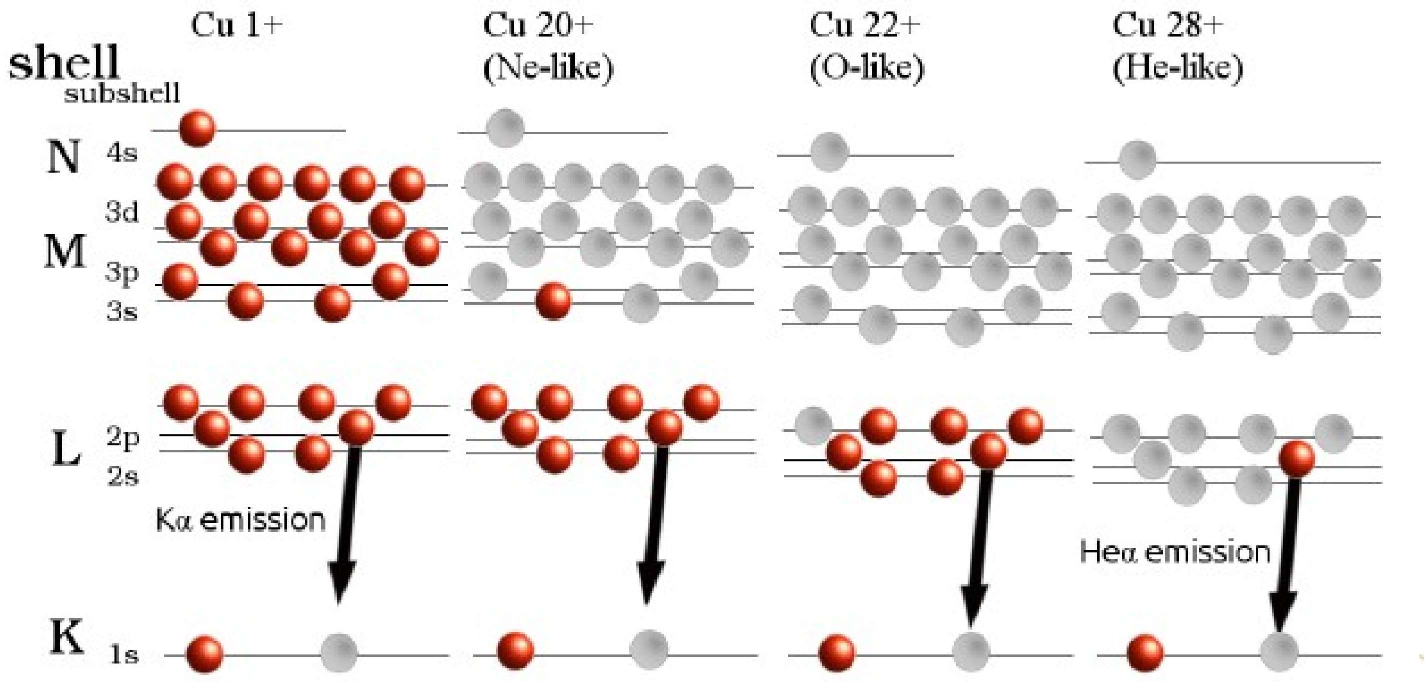
Technology applications



*R. Neutze et al., Nature (2000)

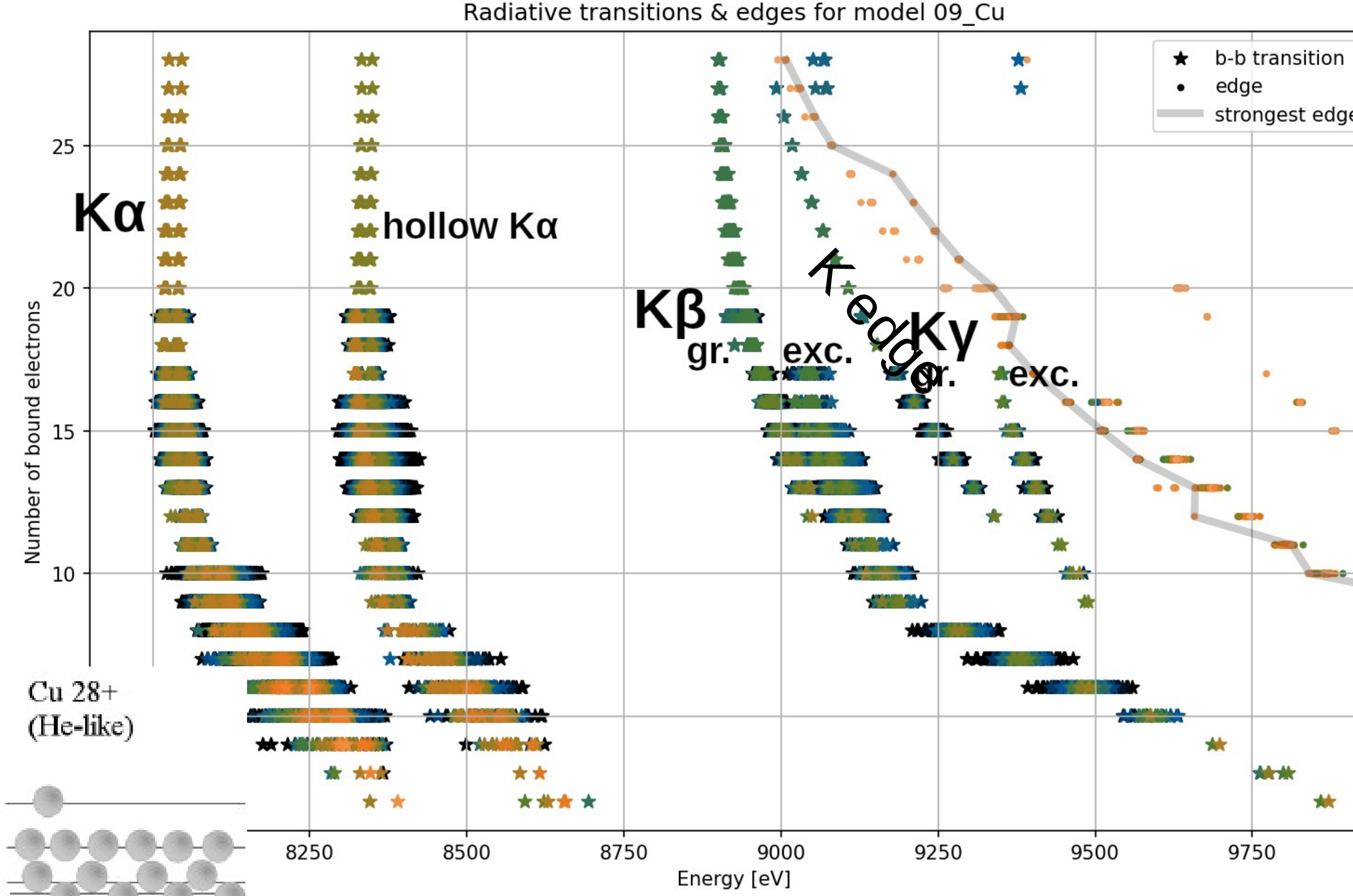
Member of the Helmholtz Association
Dominik Kraus | Institute of Radiation Physics | www.hzdr.de

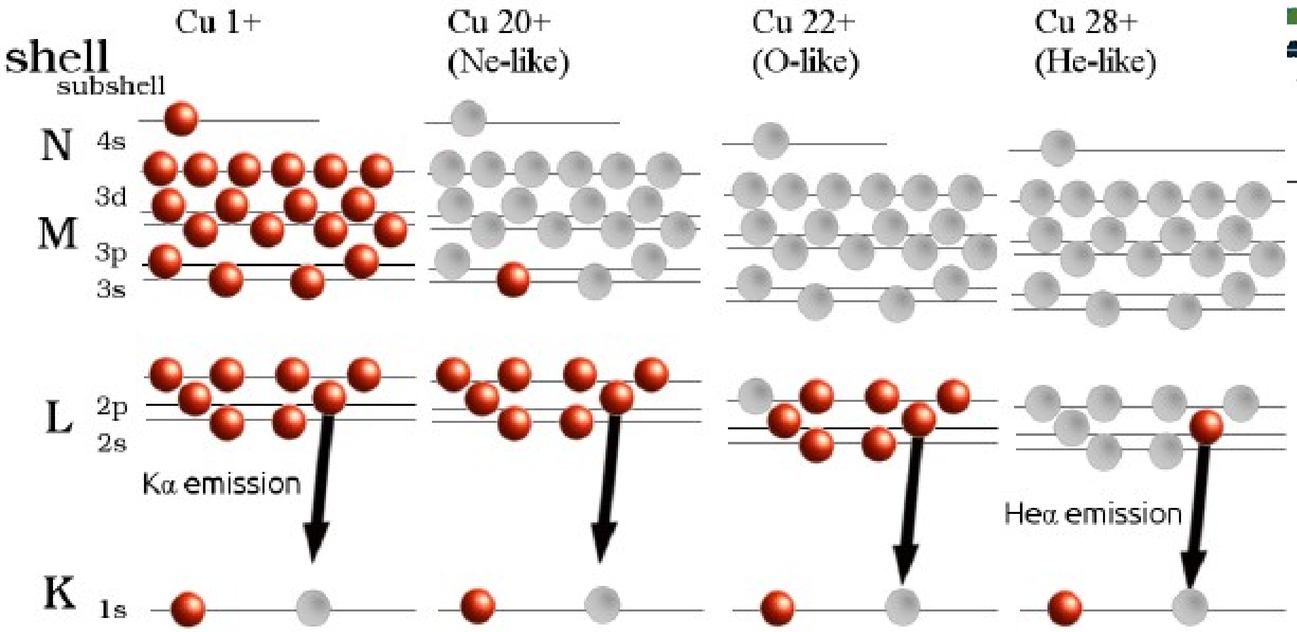
Atomic transitions



Map of transitions

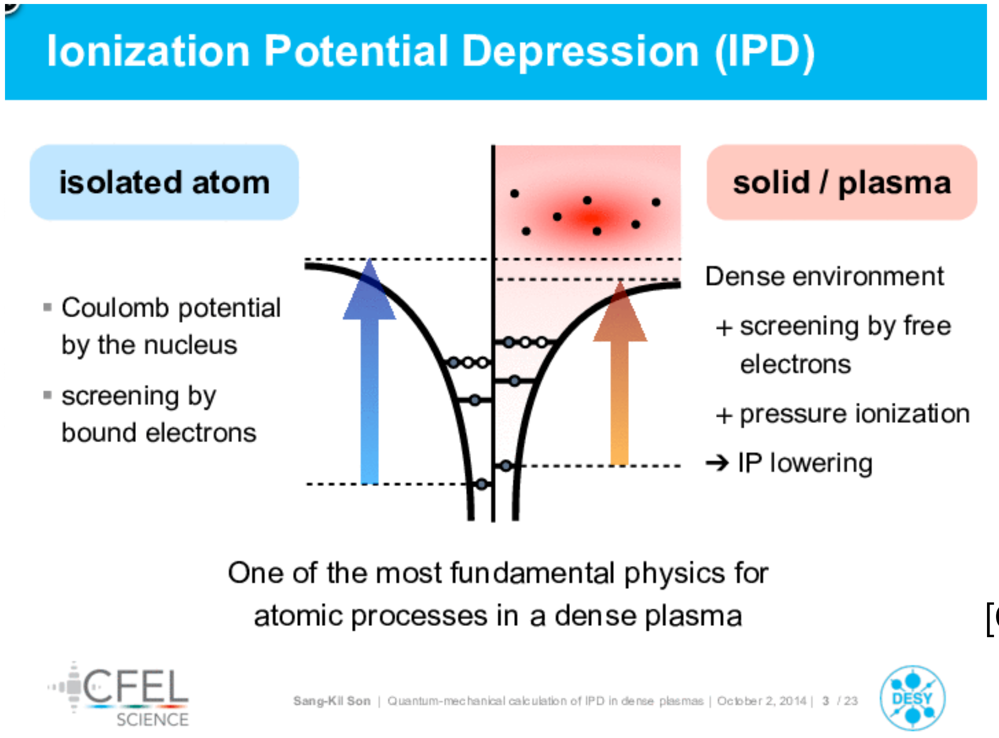
Transitions calculated by the **cFAC** code.





Ionization Potential Depression 1

- In the plasma environment, the outer levels are merged into continuum due to surrounding conditions.
- Shift of the ionization edge.
- The Ecker-Kroll model (1963) predicts higher values compared to mostly used Stuart-Pyatt model (1966).
- Similar experiments on Al and Mg have indicated the measurements are closer to the EK model.
- Extension of this type of measurements on higher charge state was still missing.



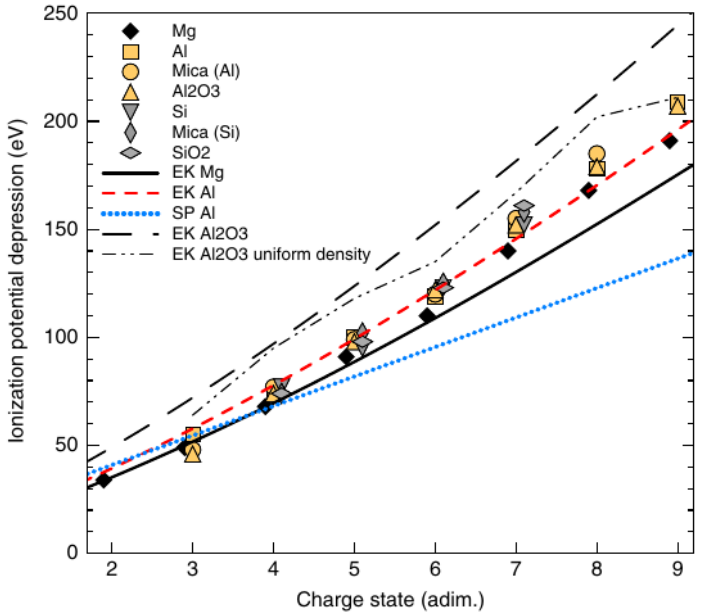


Figure 4 | IPD inferred by the *K*-edge measurements. The reduction in the ionization potential of Mg, Al and Si in the different materials is plotted as a function of the ionic charge state and is compared with the predictions of analytical models (EK and SP—see text), assuming a plasma ionization equal to the charge state. The data sets for each different active material are slightly shifted horizontally for clarity. For the alumina, detailed simulations (see Methods section) have also been performed to determine the reduction in the total (uniform) free-electron density of the material due to the different ionization balance of the oxygen ions and the predictions of the EK model in this case are labelled as 'uniform density'. The experimental resolution in FEL photon energy is 5 eV; thus, the size of the symbols is representative of the uncertainty on the IPD.

[O. Ciricosta et al., Nat Comm 7:11713, 2016.]

XFEL2806: Broad experimental collaboration, Feb 2022

HZDR (Dresden):

K. Falk, L. Gaus, O. Humphries, M. Kozlová, X. Pan, M. Šmíd, R. Štefaníková

IOP ASCR (Prague):

T. Burian, V. Hájková, L. Juha, T. Krupka,

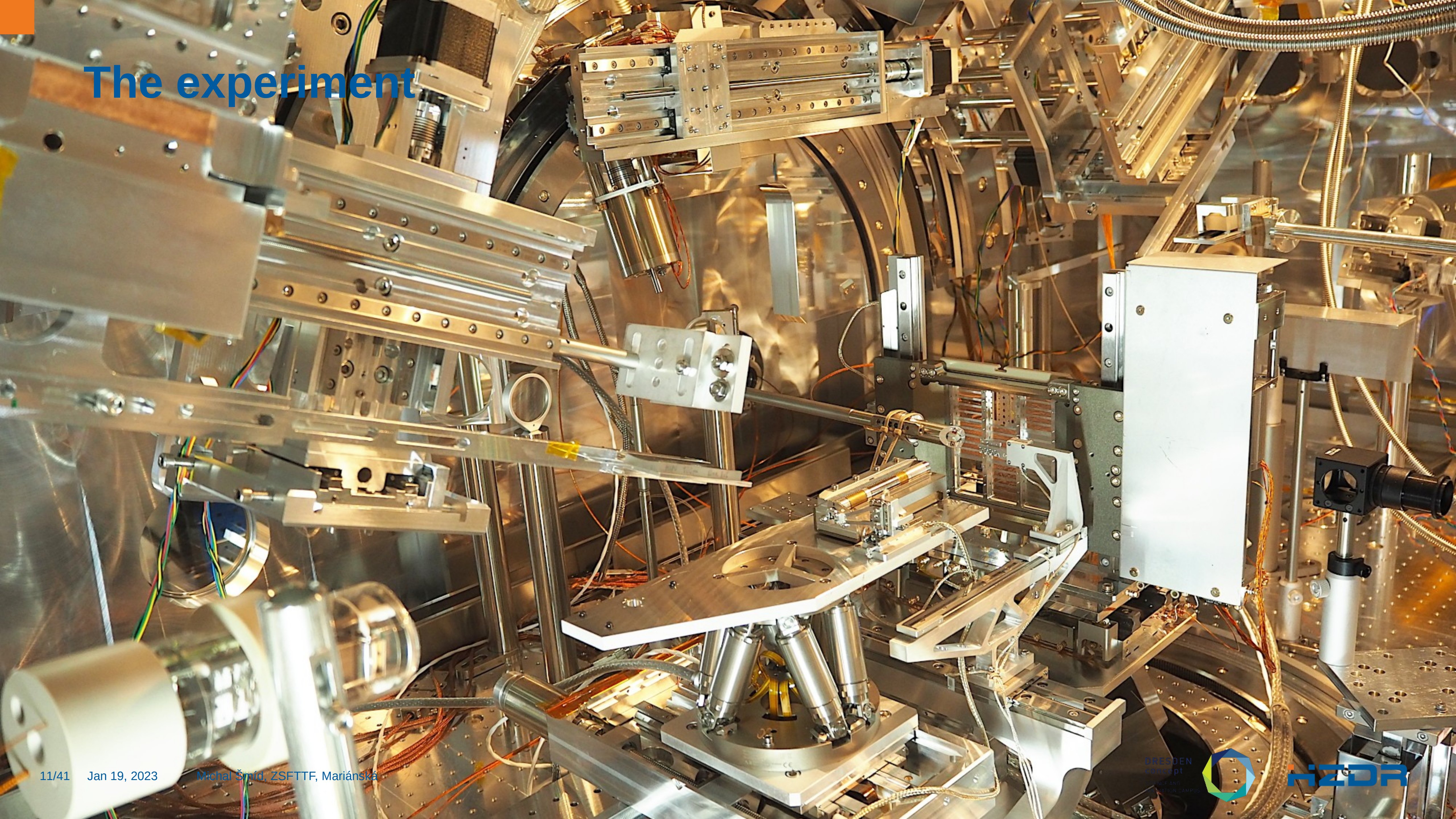
DESY (Hamburg):

W. Wang, A. Schropp

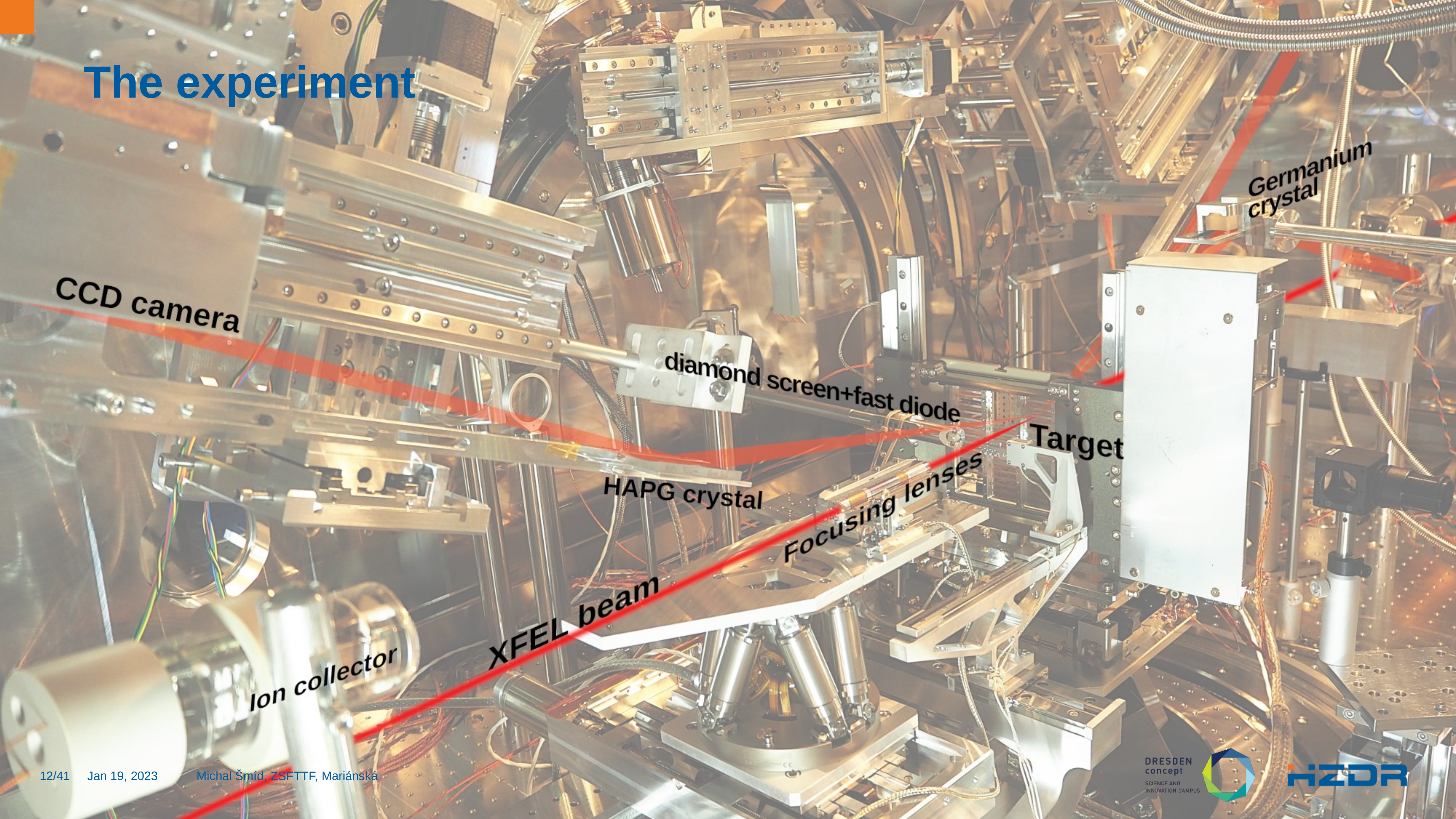
XFEL (Hamburg):

C. Bähtz, V. Bouffetier, E. Bramrink, V. Cerantola, R. Husband, J. Kaa, Z. Konôpková, M. Makita, T. Preston, K. Sukharnikov, L. Wollenweber, S. Wagner, U. Zastrau

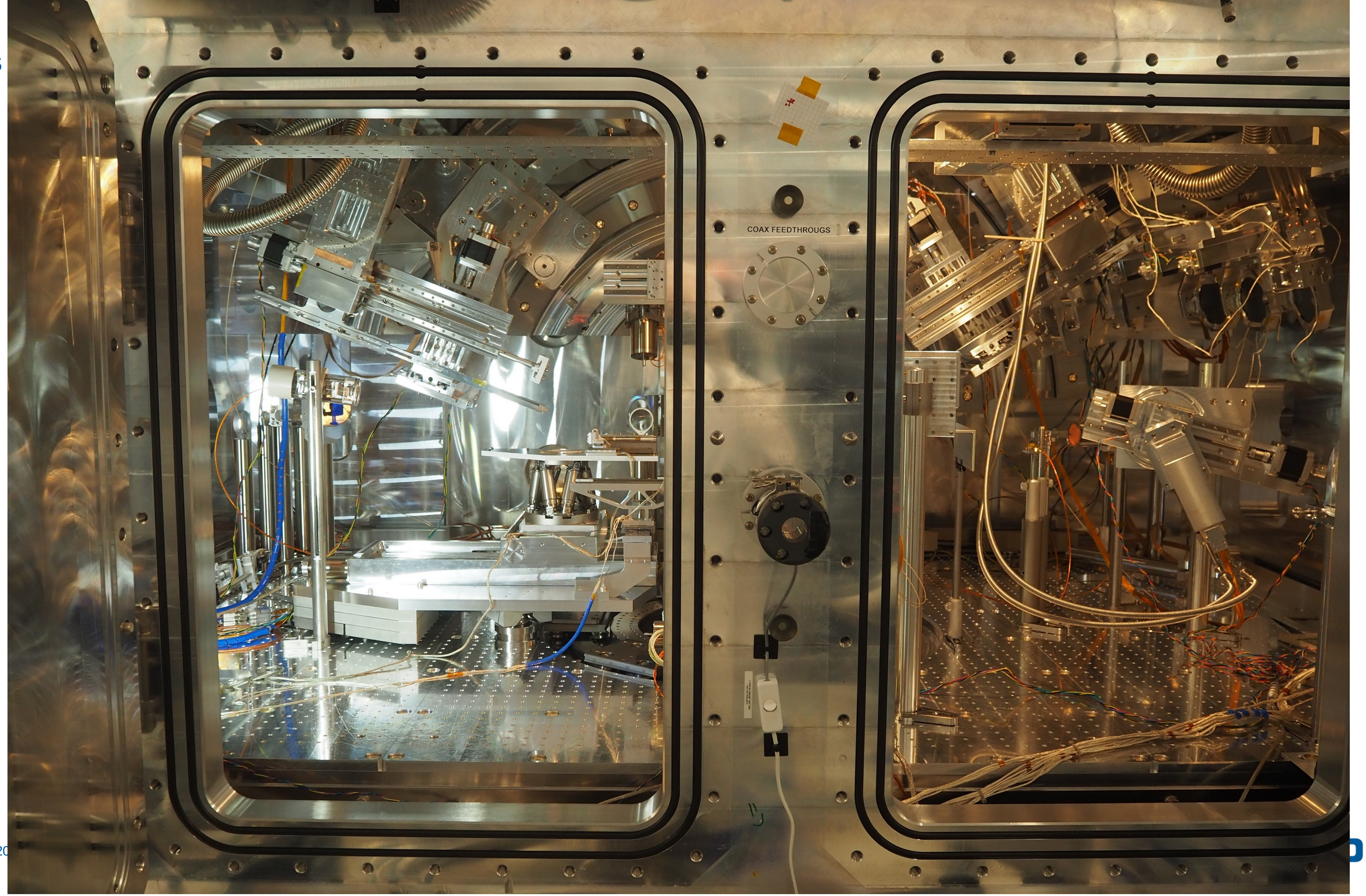
The experiment

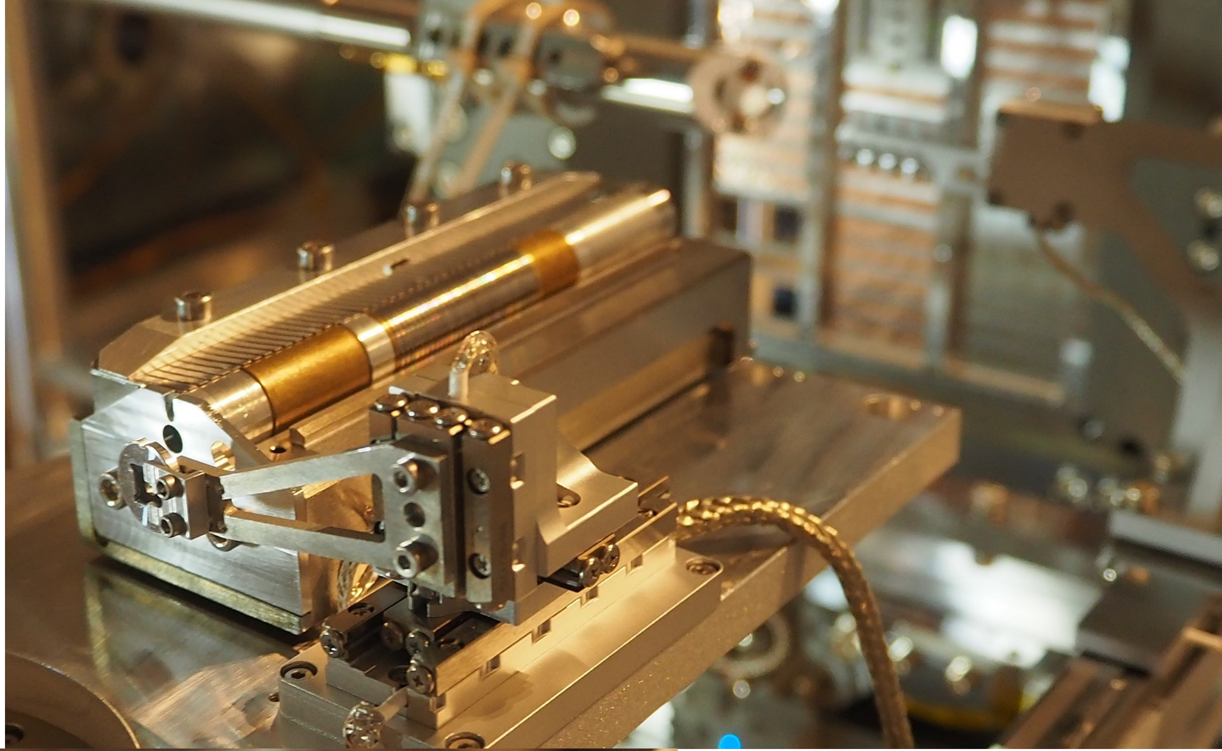


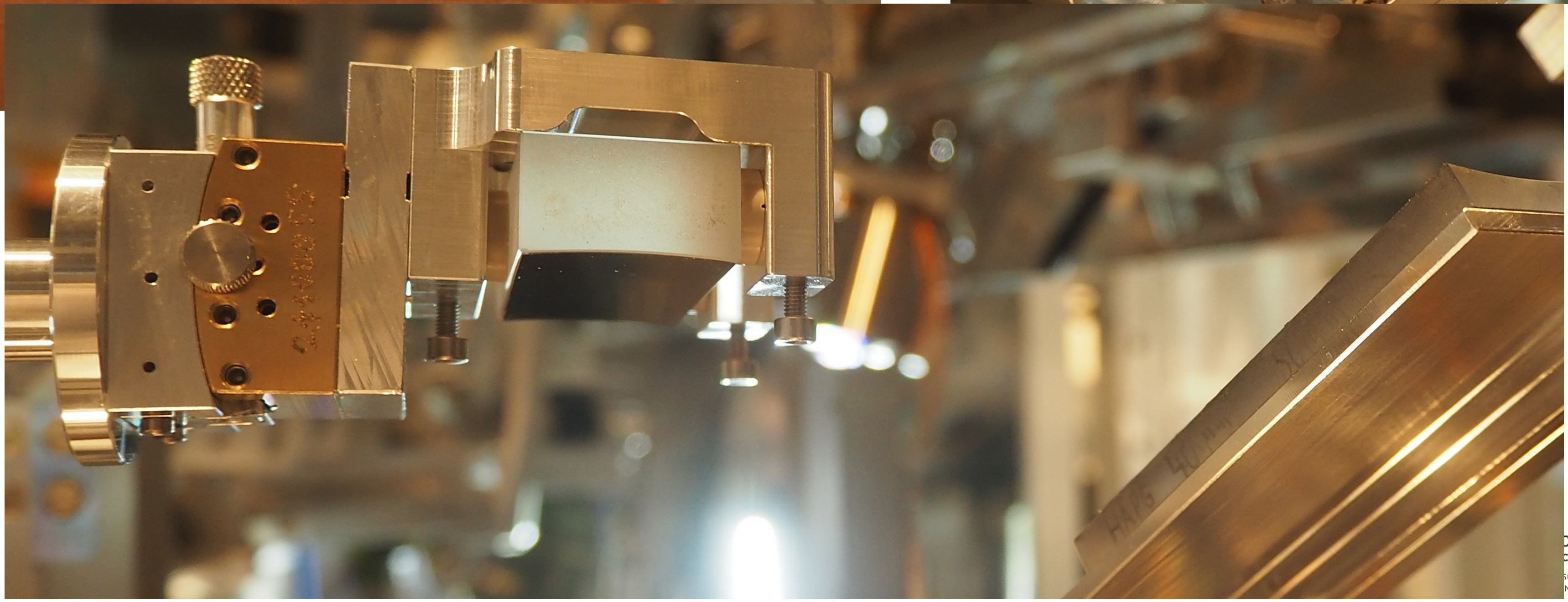
The experiment



Photos



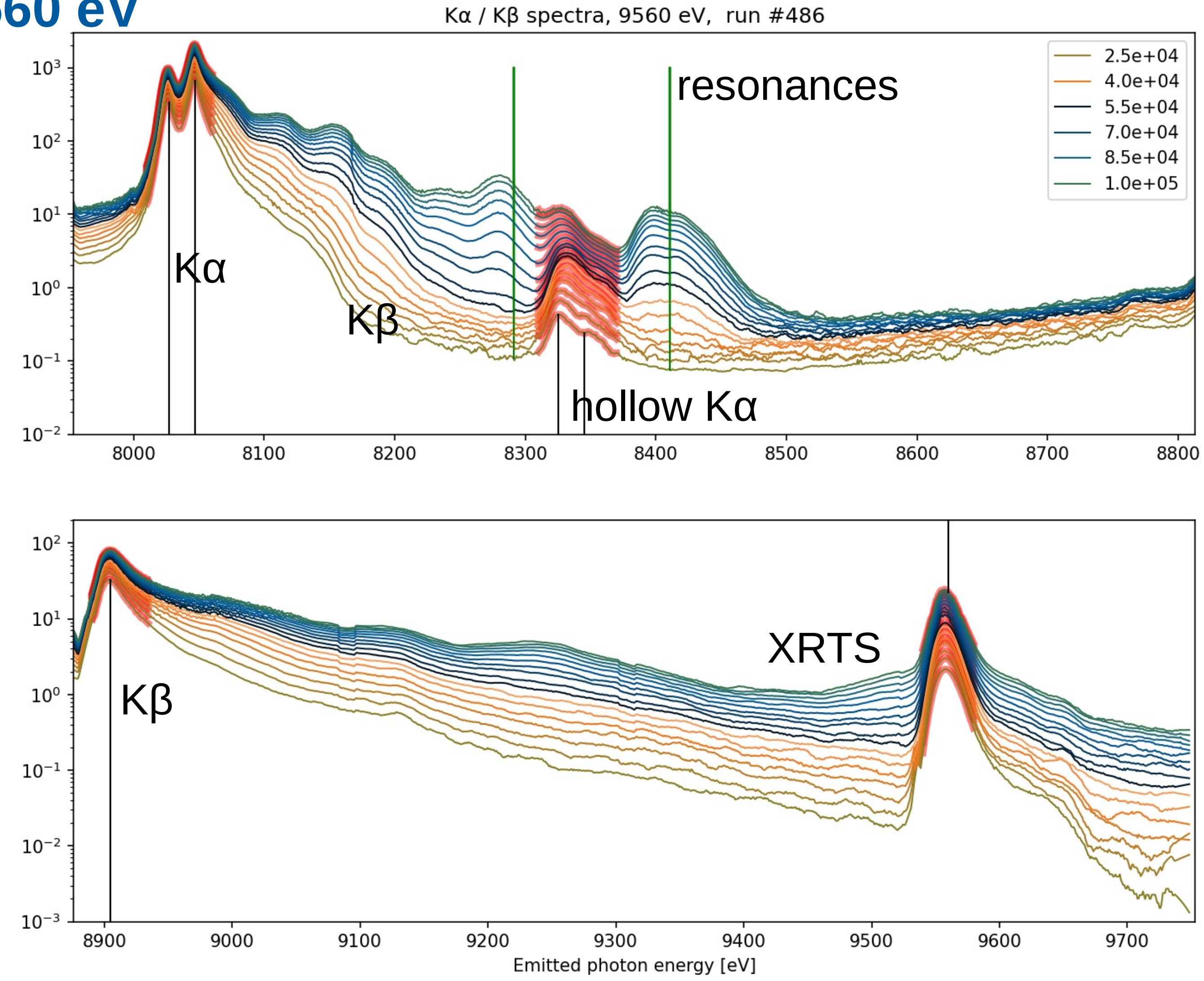


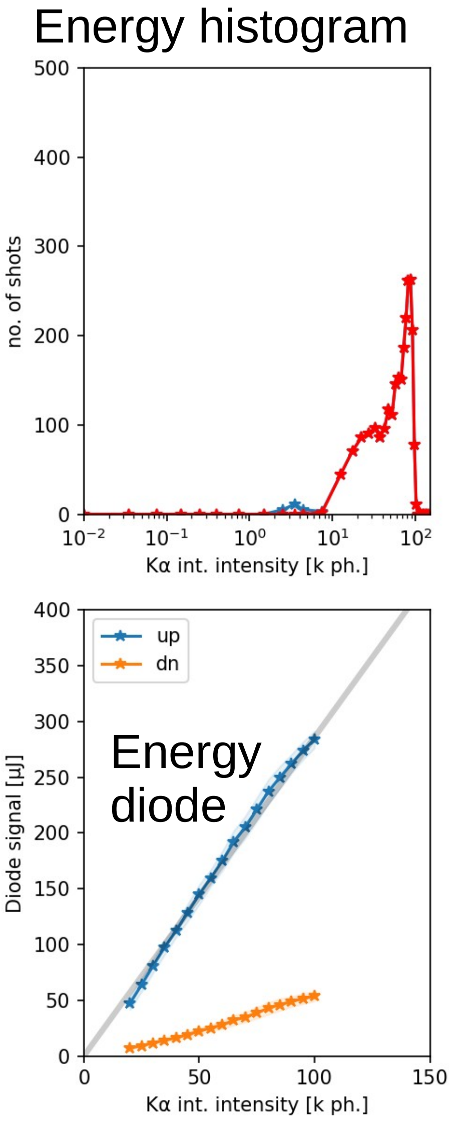


Example of spectra

XFEL photon energy 9560 eV

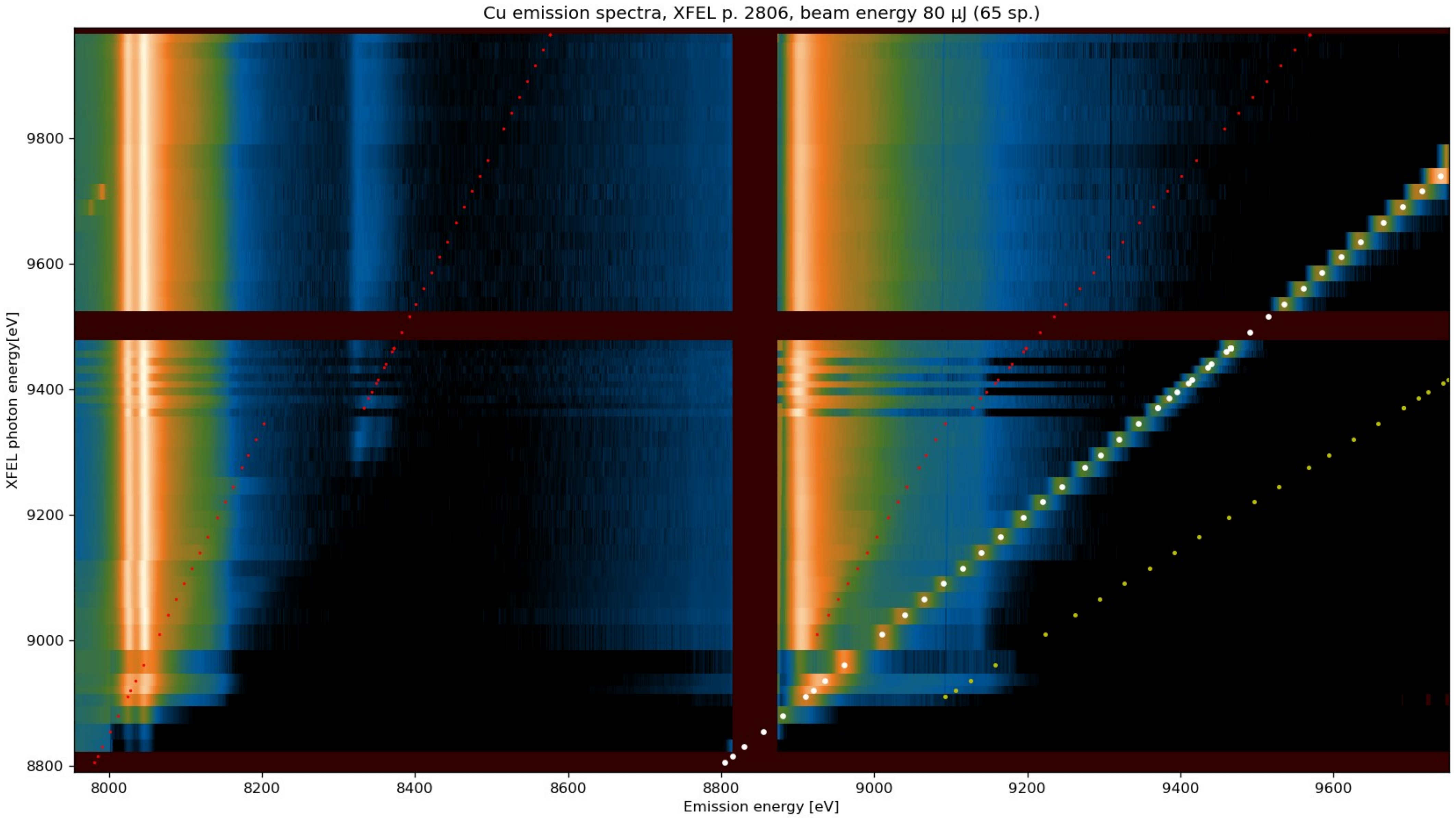
- Different lines correspond to different beam energy on target.
- Overall intensity is linearly proportional to the energy.





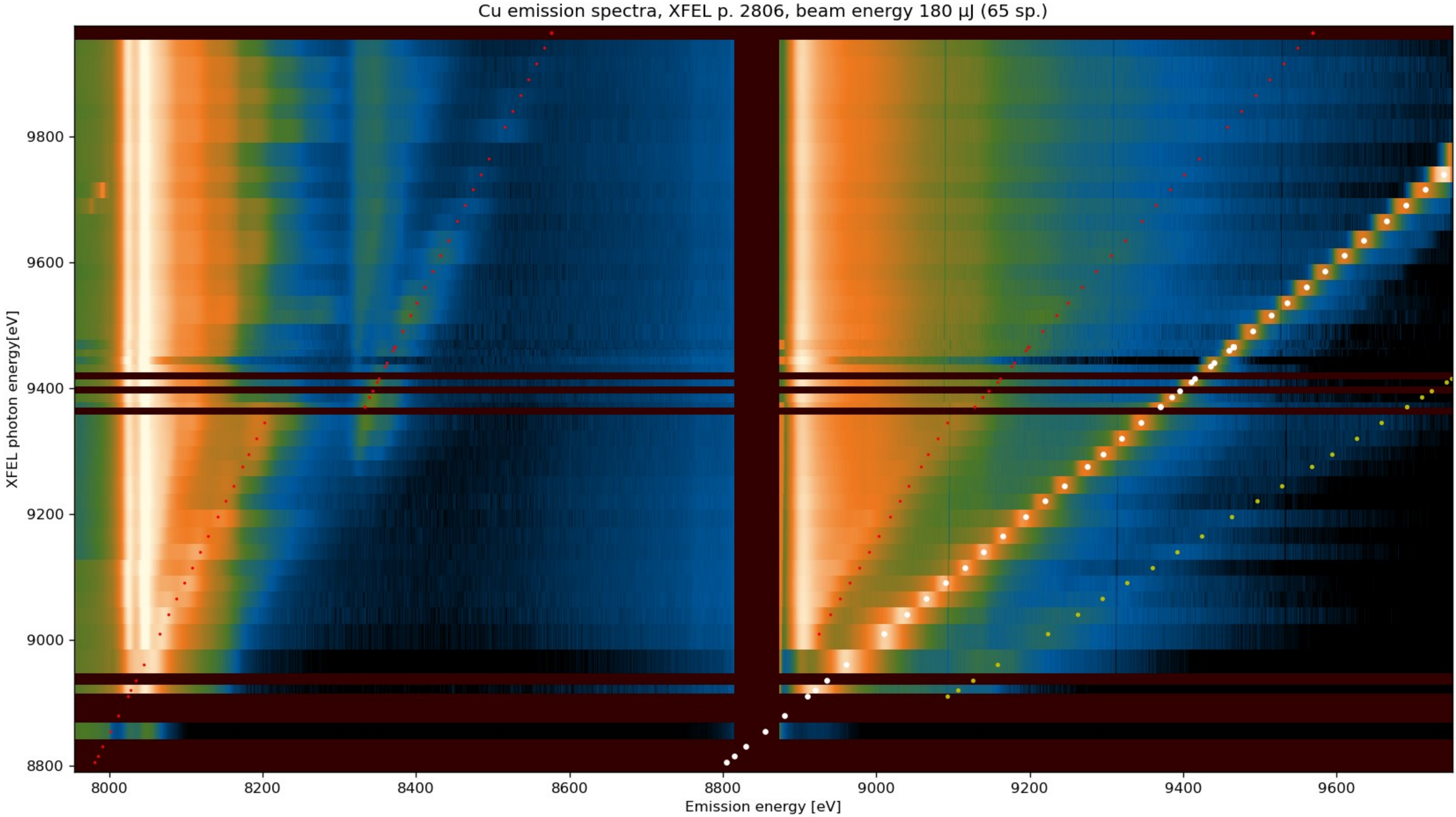
Spectra with 80 µJ on target

- Horizontal lines - various XFEL photon energies.
- White points: XFEL scattering
- Kα and Kβ seen
- Slight blue wings due to ionization
- Hollow ions already present.



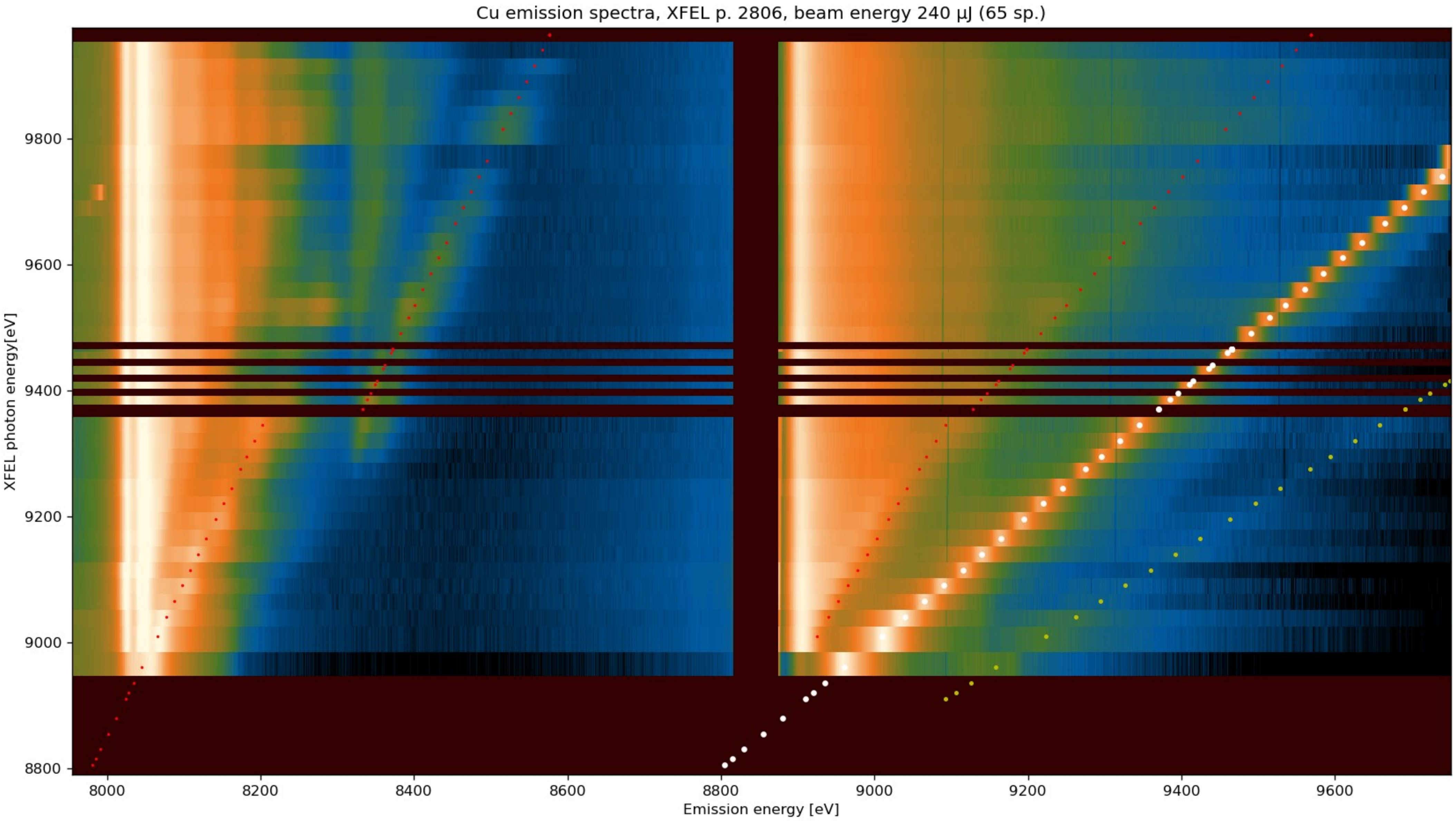
Spectra with 180 μJ on target

- Stronger heating
- Increased ionization



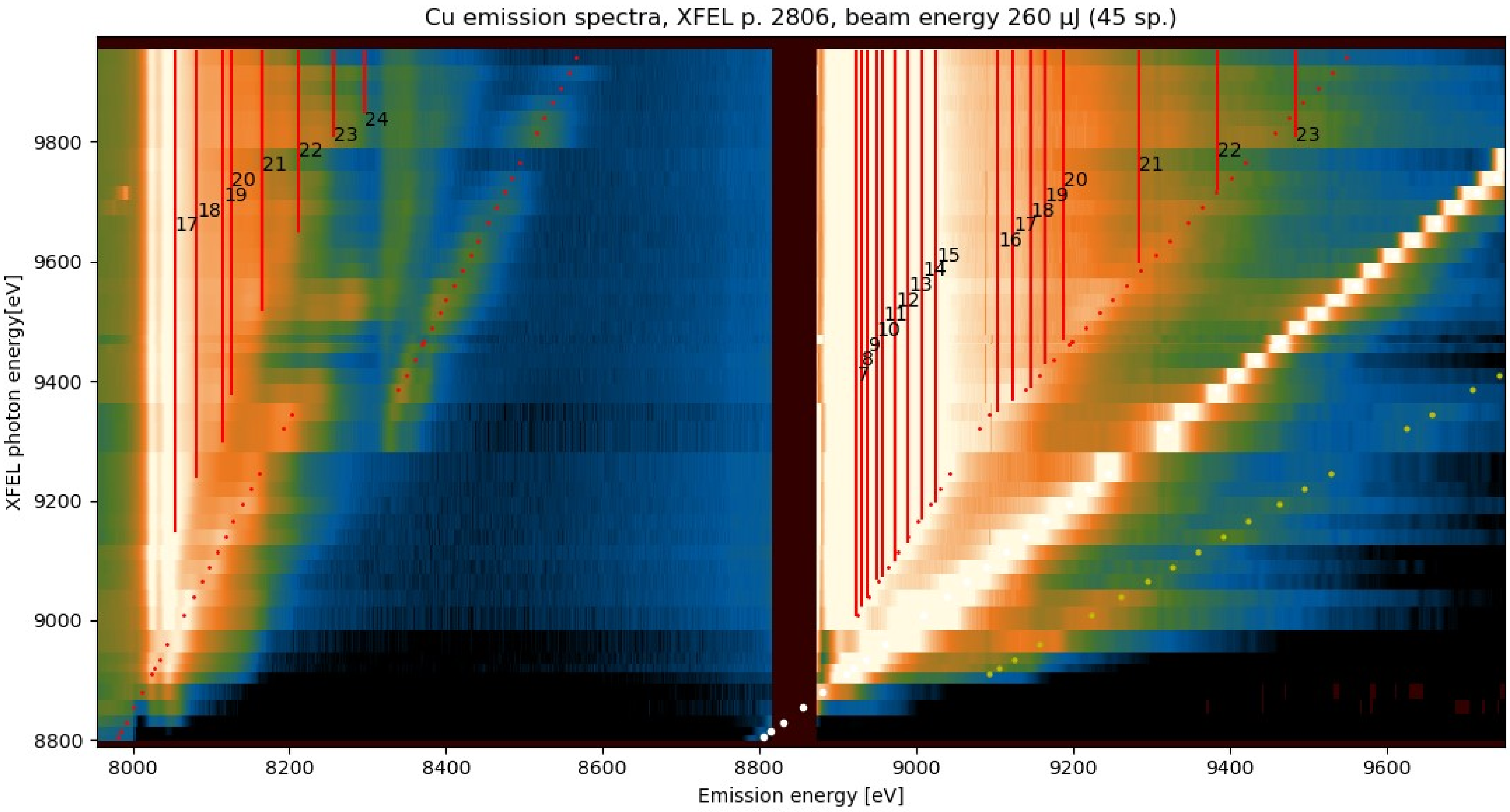
Spectra with 240 µJ on target

- ‚Workhorse‘ - good data for most photon enegrgies.
- Red dots - resonantly driven transitions.



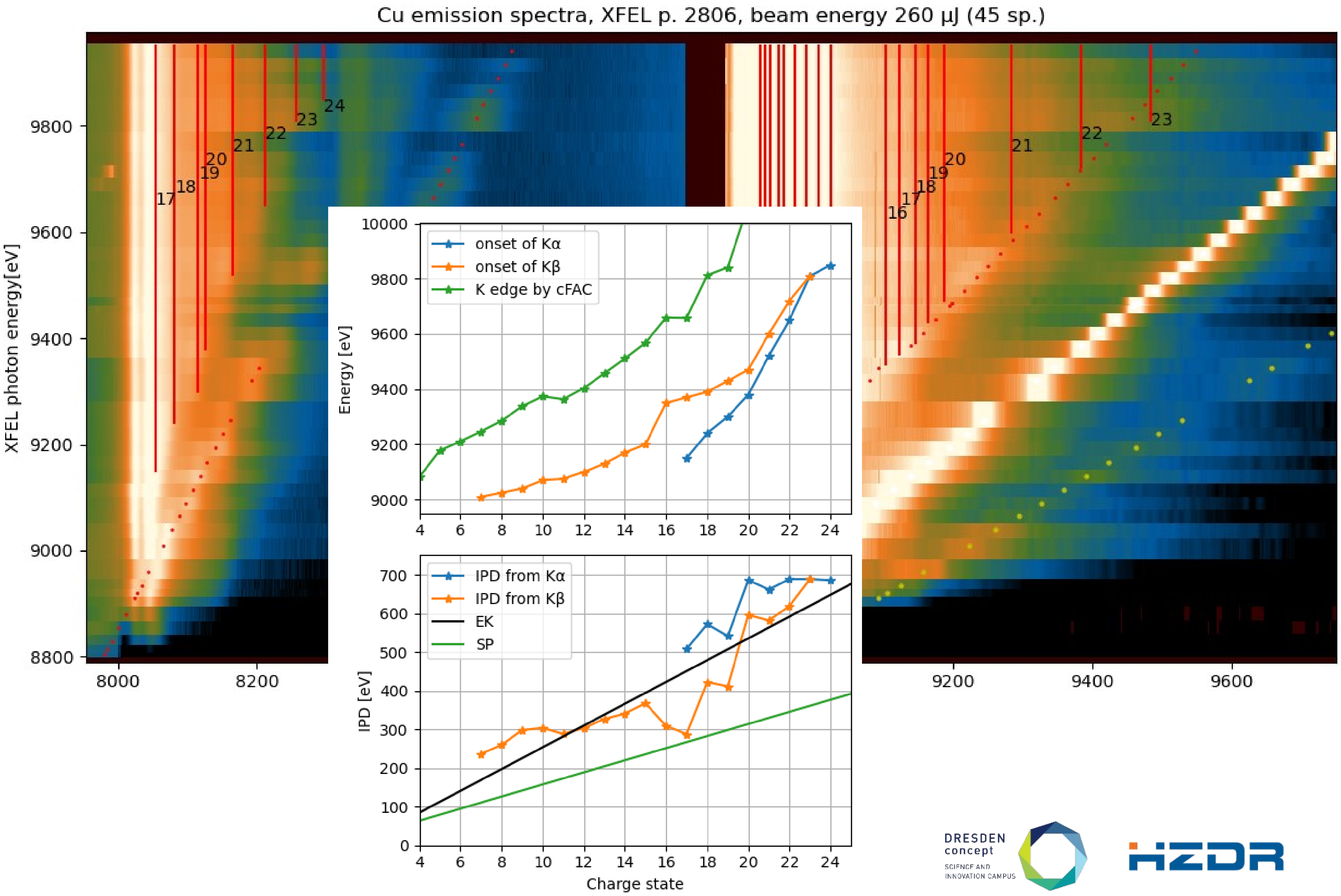
Ionization Potential Depression 2

- Positions of ionized Kα and Kβ lines from cFAC
- Not a perfect agreement yet!
- Finding the ‚onset‘ of emission of each line.
- Black number - charge state.



Ionization Potential Depression 3

- „Direct IPD measurement”
- Independent from Kα and Kβ lines.
- Very preliminary!
- Values are rather close to the EK model, as shown on previous low-charge data.

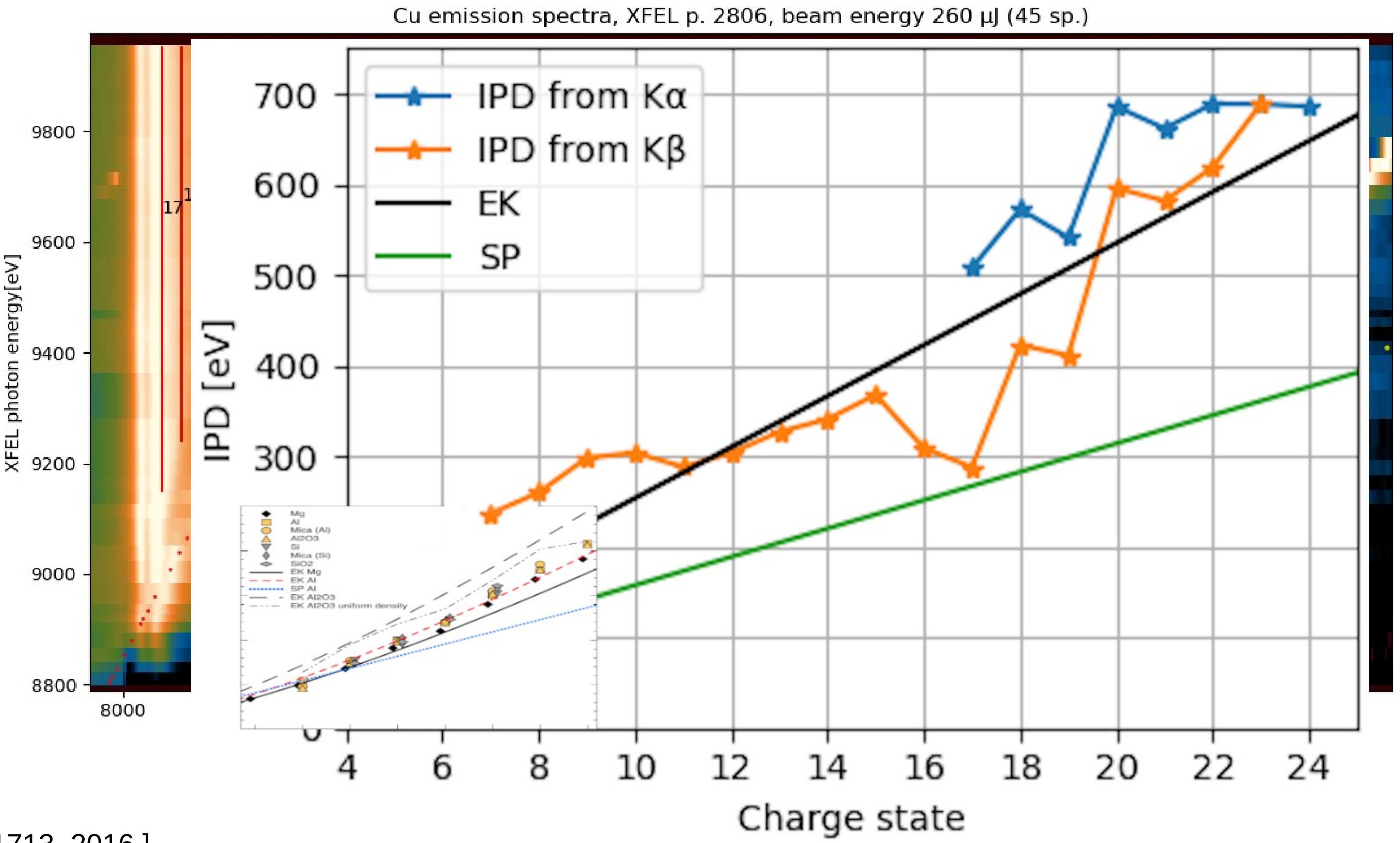


DRESDEN concept SCIENCE AND INNOVATION CAMPUS HZDR

Ionization Potential Depression 4

Differences and irregularities:

- Discrepancies in line identification.
- Not a CR model (yet).
- Inset: work on Al on lower charge states - aligned axes!



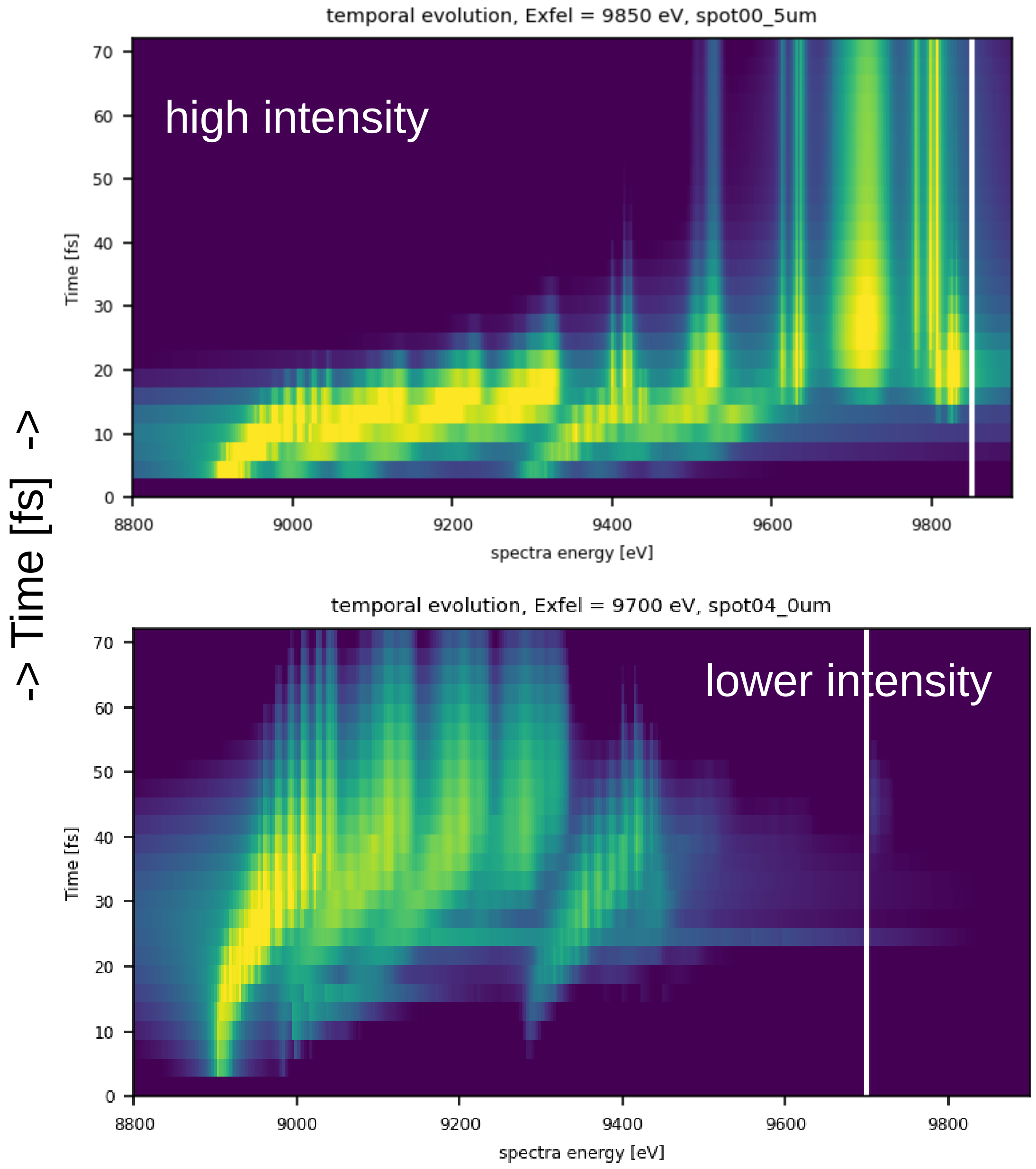
Inset: [O. Ciricosta et al., Nat Comm 7:11713, 2016.]

DRESDEN concept SCIENCE AND INNOVATION CAMPUS HZDR

SCFly simulations 1

- Time-dependent Collisional-Radiative simulation.
- Single-cell („0-D”)
- Driven by XFEL pulse only.
- Gaussian temporfal profile.

- XFEL beam heats **and** probe the matter at the same time.
- Heating is seen as shift of the lines towards higher enrgy.

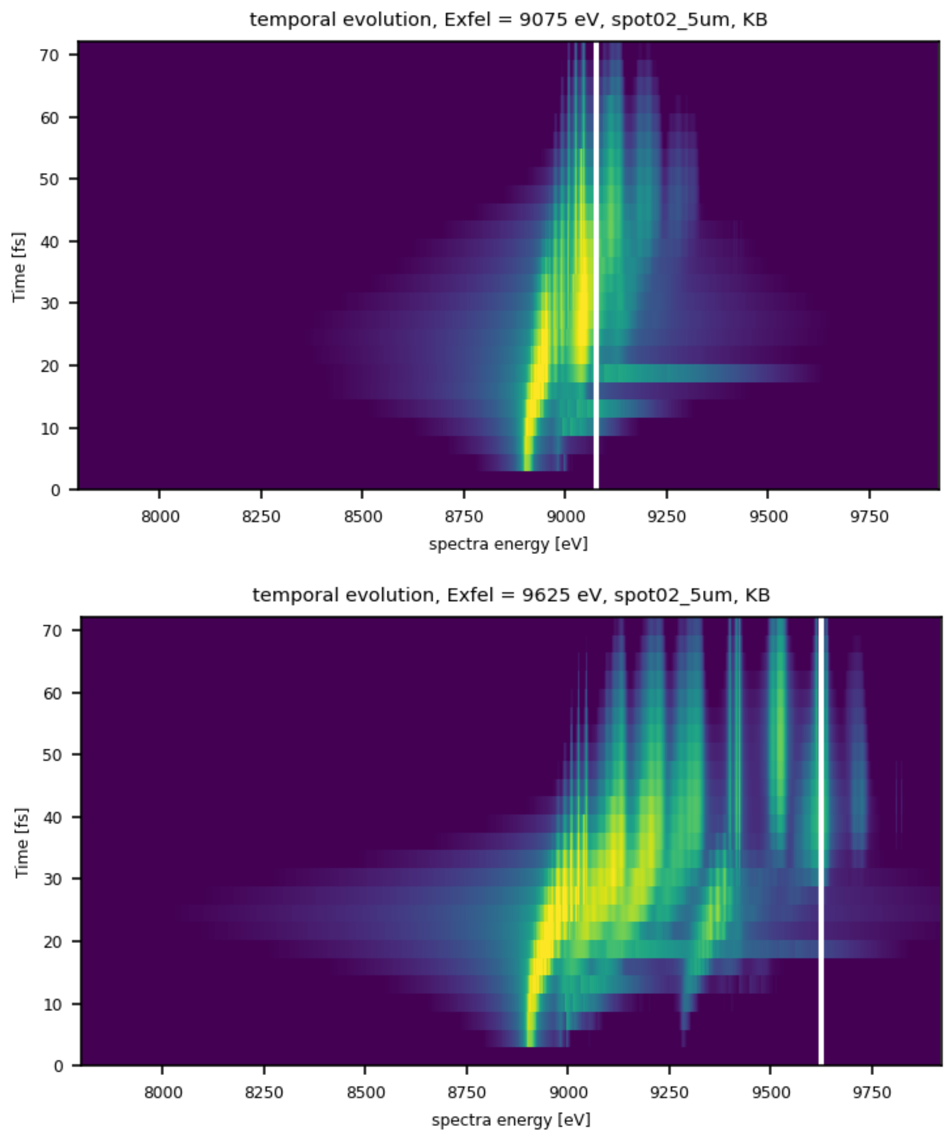


SCFly simulations 2

- These two simulations has same intensity.
- Only difference: photon enrgy of driving XFEL beam (white line).
- On upper simulation: only Kβ transitions below the XFEL energy are lit up.
- Later, XFEL is below K edges present in warmer matter and goes through.

- Detectable on transmission measurement.

-> Time [fs] ->

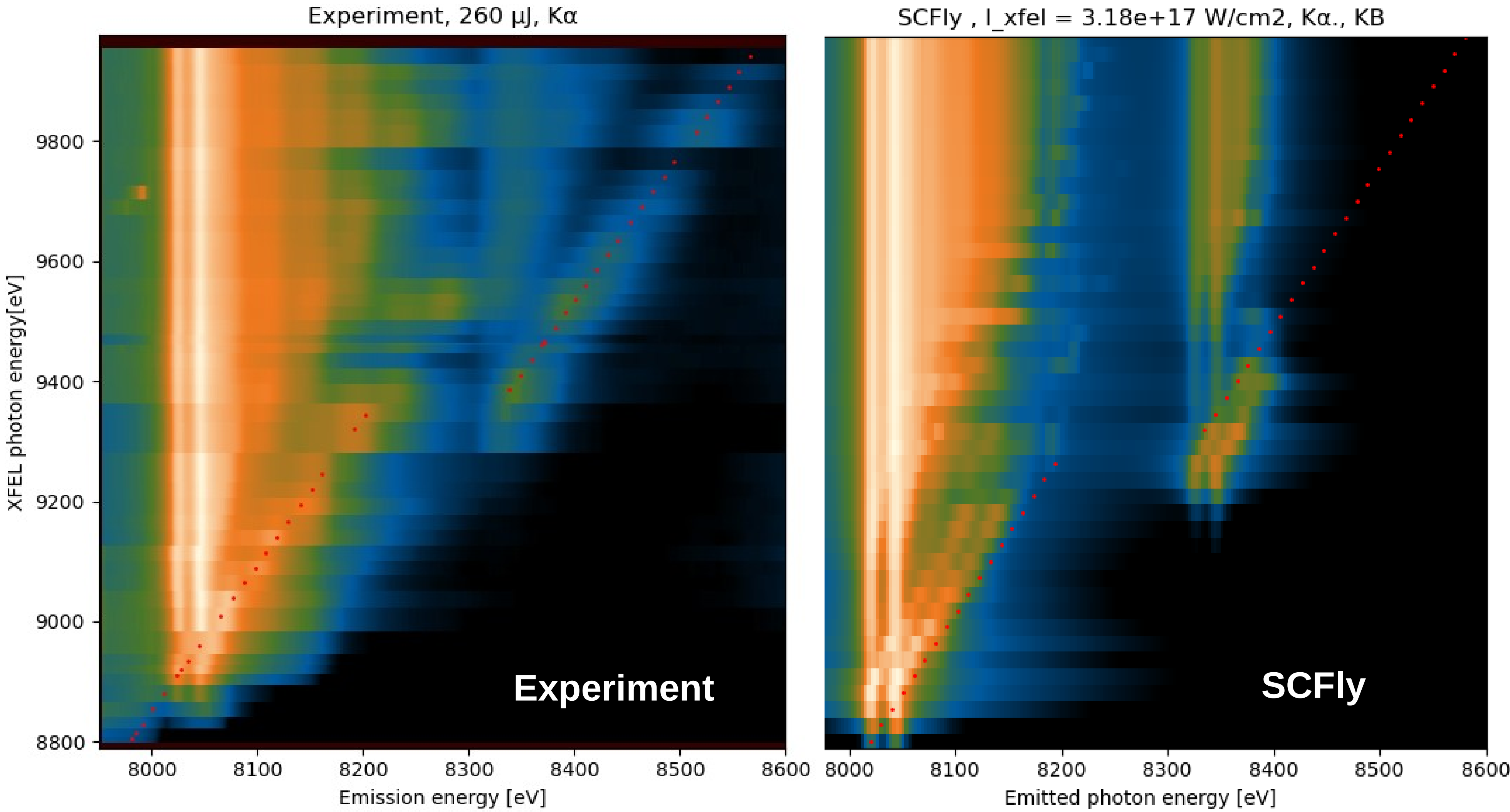


SCFly simulations 3

Amazing qualitative agreement!

- Experiment: 260 µJ
- SCFly: 3e17 W/cm2

(would correspond to ~2.3 µm dia)

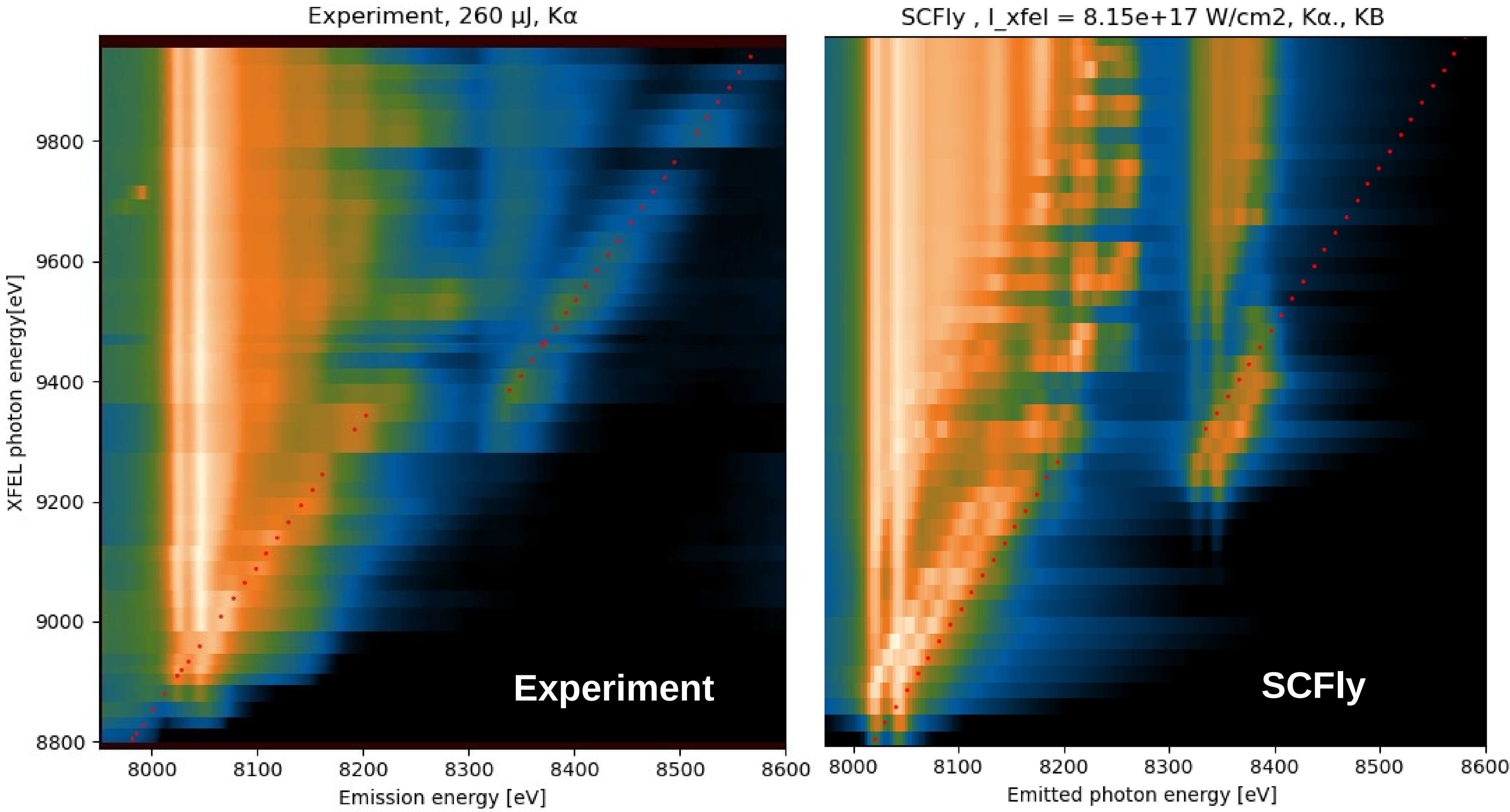


SCFly simulations 4

Amazing qualitative agreement!

- Experiment: 260 µJ
- SCFly: 8e17 W/cm2

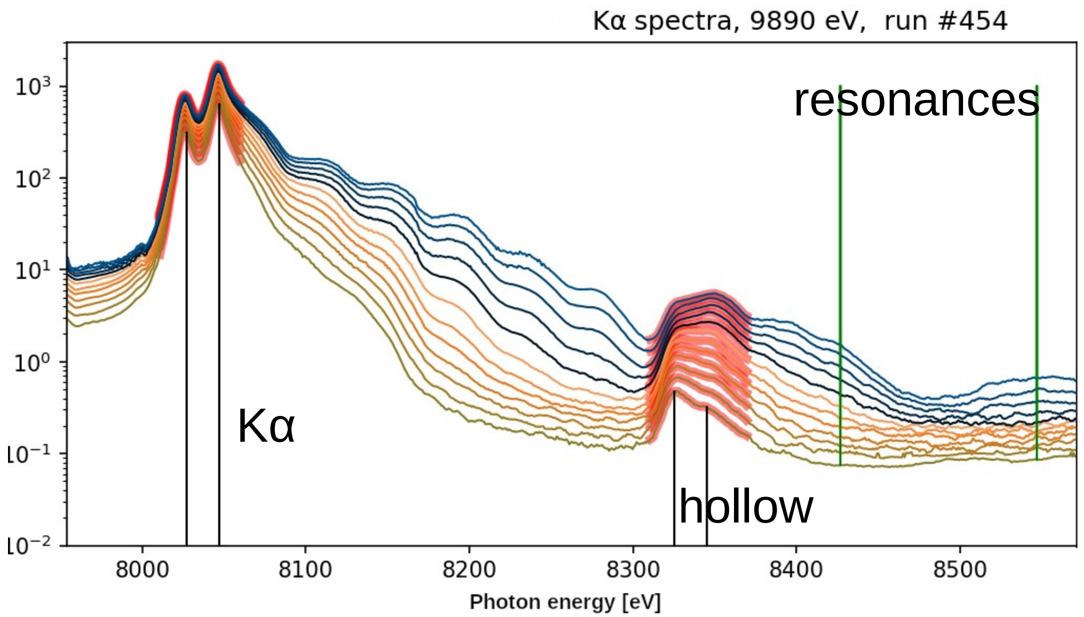
(would correspond to ~1.4 µm dia)

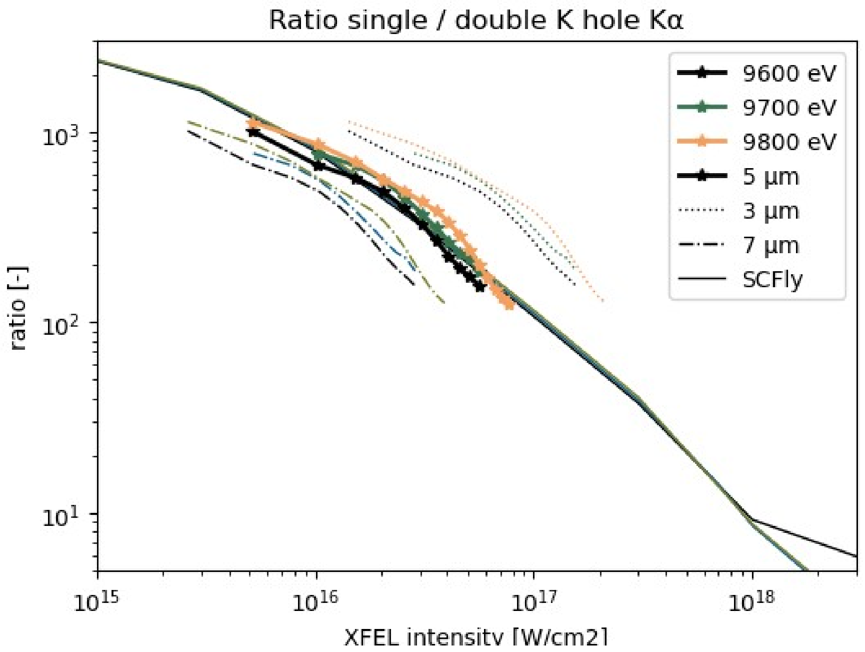


HiBEF DRESDEN concept SCIENCE AND INNOVATION CAMPUS HZDR

Hollow ion emission

- Kα: 1s2 2p5 - 1s1 2p6
- hollow Kα: 1s1 2p5 - 1s0 2p6
- Lifetime of 1s1 2p6 state is few fs
  - Either it decays as Kα
  - Or it is hitted by XFEL photon once more.
- Ratio of these lines can serve as great ***Intensity diagnostics***.
- Comparison to SCFly simulations.
- We have measurement of Energy. We assume duration 25 fs.
- In this case used to infer focal spot area -> 19μm^2 (5μm dia.)
- Still preliminary results.

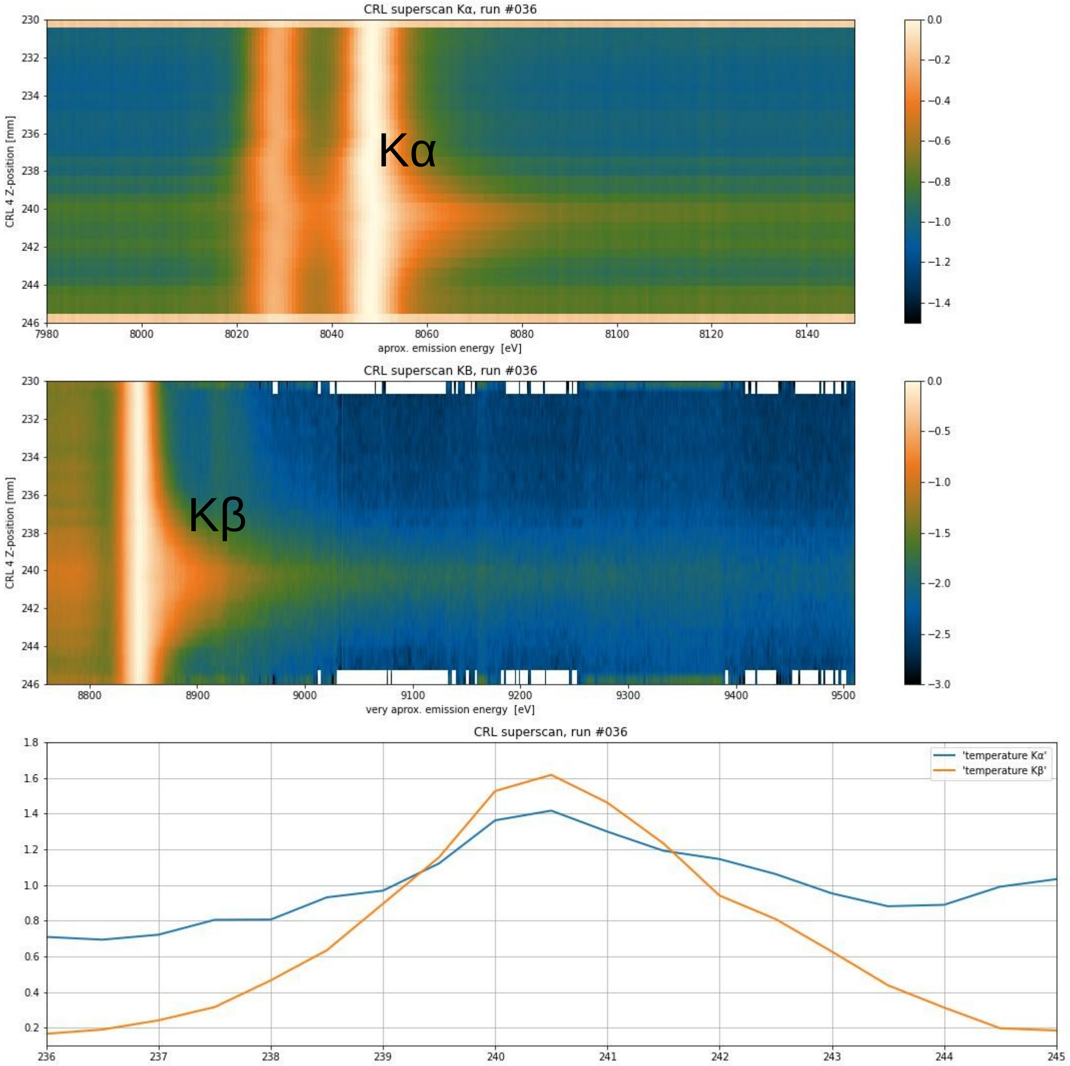




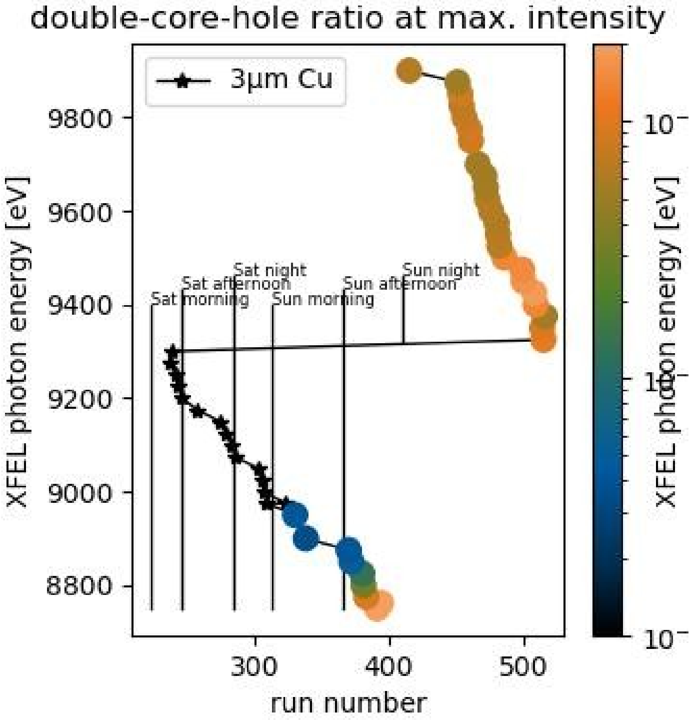
Focal spot optimization

- Big effort in automation of the experiment. (**48 hrs**!)
- We used about **45** different photon energies.
- For each 25 eV shift, the lens has to be moved ~1 mm.
- Various configuration of upstream focusing needed to keep the beam reasonable on the last lenses.
- Focusing run moves the lens gradually during the 10 Hz shooting - automatic analysis of spectra to find best focus.

position of focusing lens [mm]

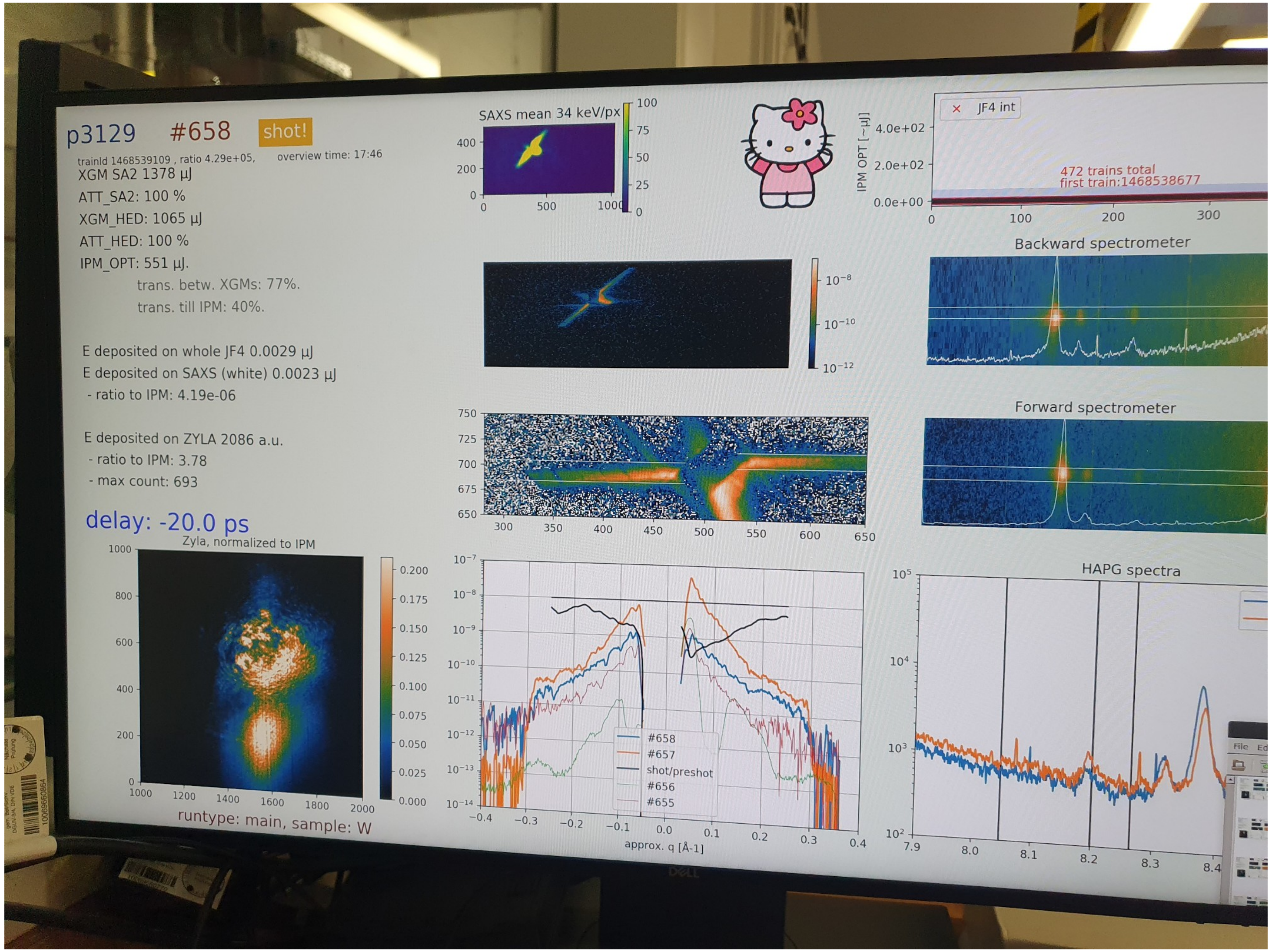


position of focusing lens [mm]



Advertisment 1 *(on-line analysis tool)*

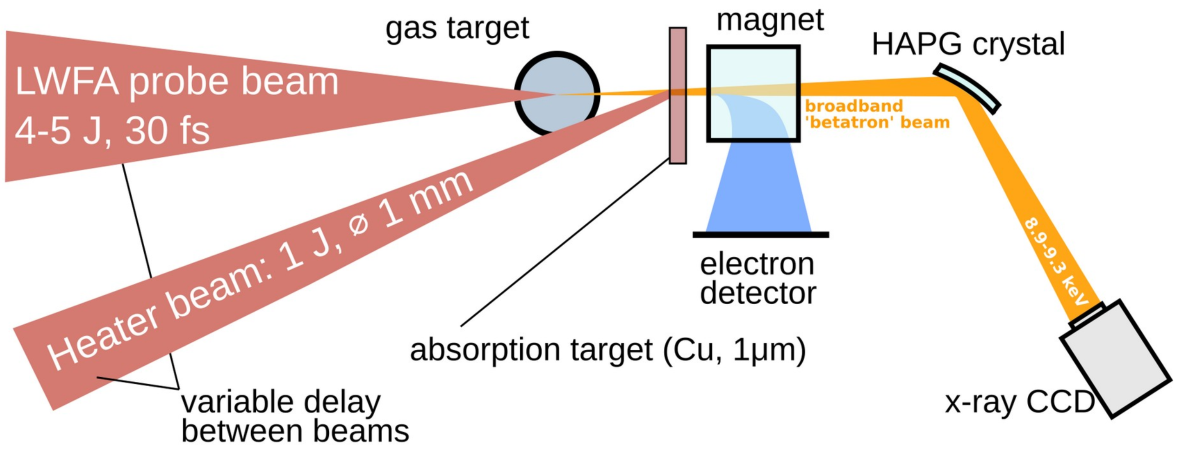
- Long term development of **user-based online analysis framework** at European XFEL
- Using library called *extra_mmm*
- Aimimg to be advanced-user friendly, to easily get the needed data from XFEL‘s system.
- In last experiment (Sep 2022) worked basic analysis fully automated
- Result on screen quickly after shot.

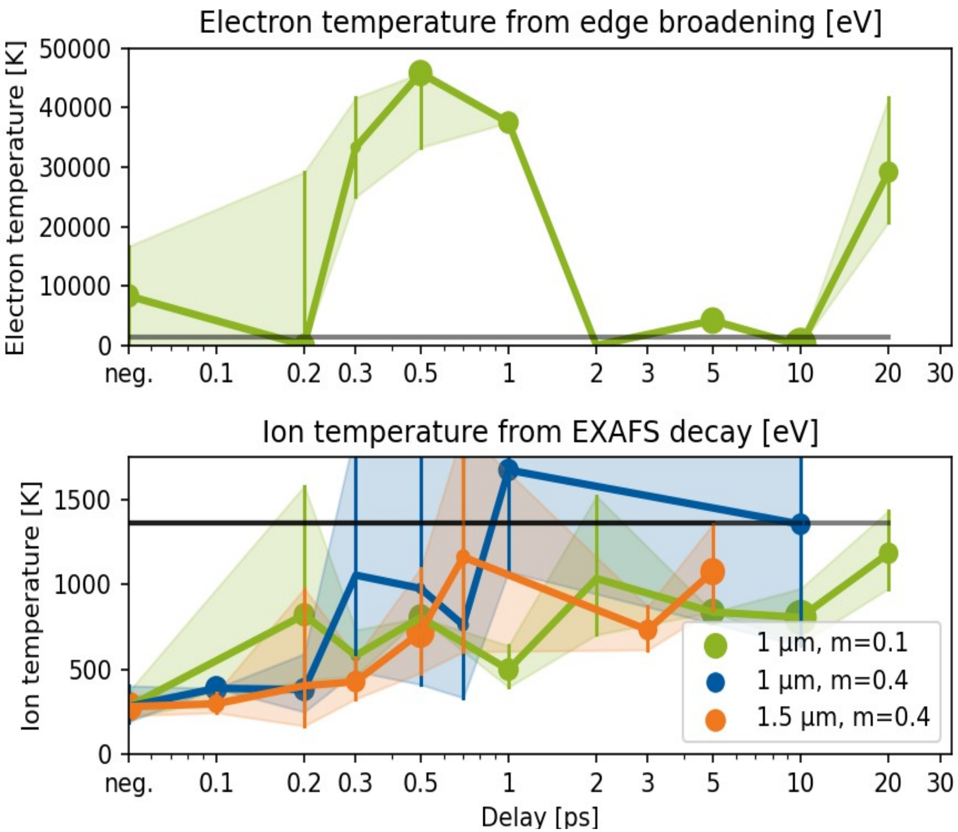


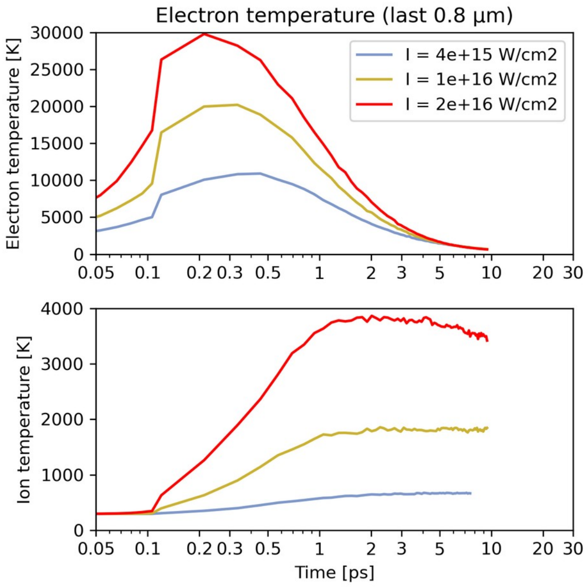
concept
SCIENCE AND INNOVATION CAMPUS

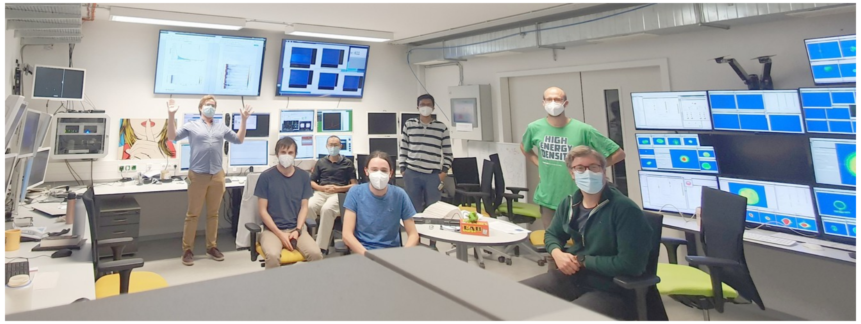
Ultrafast melting of Warm Dense Cu studied by x-ray spectroscopy

- Recent pump-probe experimental results @ **Draco** laser system @ HZDR (Dresden, Germany)
- 2 x Ti:Sa beams, Heating: ~ 2e15 W/cm^2 , 100 MJ/kg
- WDM sample backlit by `broadband x-rays from LWFA driven betatron radiation.
- HAPG / HOPG spectrometer, heavy shielding.
- Detected signal: ~ **1e6** photons per shot in the range 8800 - 9400 eV.
- Ion and electron temperatures measured by x-ray absorption spectrscopy. -compared to DFT simulations.
- **electron-ion relaxation.**

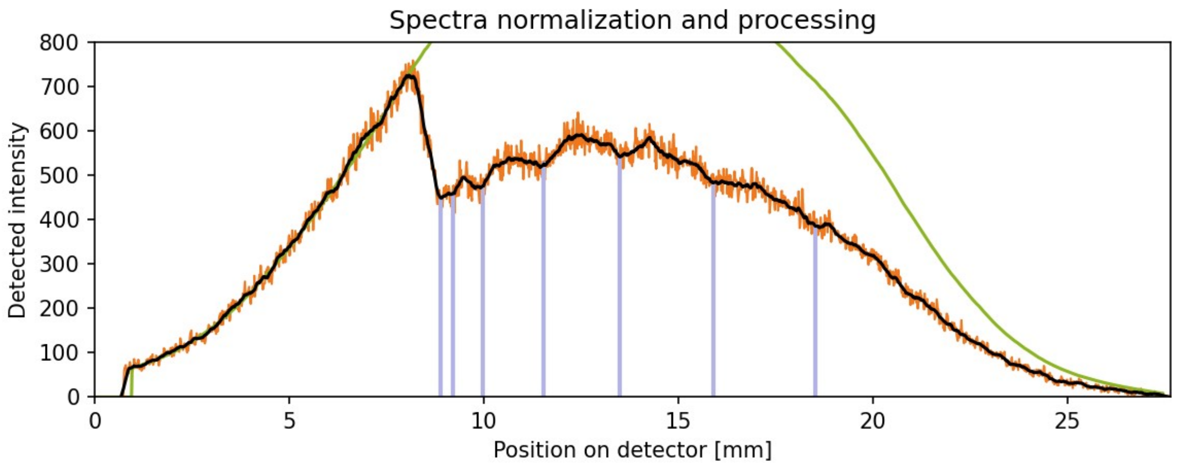


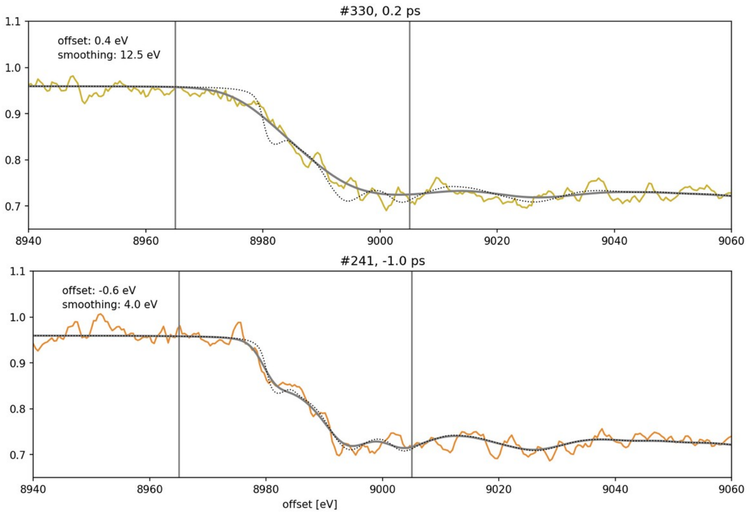


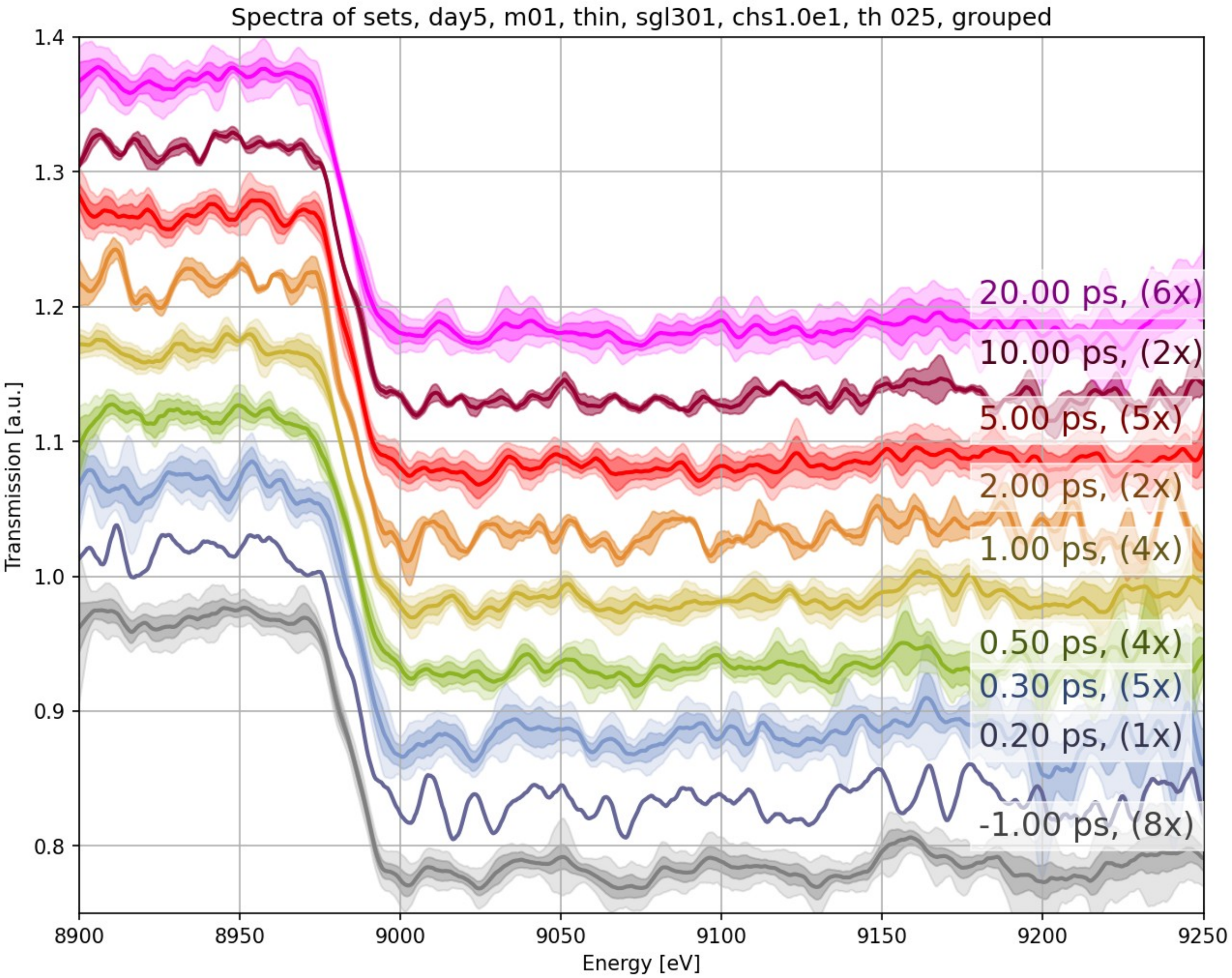




Ultrafast melting of Warm Dense Cu studied by x-ray spectroscopy

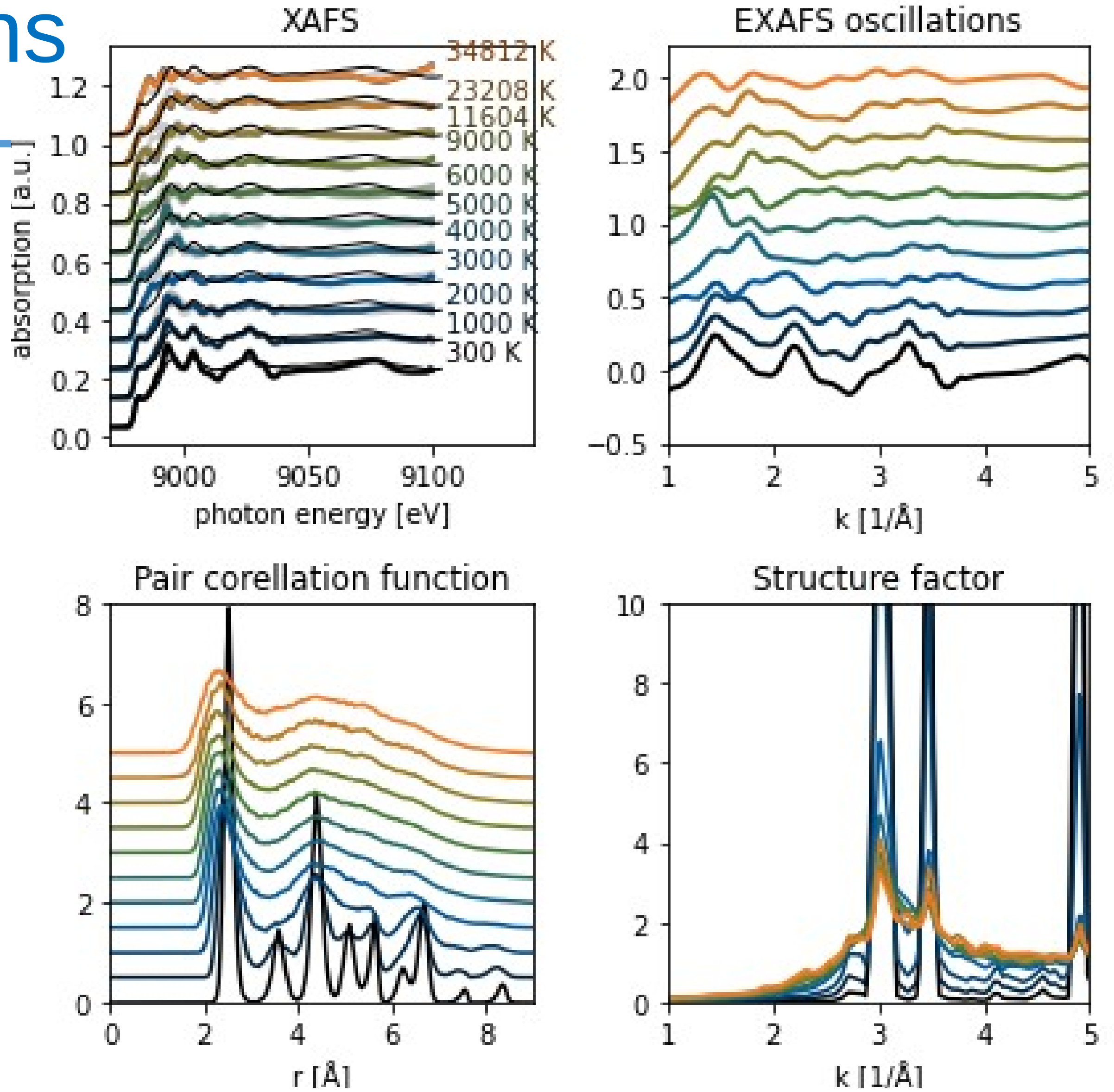






Vasp simulations

- *„The Vienna Ab initio Simulation Package: atomic scale materials modelling from first principles.”*
- https://www.vasp.at
- Simulated by Jan Vorberger (HZDR).



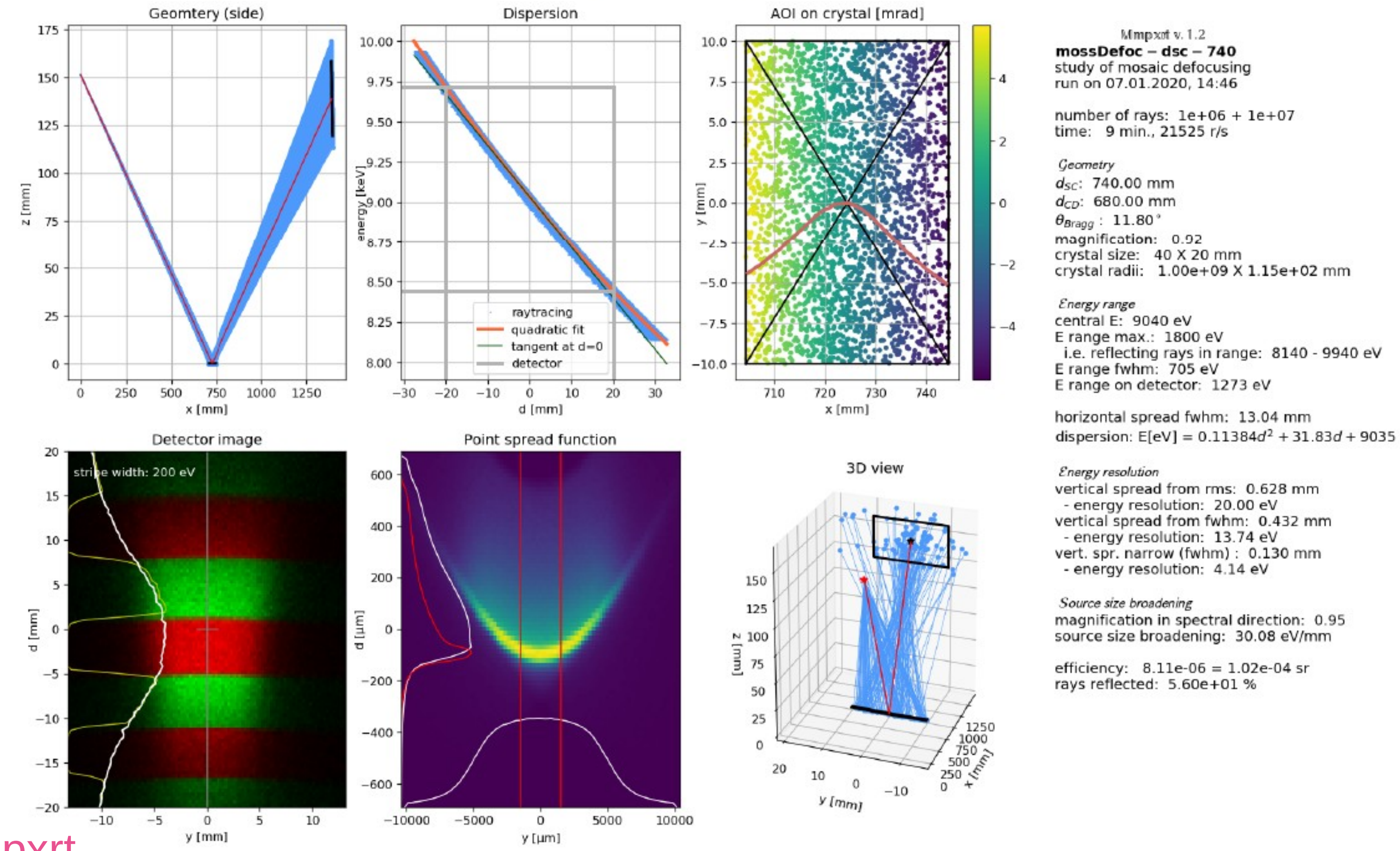
advertisment 2: **mmpxrt**

(one by last slide)

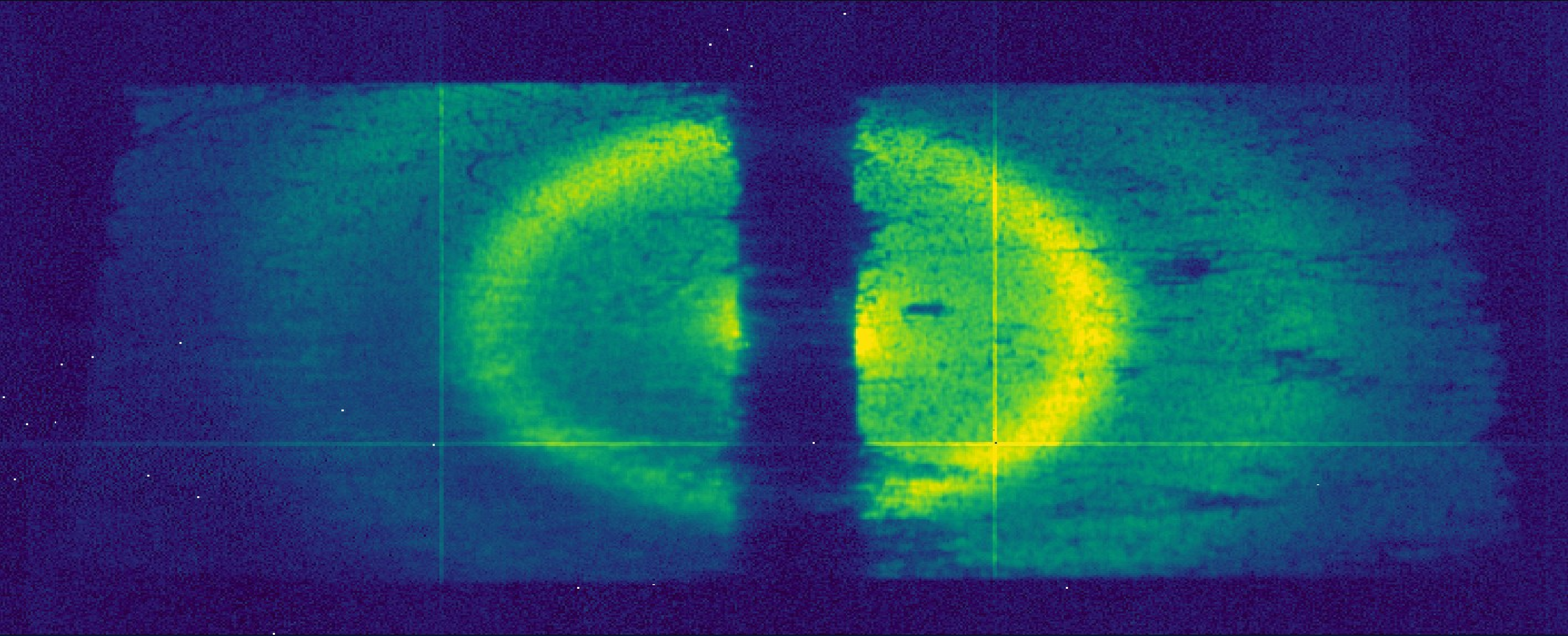
- Raytracing code
- Tool for design of x-ray spectrometers.
- Tested support of mosaic crystals.
- Open source, Python code
- Provides good flexibility and extendability.

Computer Physics Communications
Volume 262, May 2021, 107811

X-ray spectrometer simulation code with a detailed support of mosaic crystals ☆, ☆☆



https://codebase.helmholtz.cloud/smid55/mmpxrt



Mirrors for Small Angle X-ray scattering

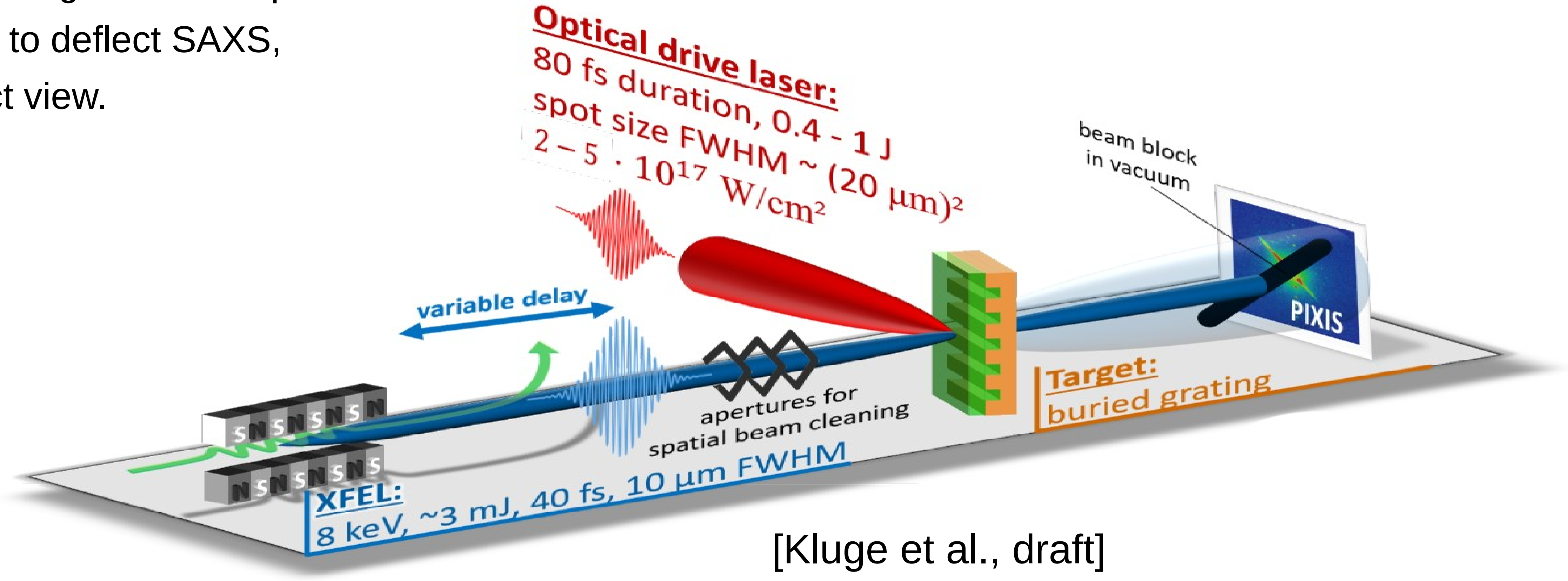
Michal Šmíd, Carsten Bähtz, Alejandro Laso García, Jörg Grenzer, Thomas Kluge, Alexander Pelka, Irene Prencipe, Melanie Rödel
and Tom Cowan
and the HED team

27.1.2020, XFEL UM

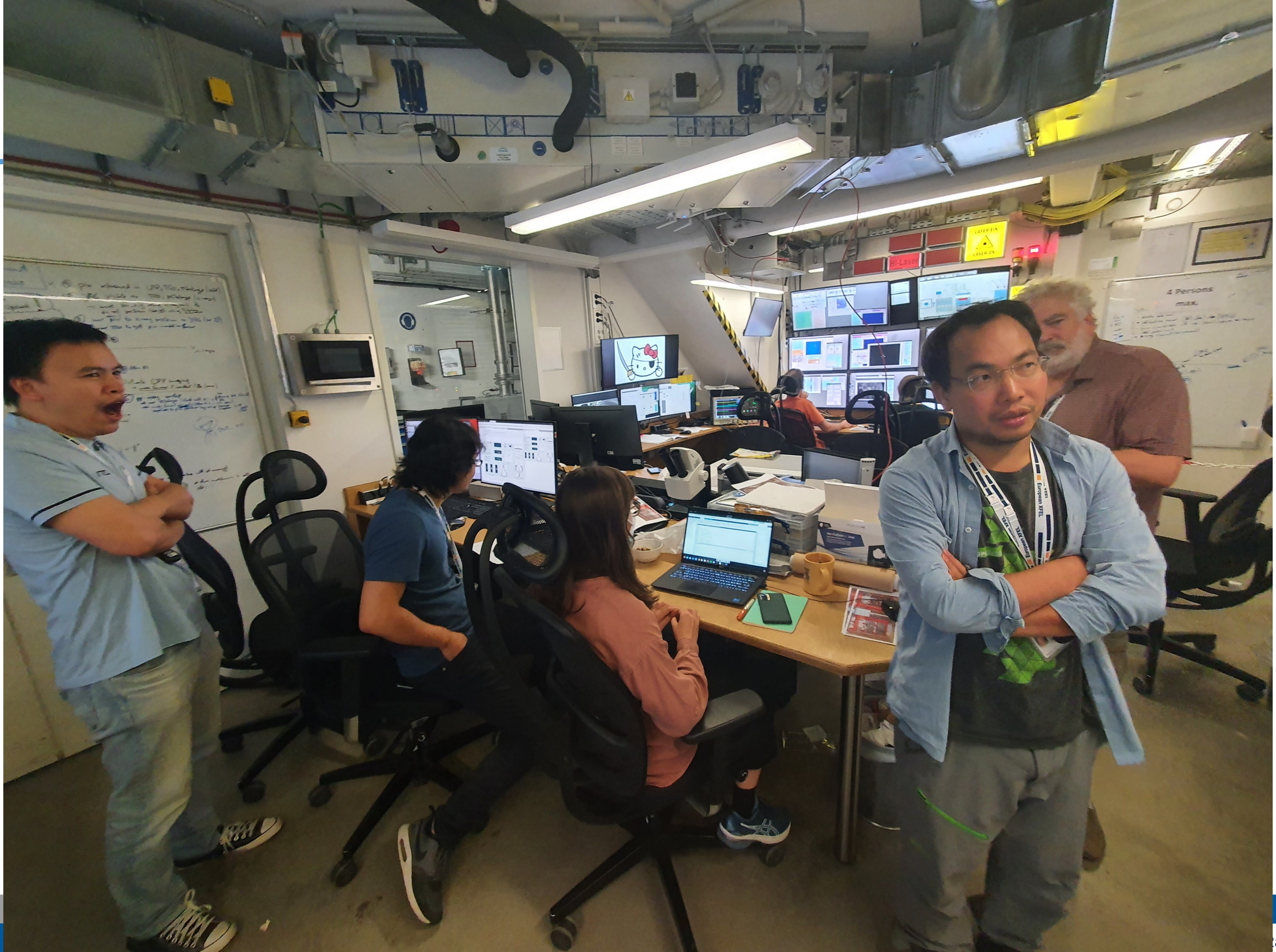
HELMHOLTZ
ZENTRUM DRESDEN
ROSSENDORF

Motivation

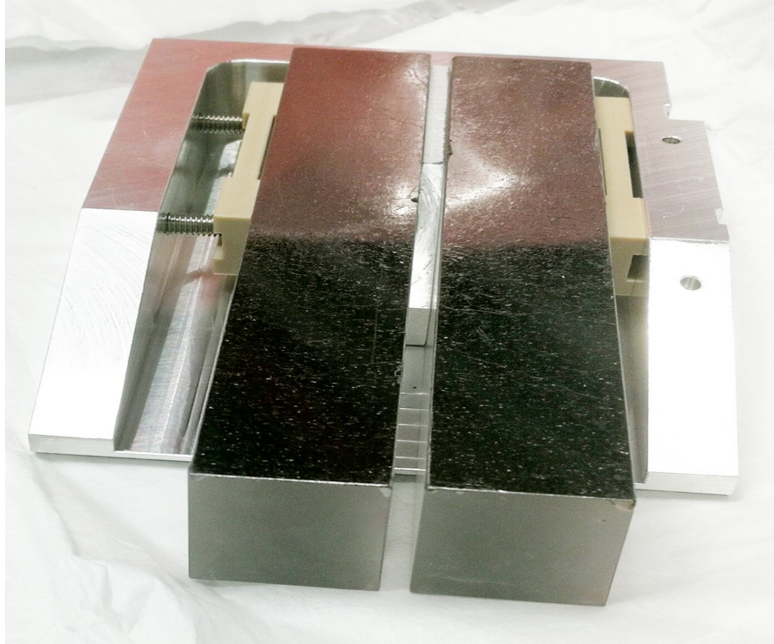
- SAXS: Diagnostics of nm size structures on target
- Detector usually open towards laser-irradiated target
  ->Strong background from plasma emission
- Use mirror to deflect SAXS,
  block direct view.

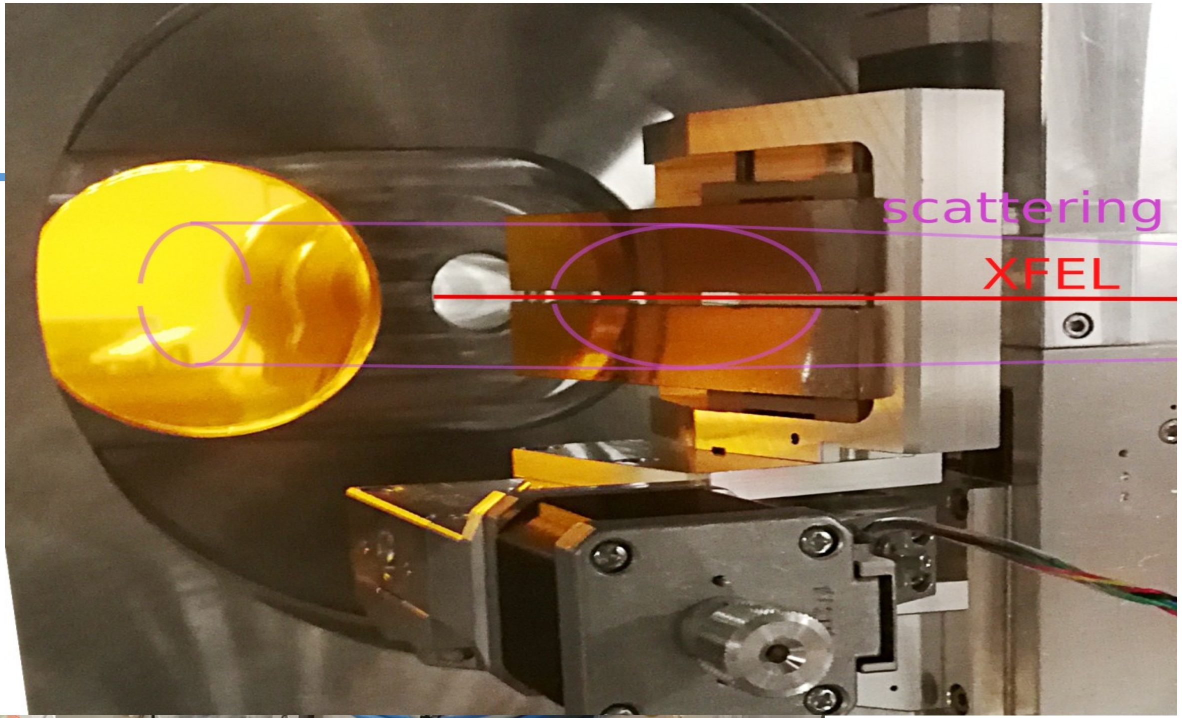


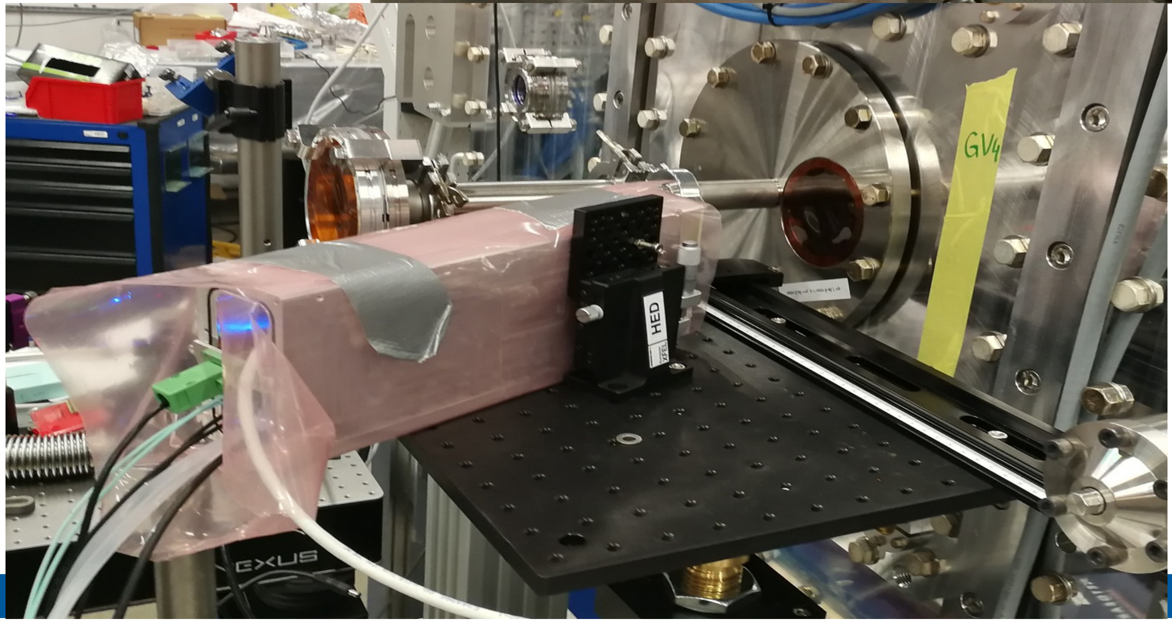
[Kluge et al., draft]


HI-Laser
4 Persons max.
European XFEL

HAPG mirror

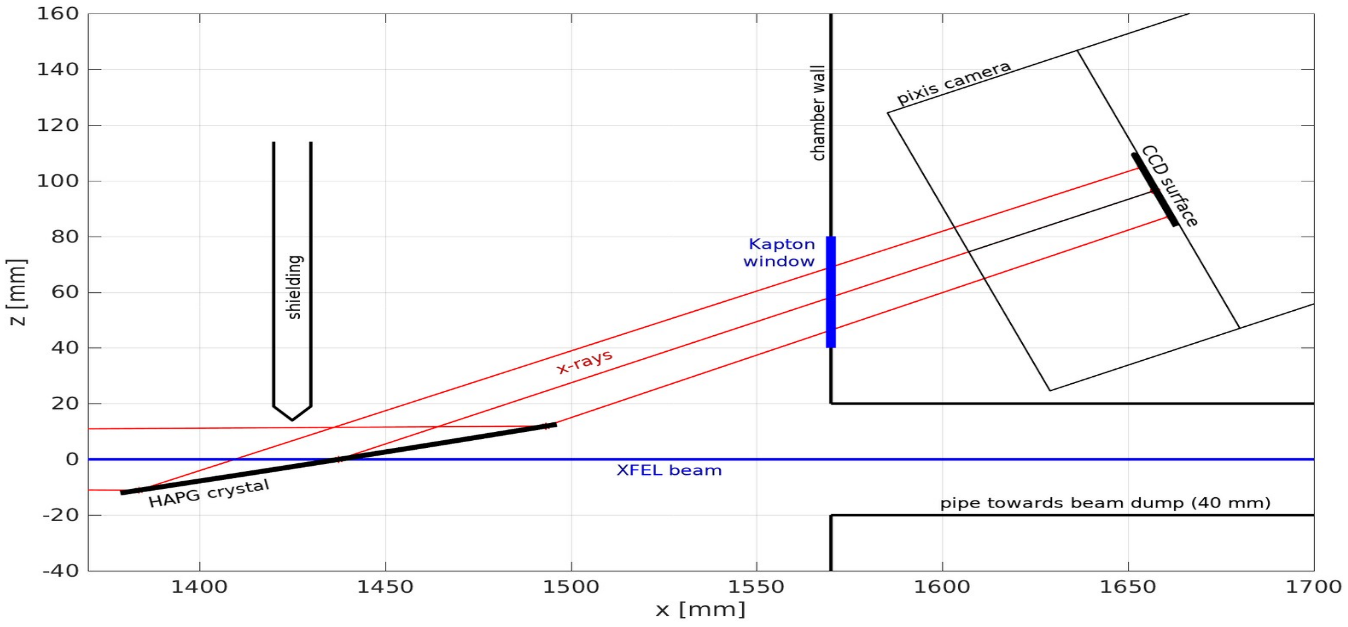


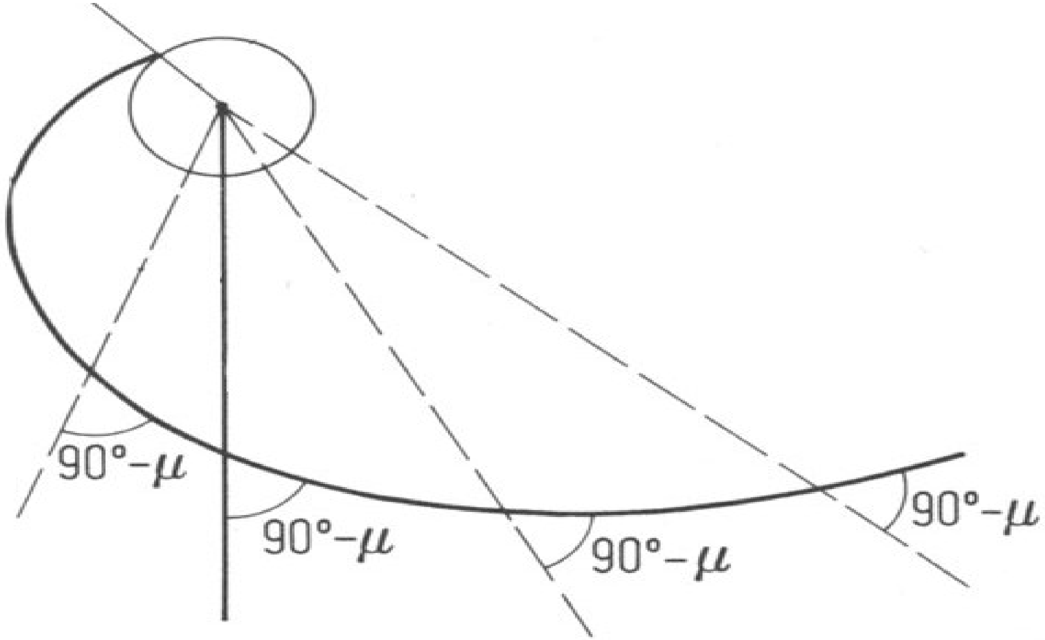




Design

- X-ray optics: very narrow acceptance angle.
- Geometry ensuring identical incidence angle of rays from point : **logarithmic spiral**.
- **Circle**: good approximation, but not perfect. Would not work with perfect crystal.
- **HAPG** mosaic crystals: broader acceptance angle



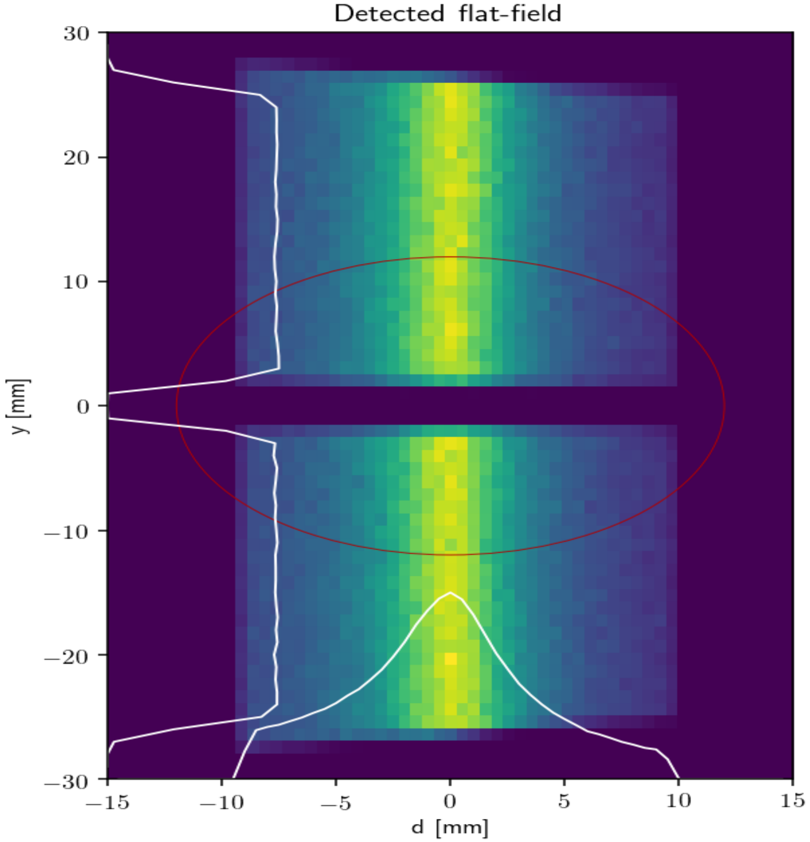


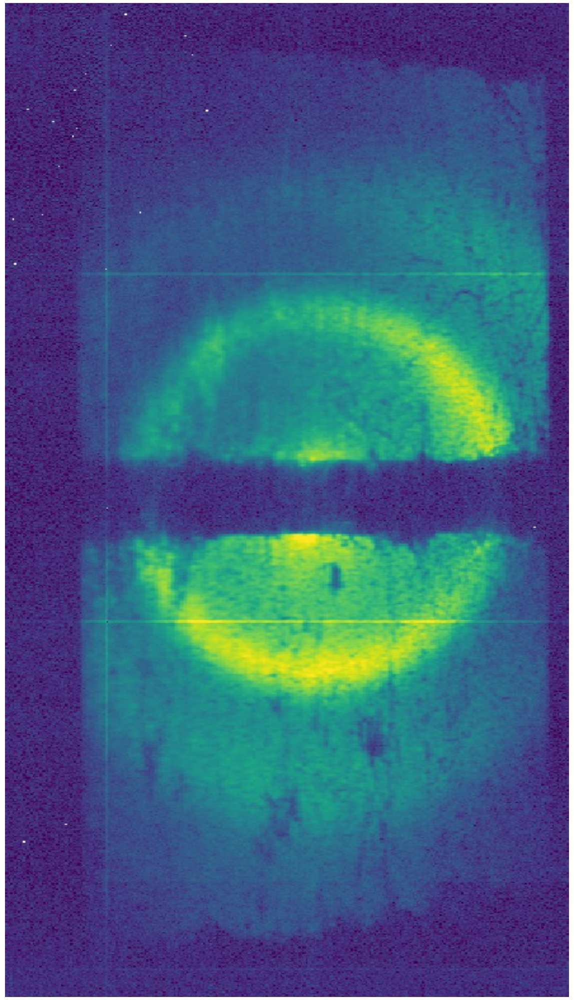
[pictures from wikipedia, caltech.edu]

Non-optimal energy

- Radius of curvature is optimized for **8150** eV
- Test was performed also on **9500** eV
- Reflectivity should be significantly dropping towards horizontal edges
- Experimental performance: significantly better
- Probably due to higher-then-desired mosaicity.

Raytracing for 9500 eV





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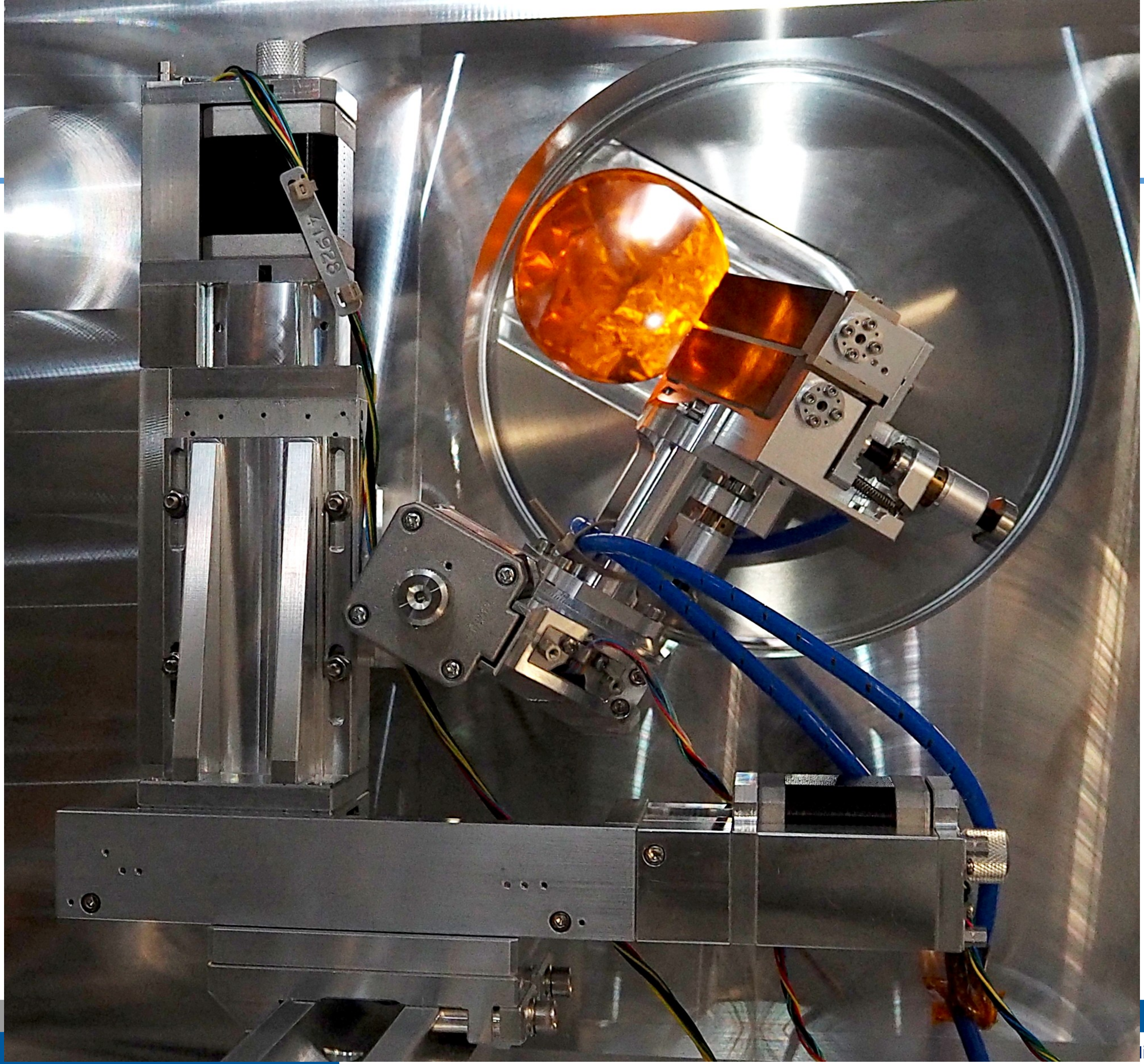
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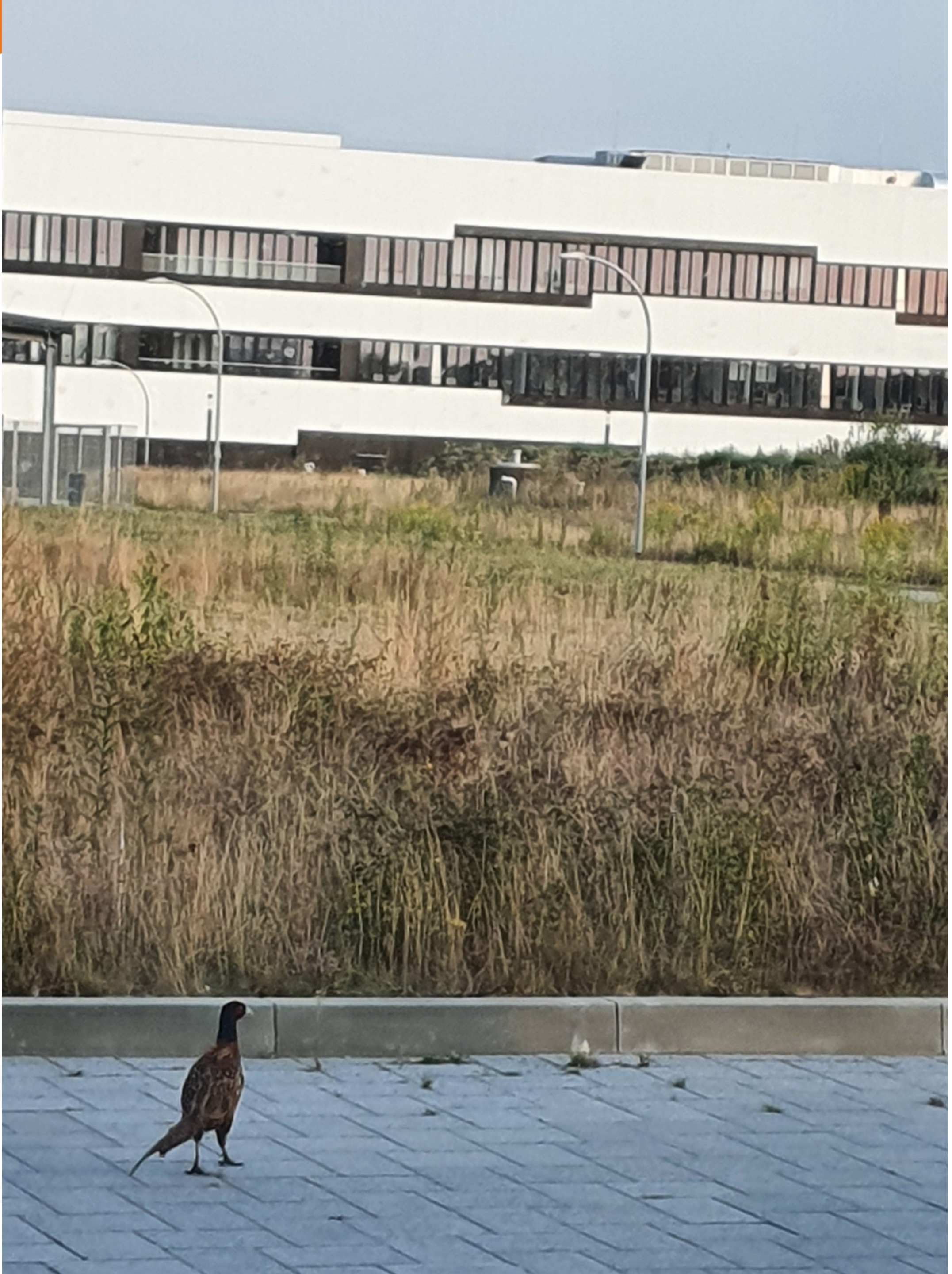

Konec

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