The color of x-rays

seeding, two-color mode and spectroscopy at the HED instrument

Ulf Zastrau

Leading scientist

Group leader HED

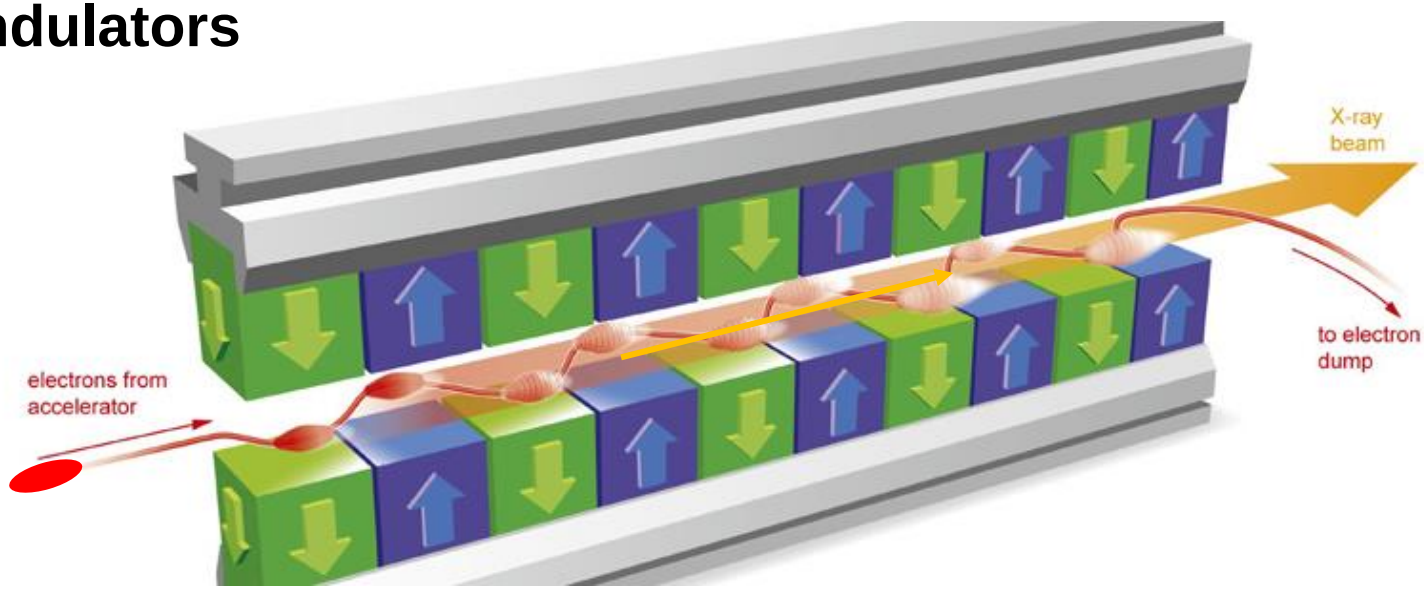
European XFEL

HED High-Energy Density science

HiBEF

Satellite meeting, UM 2022 – Jan 25st, 2022

Undulators



$$K = \frac{e B_0 \lambda_u}{2\pi m_e c}$$

Moving coordinate system (*)

$\lambda_u^* = \lambda_u / \gamma$ length contraction

electron oscillates with $\omega^* = 2\pi \frac{c}{\lambda_u^*} = \gamma \cdot \frac{2\pi c}{\lambda_u}$

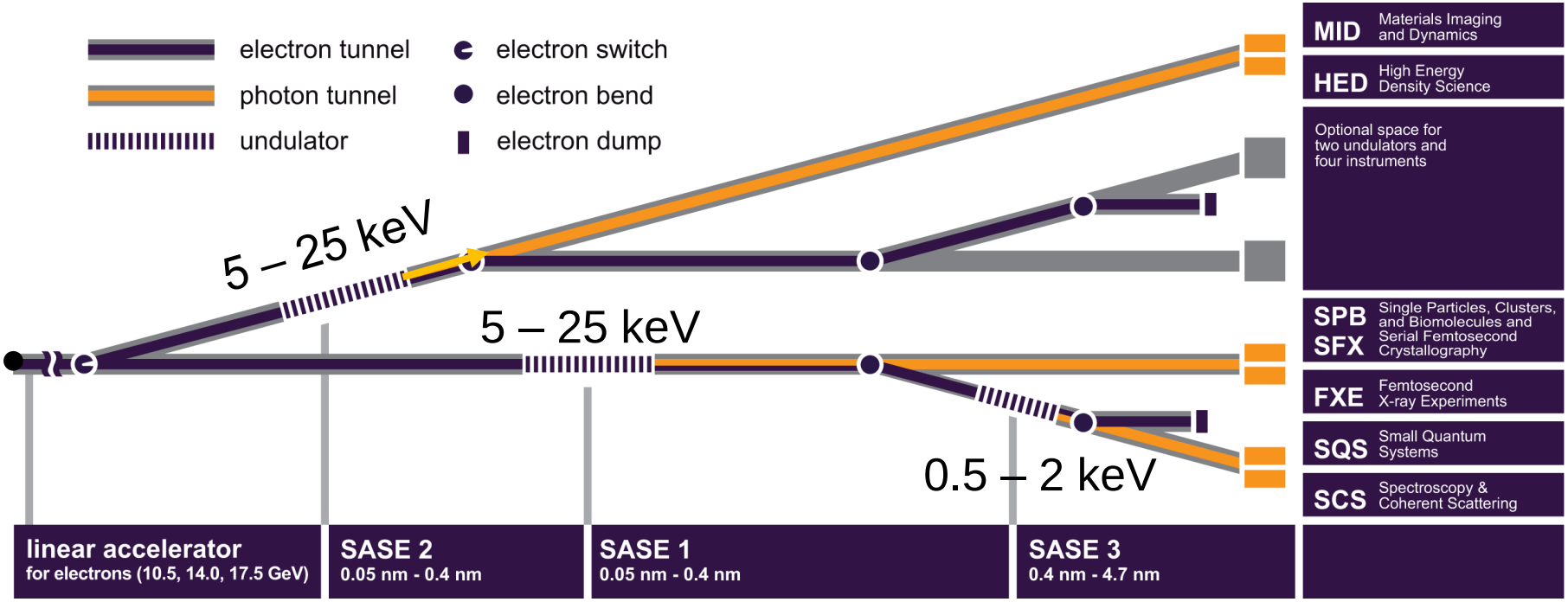
Lorentz transformation of radiation to lab-system

$$\Rightarrow \lambda_\ell \approx \frac{\lambda_u^*}{\gamma} = \frac{\lambda_u}{\gamma^2}$$

$$\boxed{\lambda_\ell = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2}\right)}$$

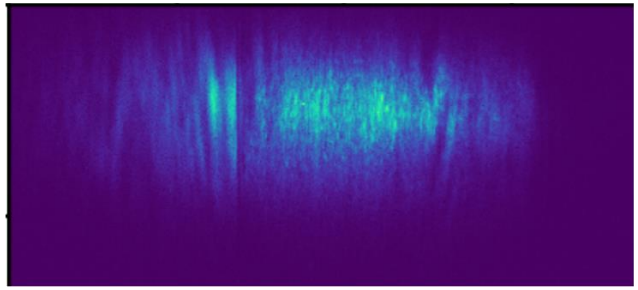
monochromatic radiation

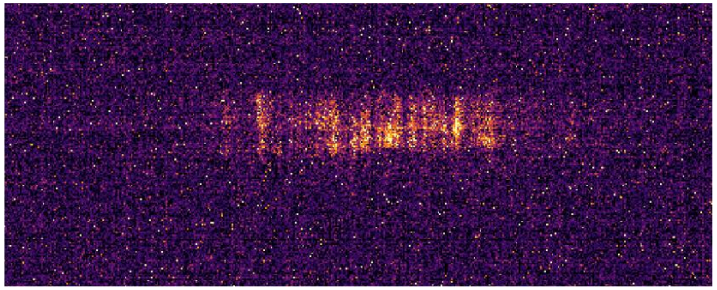
European XFEL: beamlines and instruments

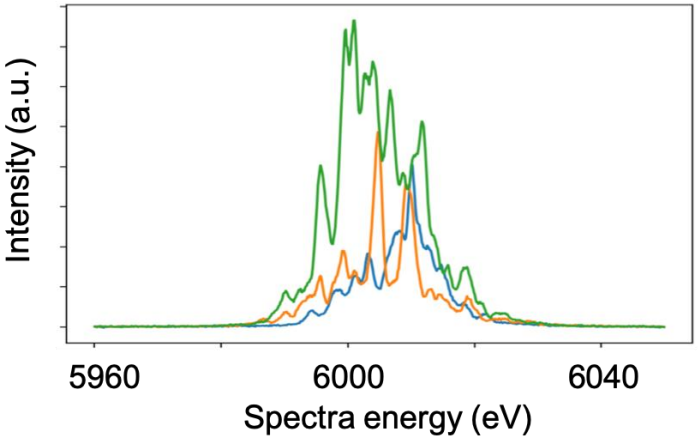


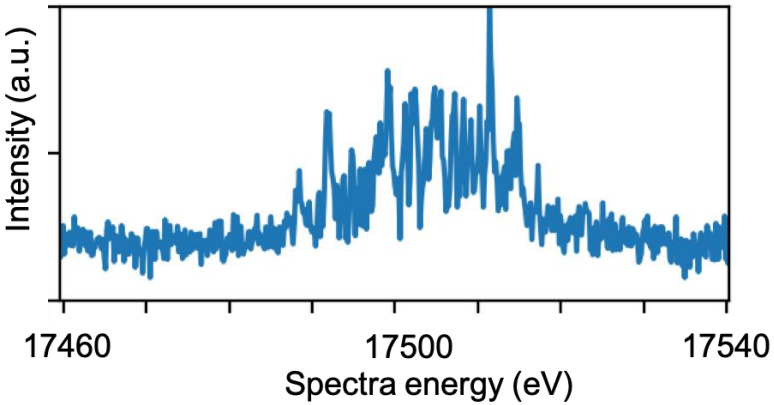
Electron energy setpoints: 8, 11.5, 14, 16.3 GeV

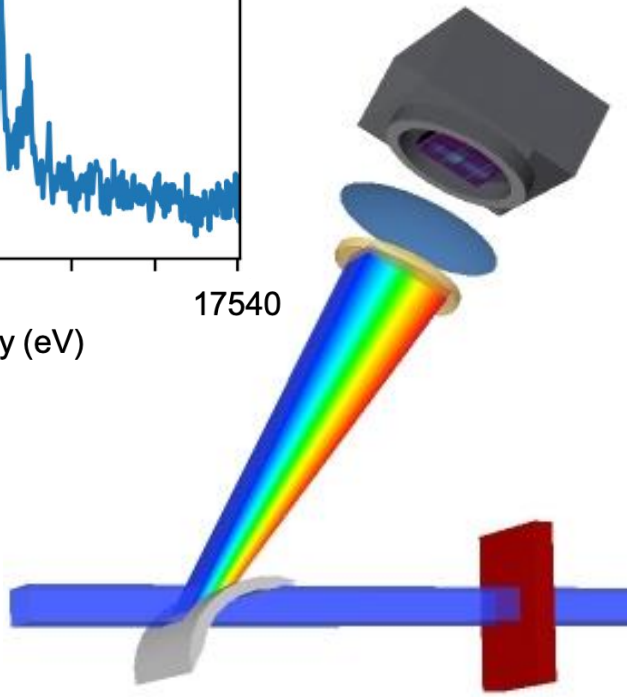
Typical SASE spectra









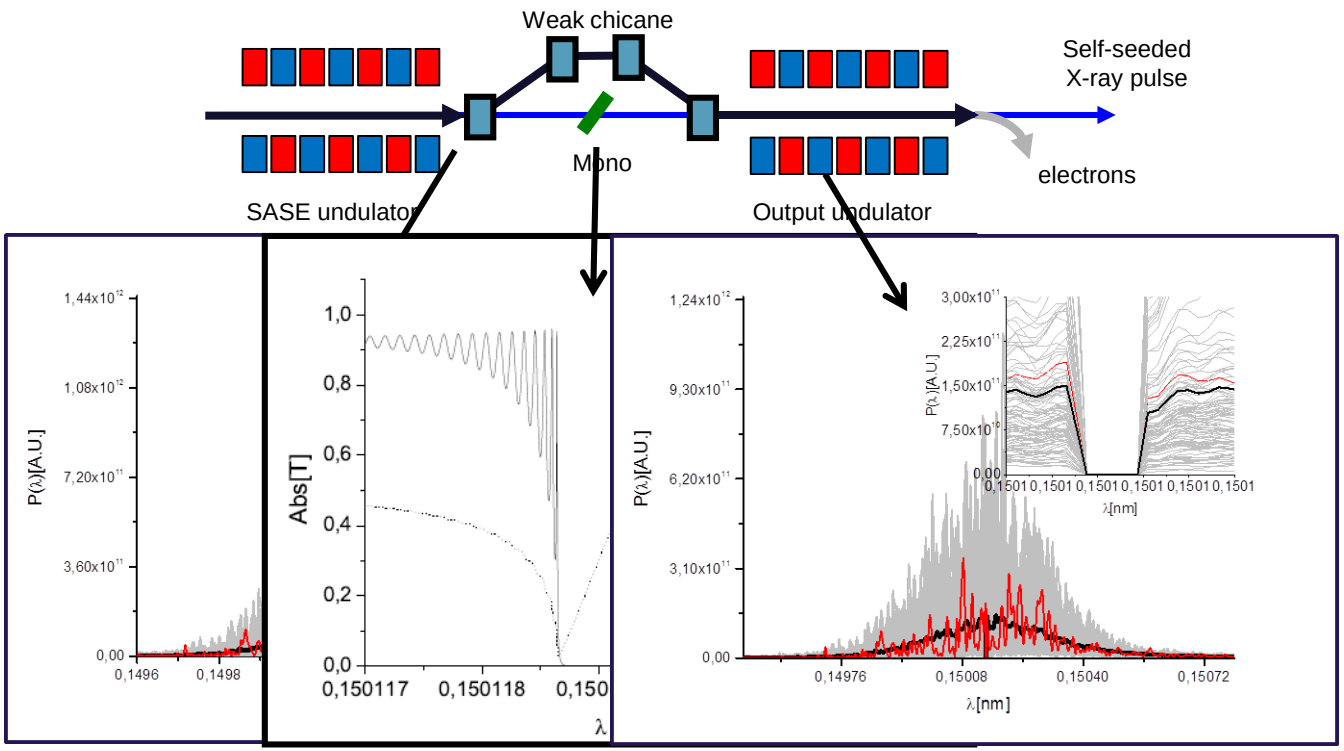


Zastrau, Appel, Baehtz et al., J. Synchrotron Rad. (2021). 28, 1393–1416

M. Harmand et al. Arxiv 2020

Courtesy G. Geloni et al.

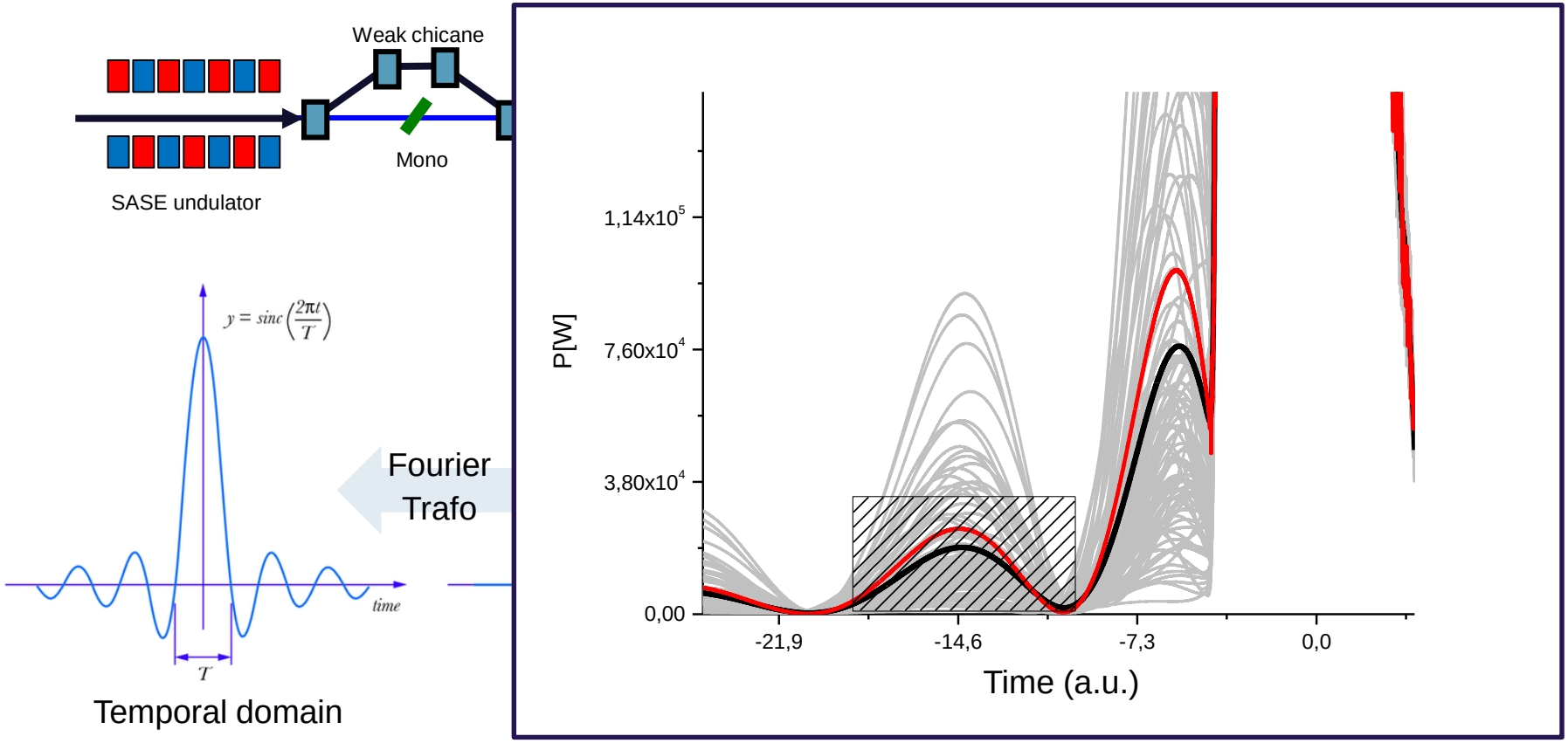
Hard X-ray Self Seeding - Principle



G. Geloni, V. Kocharyan, E. Saldin 'A novel self-seeding scheme for hard X-ray FELs', Journal of Modern Optics 58, 16 1391 (2011)

Courtesy G. Geloni et al.

Hard X-ray Self Seeding - Principle



G. Geloni, V. Kocharyan, E. Saldin ‘A novel self-seeding scheme for hard X-ray FELs’, Journal of Modern Optics 58, 16 1391 (2011)

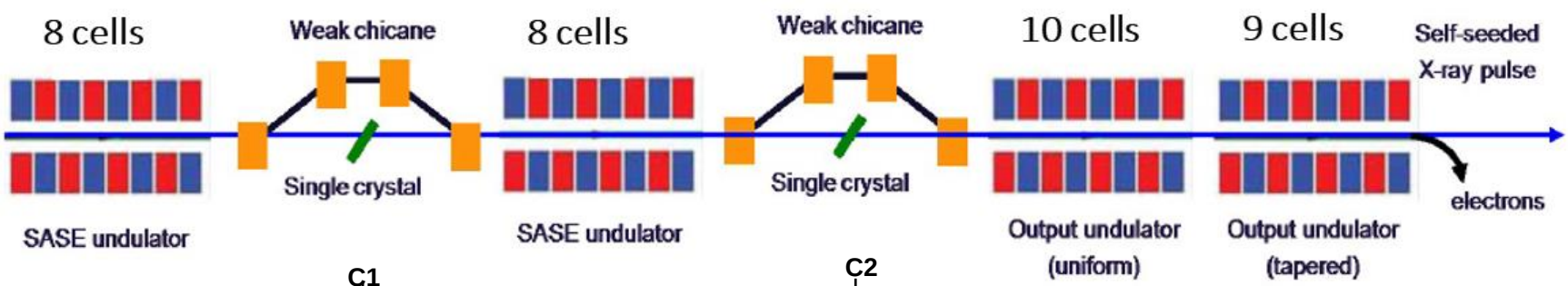
Courtesy G. Geloni et al.

HXRSS system at EuXFEL

Long undulators (175m magnetic length at SASE2) → Tapering

High repetition-rate. Overall, more pulses but:
Larger heat-load. For example HXRSS:
→ ω-shift beyond Darwin width (conservative)
→ Spectrum broadening
Two sources:
→ SR
→ FEL-based : depends heavily on photon energy

The double-chicane setup can be used to ease the FEL-based heat load



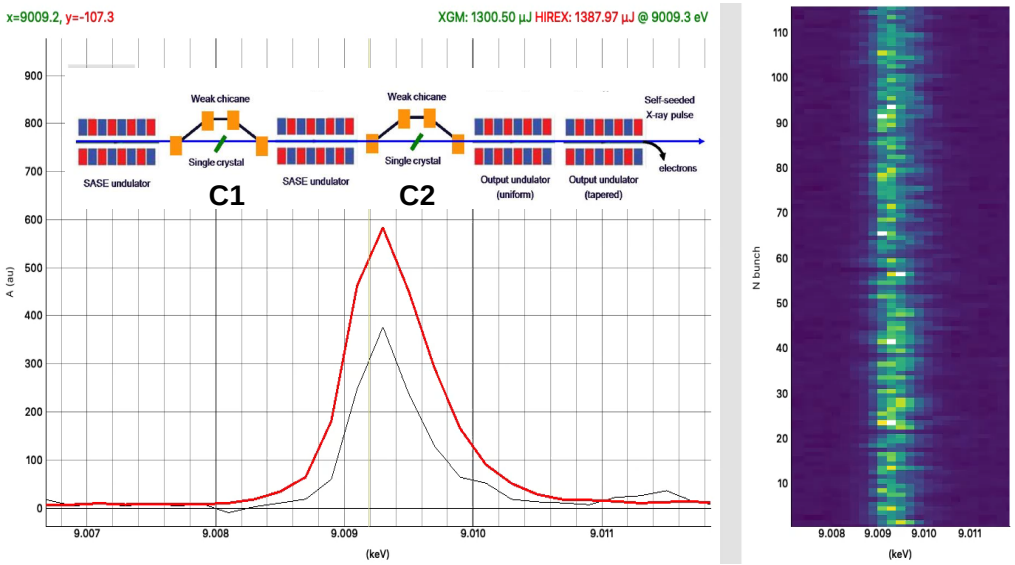
C1
↓
SASE
-"large" BW s_{SASE}
- Power P

C2
↓
Seeded
-"narrow" BW s_{seed}
- Power P

Larger spectral density (seeded signal) Compared to one-chicane

October 2020: Seeding up to 1300uJ

Courtesy G. Geloni et al.



Up to 1300uJ total energy in the pulse, C400, at 9keV nominal photon energy.

Background was measured by pitching crystal out of bandwidth, and amounted to about 500uJ

Measured FWHM bandwidth was ~ 0.7eV.

Resolution: 0.2eV/pixel

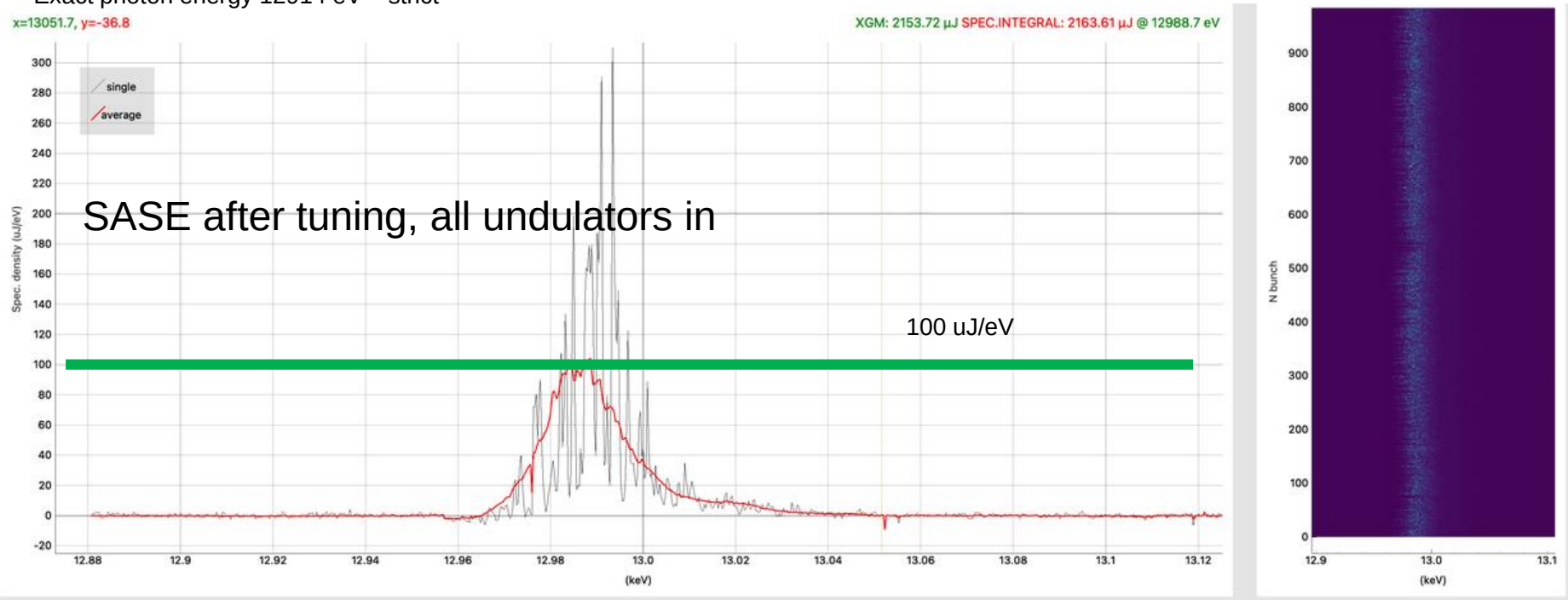
Black line: single shot spectrum. Red line: average spectrum over the same pulse in different trains

We went up to 400 pulses per train at 2.2MHz (decreasing amplification not to destroy the hirex spectrometer) : no heat loading effect visible at 9keV

Courtesy G. Geloni et al.

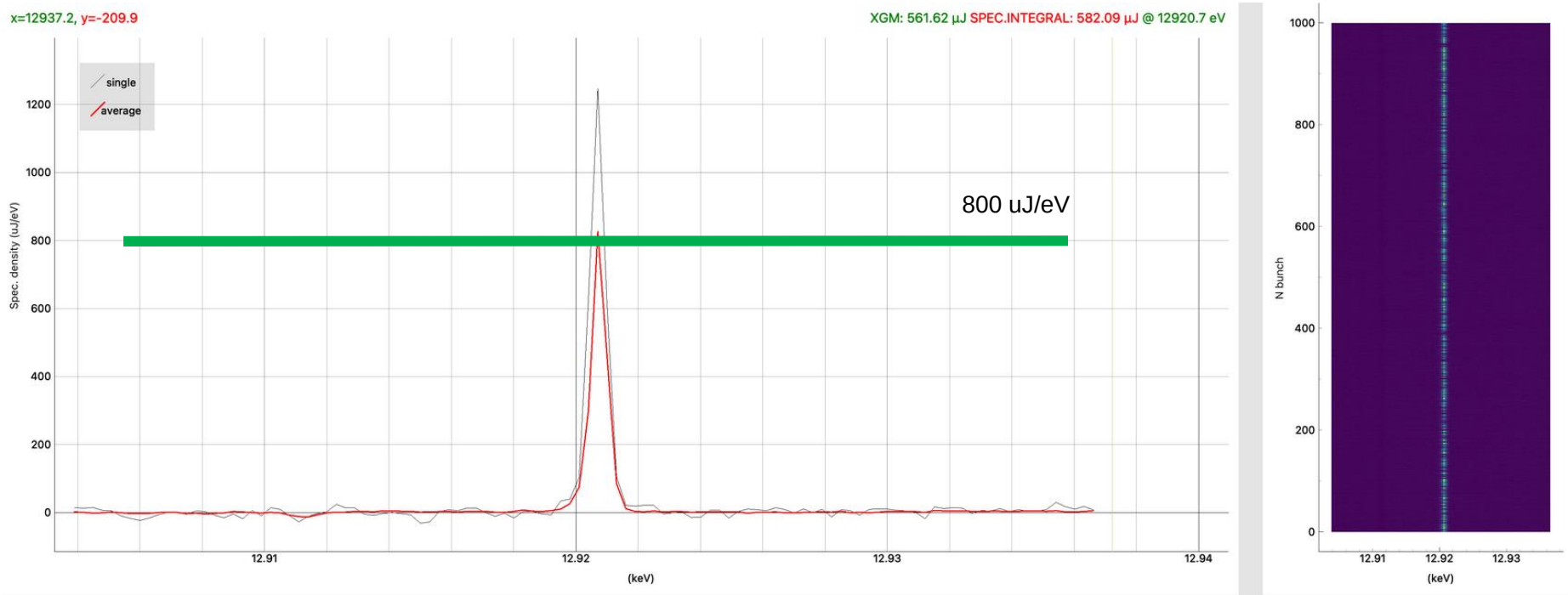
Update on HXRSS performance:
→User delivery at HED after BBA, 16.3GeV

Wanted 1-10 pulses
Exact photon energy 12914 eV – strict



Update on HXRSS performance:
→User delivery at HED after BBA, 16.3GeV

Courtesy G. Geloni et al.



Seeded: x8 higher spectral density

Special Operation Modes

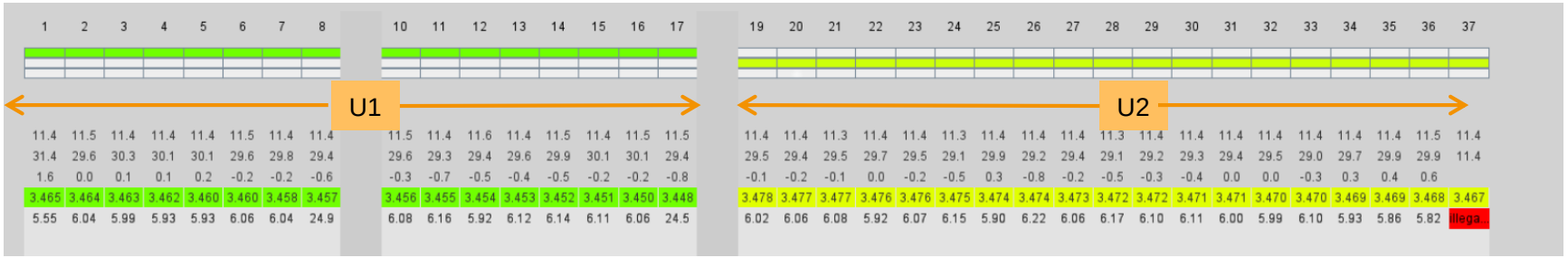
delivery modes beyond SASE at a nominal electron energy of 14 GeV.
Please contact the FEL R&D group for further details.

2 Pulse Options – SA2 Self-Seeding

7 - 10 keV	BW ~1eV FWHM 400-700uJ in the seeded BW	Has been delivered to users several times Up to 400 bunches/train with rep-rate up to 2.25MHz with some decay in intensity along the pulse train.
10 - 14 keV	BW ~1eV FWHM 200-400uJ in the seeded BW	
14 - ? keV	To be investigated	

Undulator setup

Courtesy G. Geloni et al.



Long undulators
(175m magnetic length at SASE2)

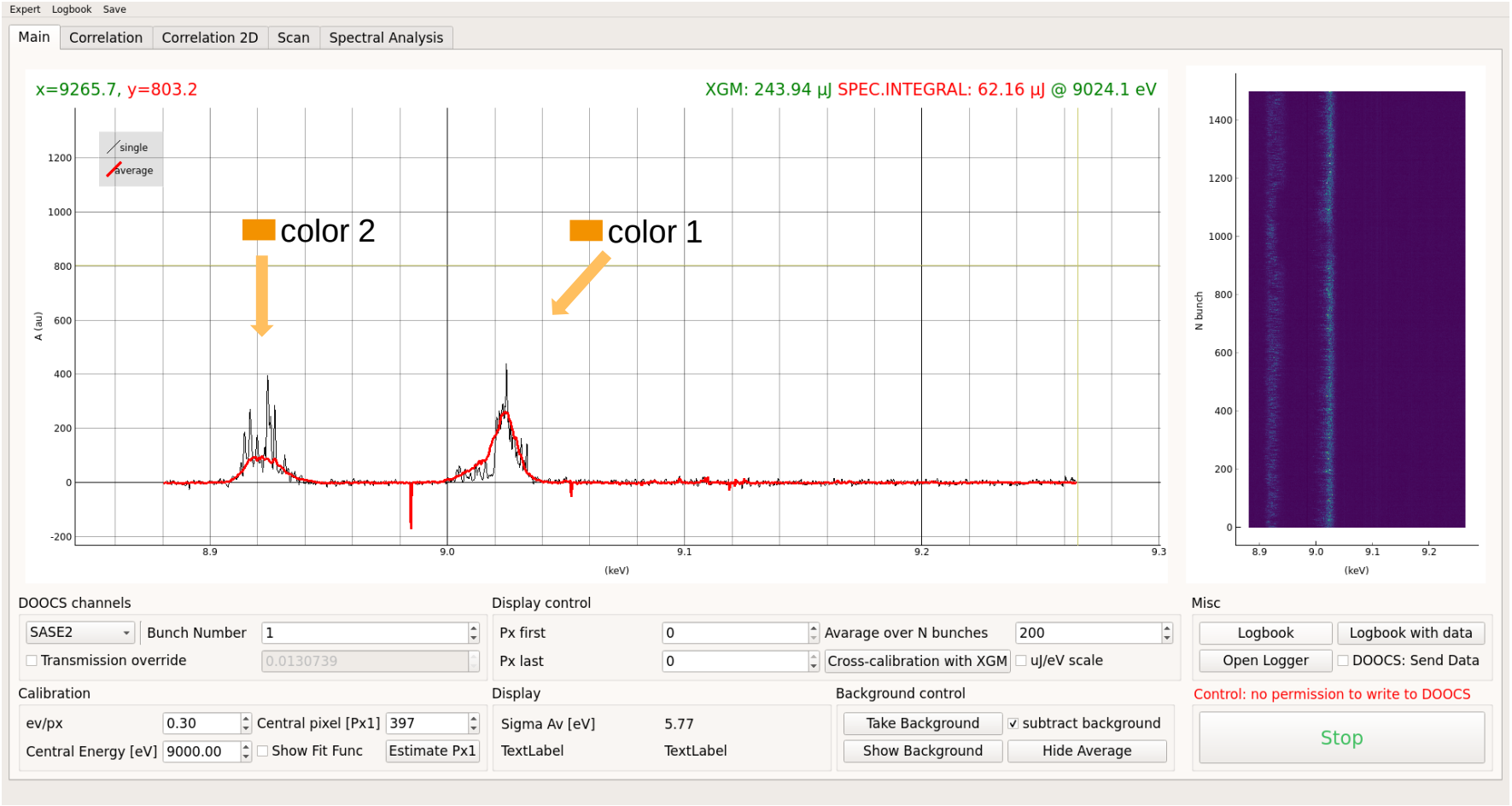
- 9 keV with 100 eV separation
- Concept
  - undulator gain length at 9 keV is shorter than 175 m
  - Split undulators in 2 parts, with different gap (change K)

$$\lambda_e = \frac{\lambda_u}{2\gamma^2}\left(1+\frac{K^2}{2}\right)$$

Two color pulses

Courtesy G. Geloni et al.

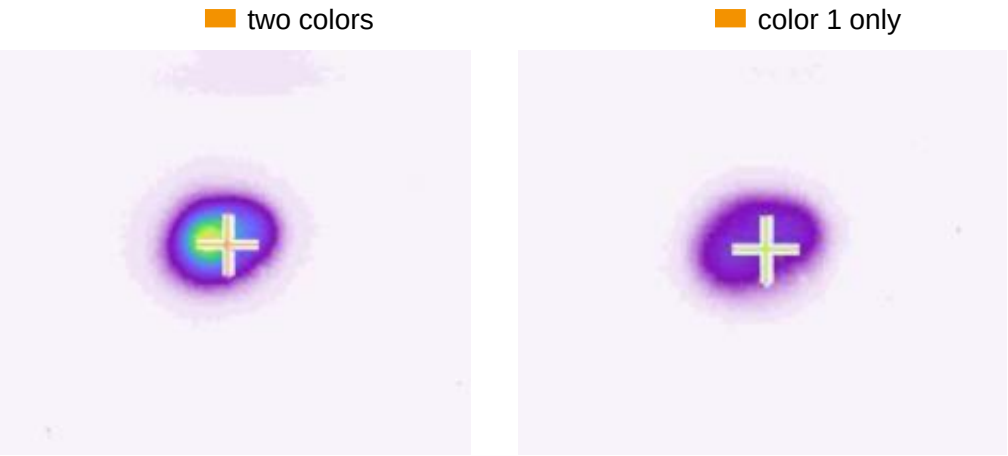
- above 100uJ each color, slightly different bandwidth

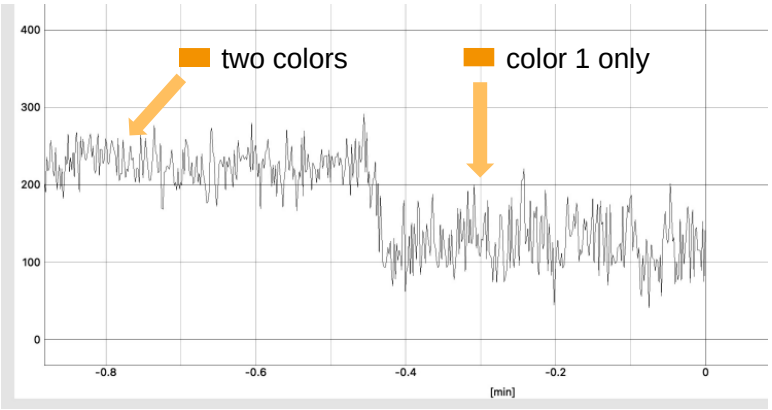


Two color pulses

Courtesy G. Geloni et al.

- above 100uJ each color
- different bandwidth
- good overlap





Special Operation Modes

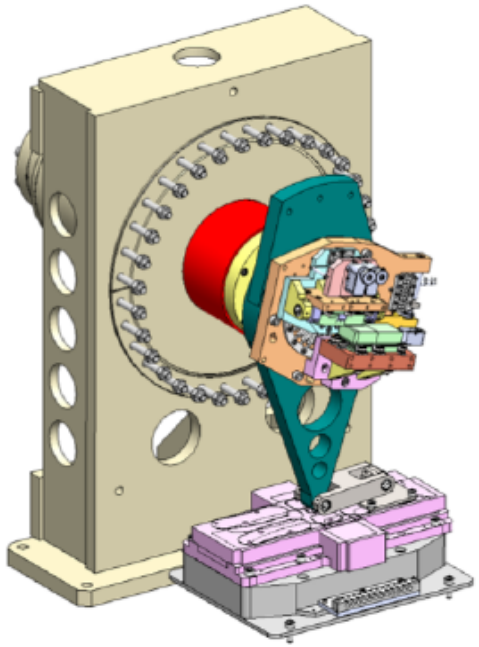
delivery modes beyond SASE at a nominal electron energy of 14 GeV. Please contact the FEL R&D group for further details.

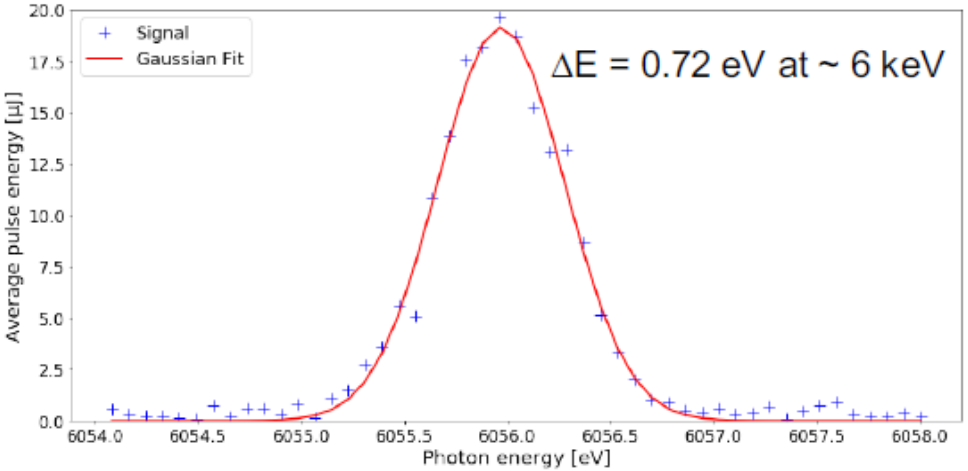
- **2 Pulse Options – SA2 split undulators**

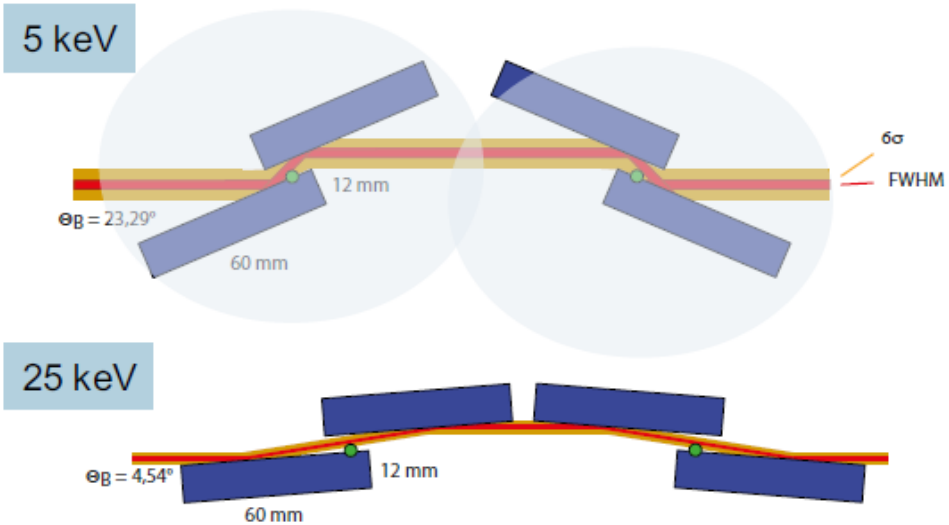
7 - 10 keV	>100 uJ/pulse •Pulse length of maximal 30 fs for each color •Delay between 5 fs and 300 fs (temporal pulse overlapping possible with a minimal color separation of 50 eV) •No zero-delay-crossing	This setup has been tried several times in machine setup

Monochromator

- 4-bounce, Si_{111} crystals
- Beam size: 6σ
- Energy range: 5 - 25 keV (24.5° - 4.5°)
- Working range up to now: 6 - 9 keV
- Cryogenically cooled
- $\Delta E/E = 10^{-4}$



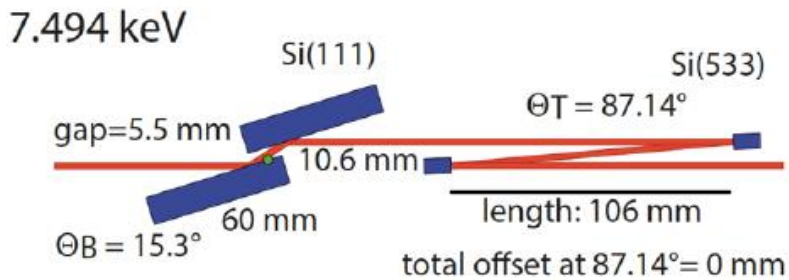


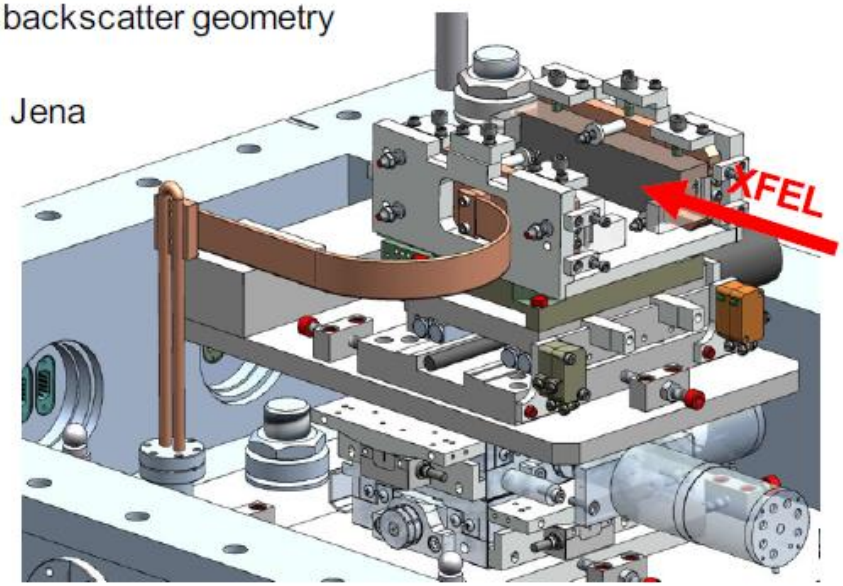


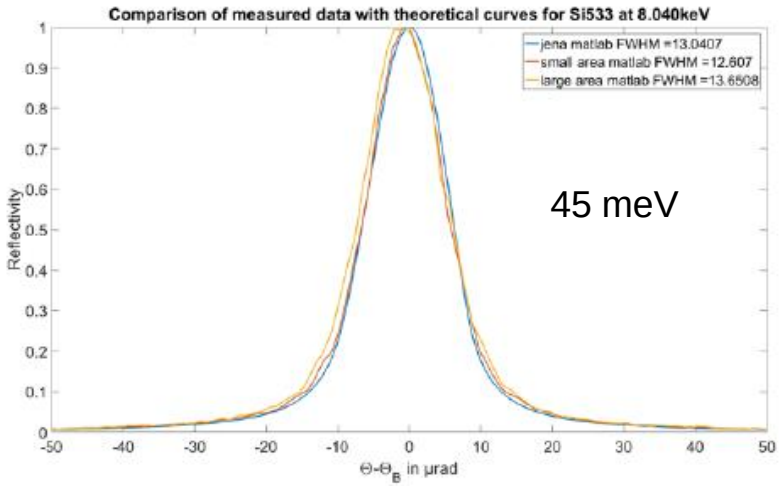
Zastrau, Appel, Baehtz et al., J. Synchrotron Rad. (2021). 28, 1393–1416

High-resolution monochromator

- First 2 crystal of standard mono + Si_{533} crystals in backscatter geometry
- Design being finalized by FMB Oxford
- Crystal was cut, prepared by X-ray optics group in Jena







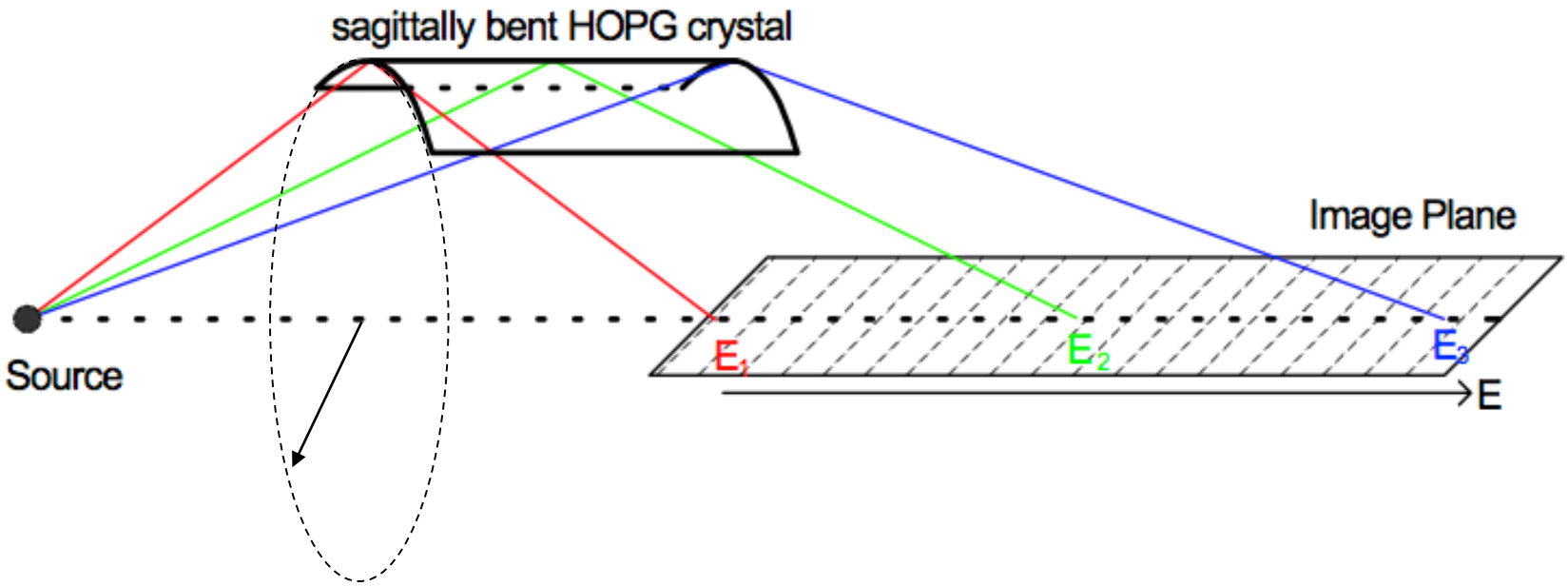
Four different bandwidths:

- $\Delta E/E = 10^{-3}$: SASE
- $\Delta E/E = 10^{-4}$: Si_{111} monochromator
- $\Delta E/E = 10^{-4}$ - 10^{-5}: seeded (E: 5 - 14 keV)
- $\Delta E/E = 10^{-6}$: Si_{533} ➔ 7.494 keV

Wollenweber et al., Review of Scientific Instruments 92, 013101 (2021)

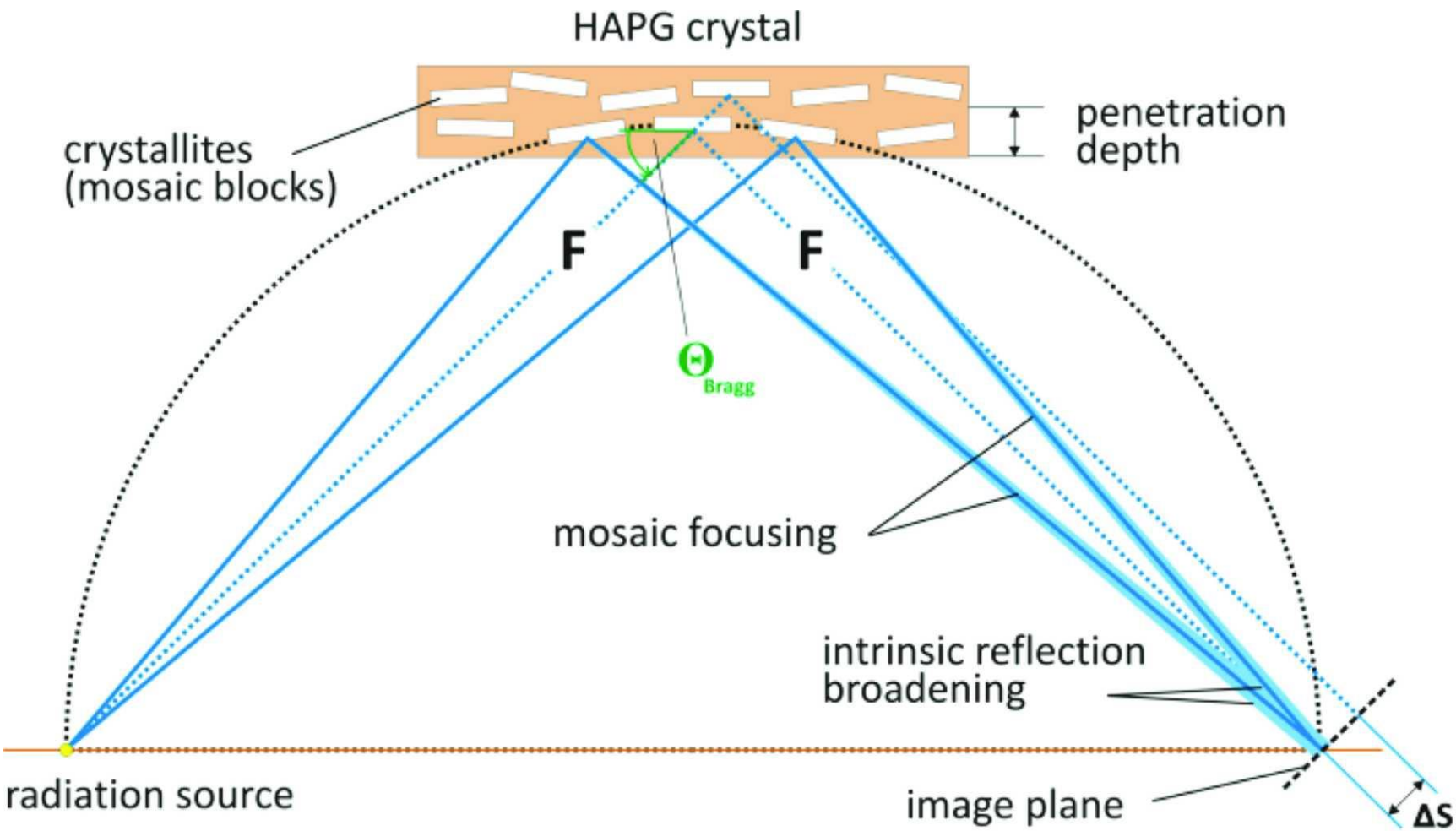
Von-Hámos scheme

Cylindrically bent crystal, source point and spectrum are located at the cylinder axis.



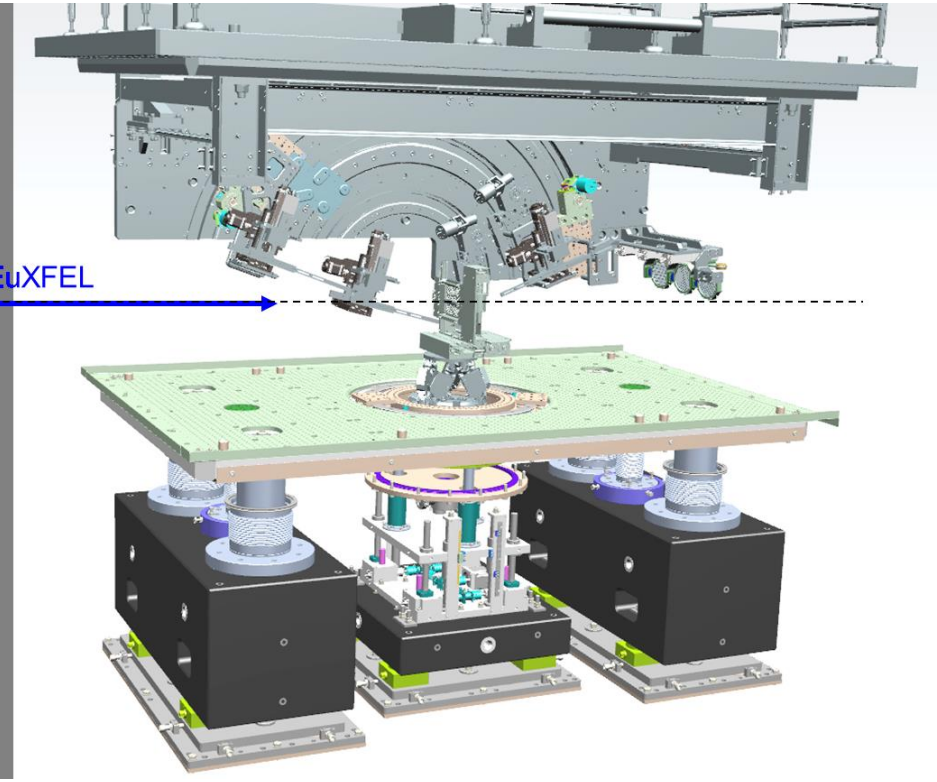
Röntgenspektroskopie und Abbildung mittels gekrümmter Kristallreflektoren. I. Geometrisch-optische Betrachtungen
(x-ray spectroscopy and imaging using curved crystal reflectors. I. geometrical-optical view.)
Hámos, L. V., Annalen der Physik, vol. 409, Issue 6, pp.716-724

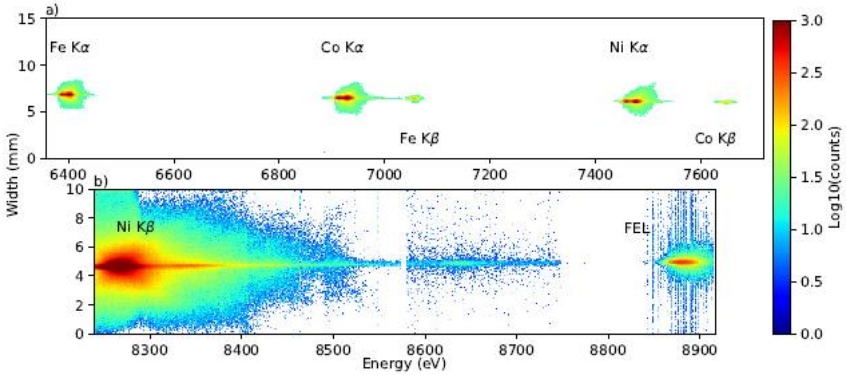
Mosaic crystals – dispersive focusing, broad R curve

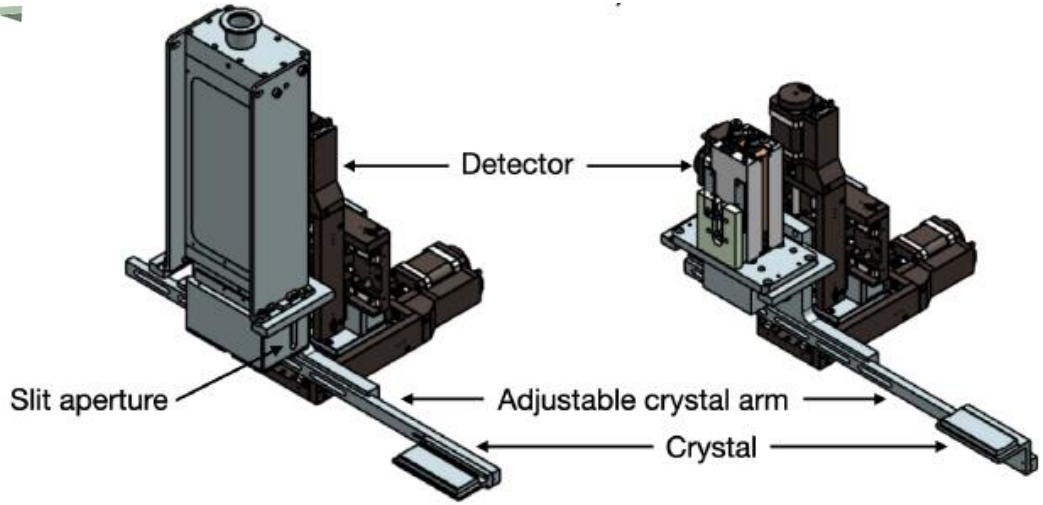


Mosaic graphite von-Hamos spectrometer

Inside IC1, we offer von-Hamos HAPG spectrometers



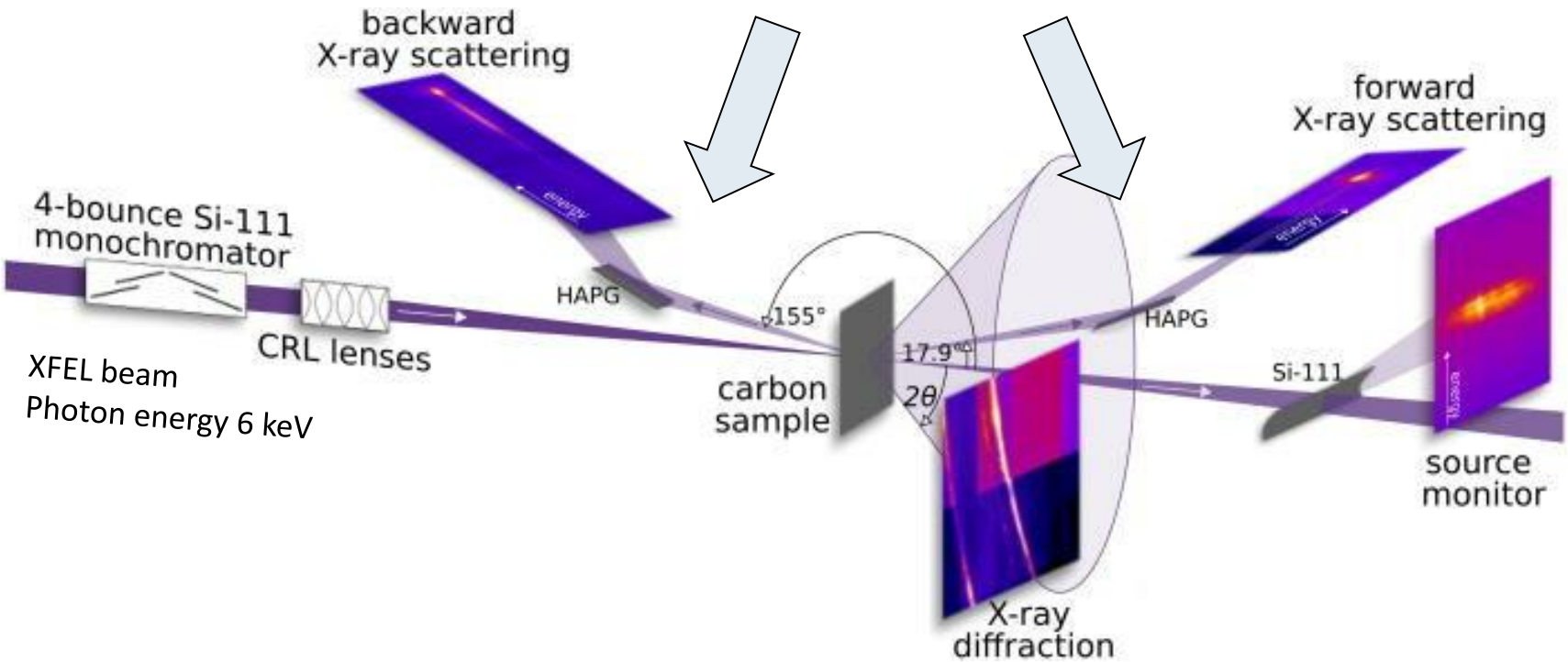




Preston et al., Journal of Instrumentation, Volume 15 (2020)

X-ray inelastic scattering (Kraus, Voigt et al.)

Using HEDs HAPG spectrometers



XFEL beam
Photon energy 6 keV

Voigt et al., Physics of Plasmas 28, 082701 (2021)

Demonstration of an x-ray Raman spectroscopy

Voigt et al., Physics of Plasmas 28, 082701 (2021)

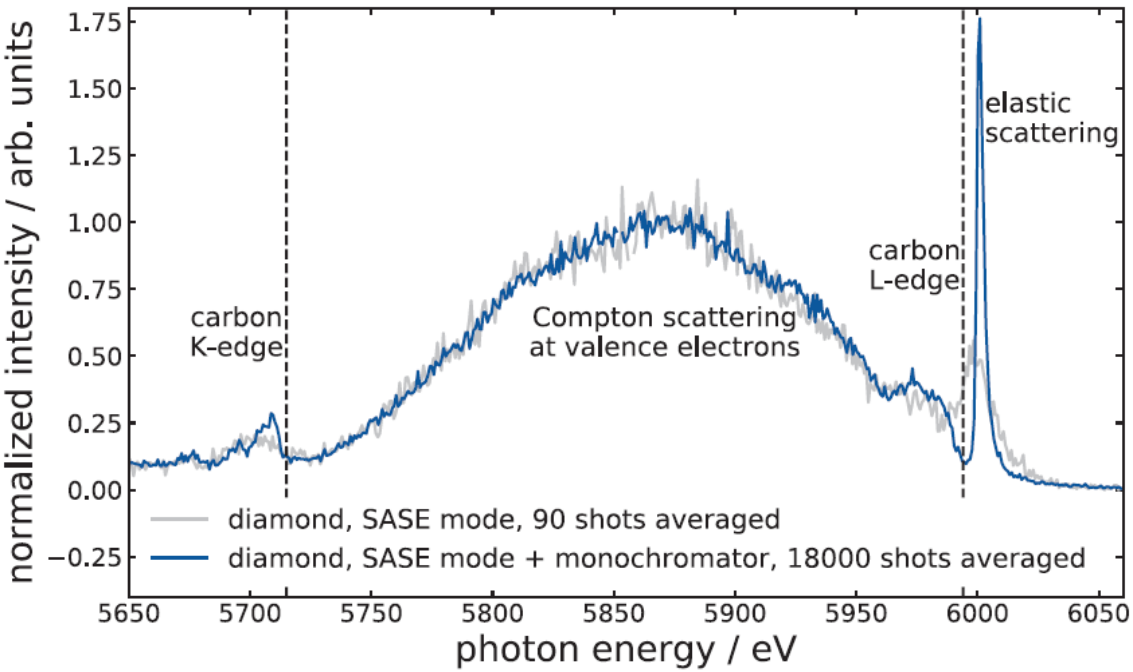


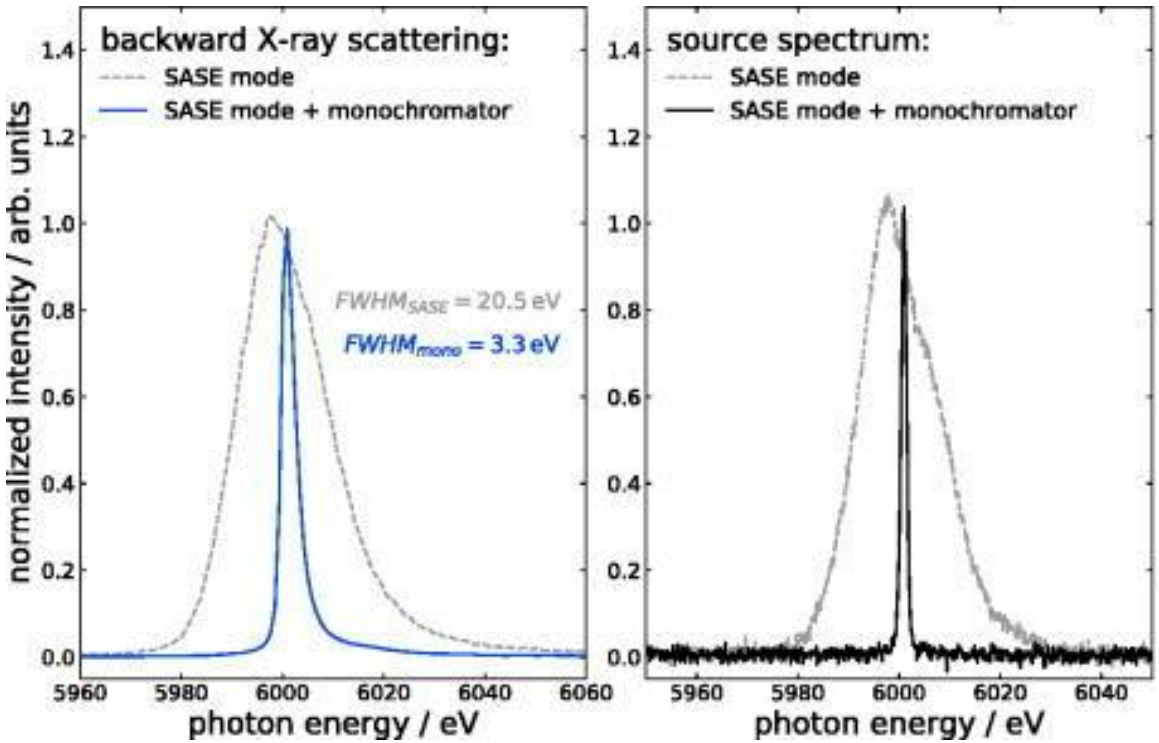
FIG. 2. Backward x-ray scattering spectrum from diamond normalized to the inelastic signal maximum. Gray: SASE mode (average x-ray pulse energy of 1650 μJ). Blue: monochromatic x-rays (average x-ray pulse energy of 17 μJ). Dashed lines indicate the carbon K-edge at $\sim$285 eV and L-edge energies at $\sim$6 eV below the elastic scattering peak.

User quote: "*High quality spectra have been obtained showing the outstanding capabilities* of the HED instrument ready to be exploited once the HIBEF drivers are available*."

* Preston et al., "Design and performance characterisation of the HAPG von Hámos Spectrometer at HED", JINST 15 (11), P11033 (2020)

PI: Dominik Kraus, Univ. Rostock

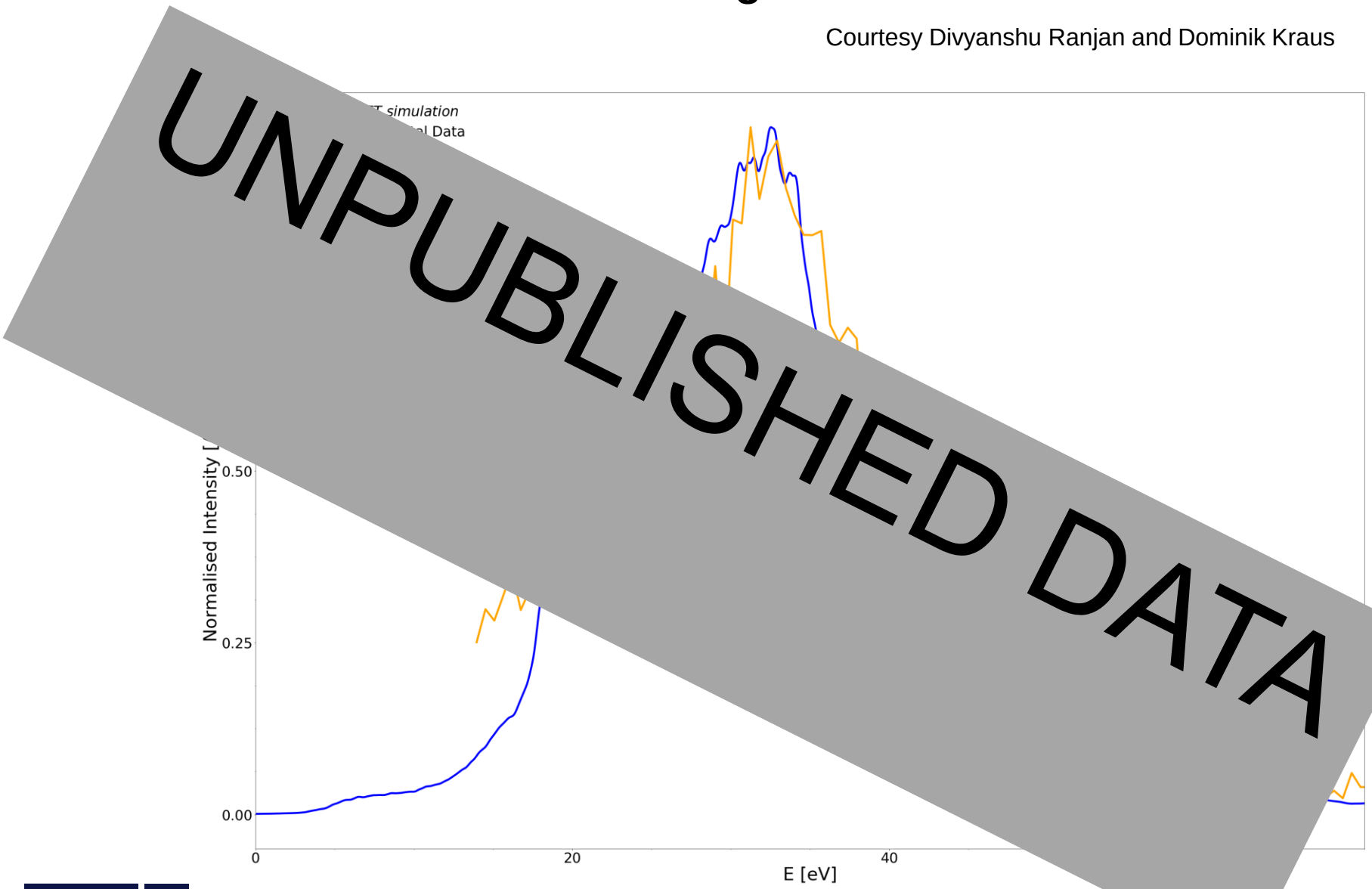
Few-eV resolution inelastic x-ray scattering with HAPG



Voigt et al., Physics of Plasmas 28, 082701 (2021)

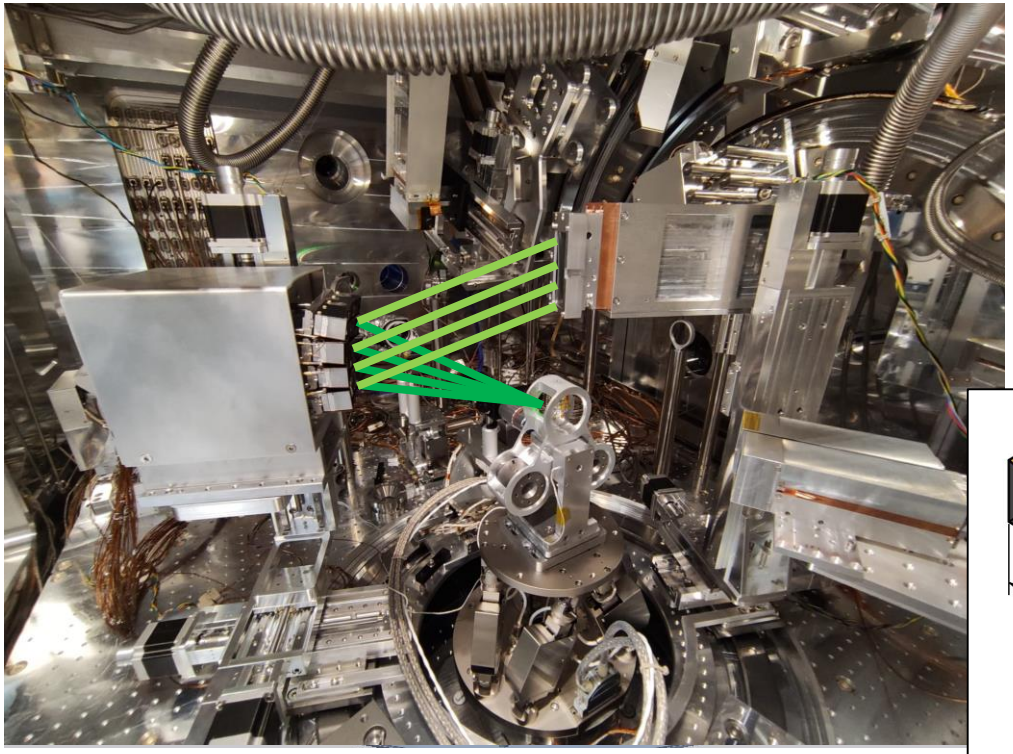
Monochromatized SASE scattering from diamond

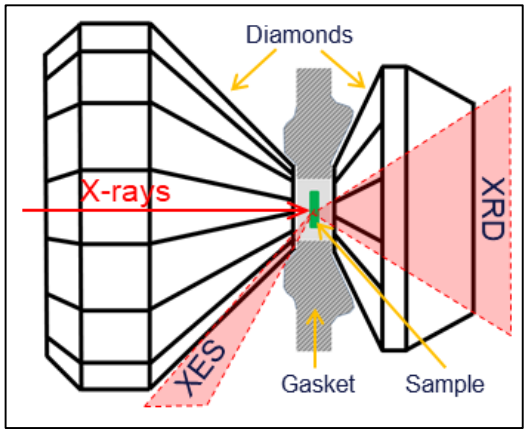
Courtesy Divyanshu Ranjan and Dominik Kraus



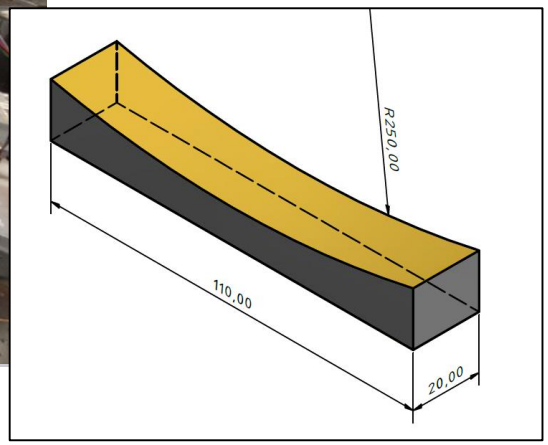
vH spectrometer for measurements from DACs in IC1

Courtesy J. Kaa





Kaa et al. 2022, submitted



Available crystal cuts:

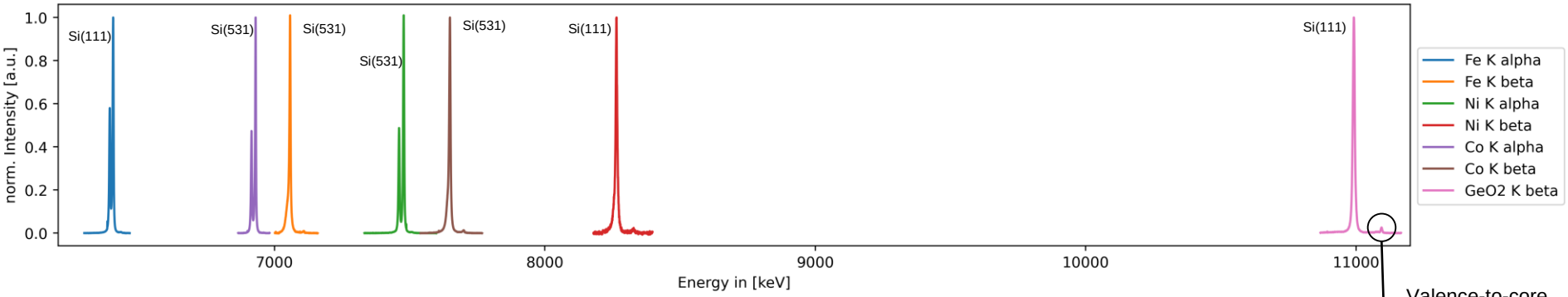
- **Si(531)**
- **Si(111)**
- Si(533)
- Si(511)
- Ge(220)
- Ge(111)

Si531 and Si111 available now, the others from mid-2022

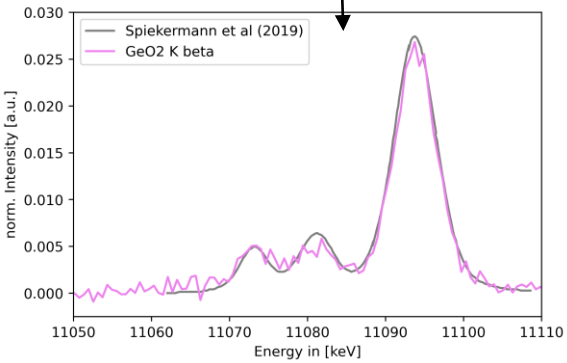
Spectrometer specification on free standing foils

Courtesy J. Kaa

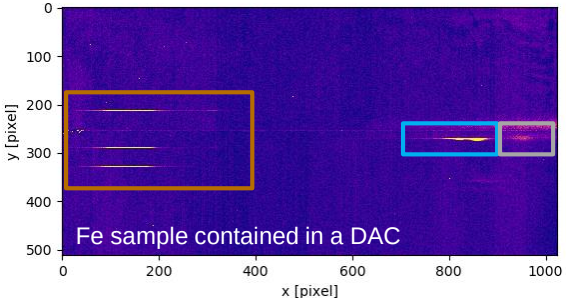
5 min aquisition time



Valence-to-core signal

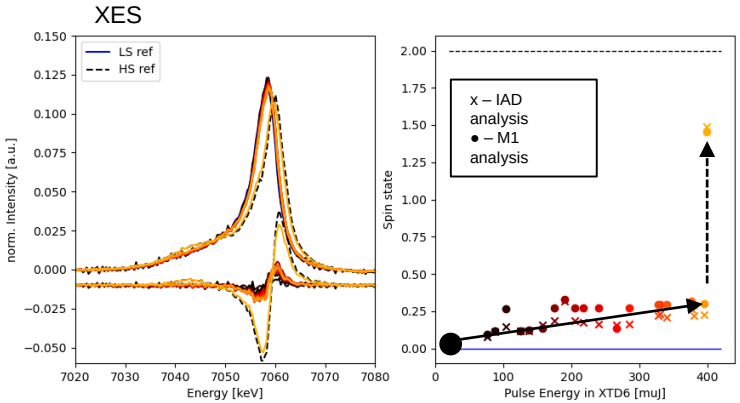


- Energy range: 6 keV - 12 keV
- Energy dispersion: ~0.4 eV/pixel (JF detector)
- Instrumental broadening: ~0.5 - 1 eV
- Multi-fluorescence spectroscopy e.g.:
  - Si(531) for Fe K beta
  - Si(333) for Fe K alpha
  - Si(444) for Re L alpha (~12 keV)

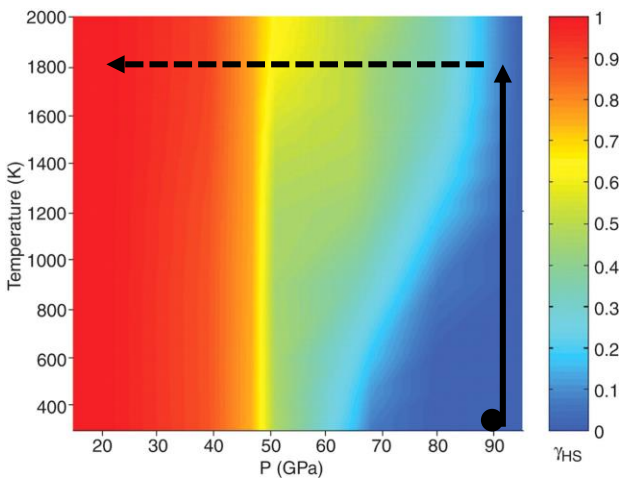


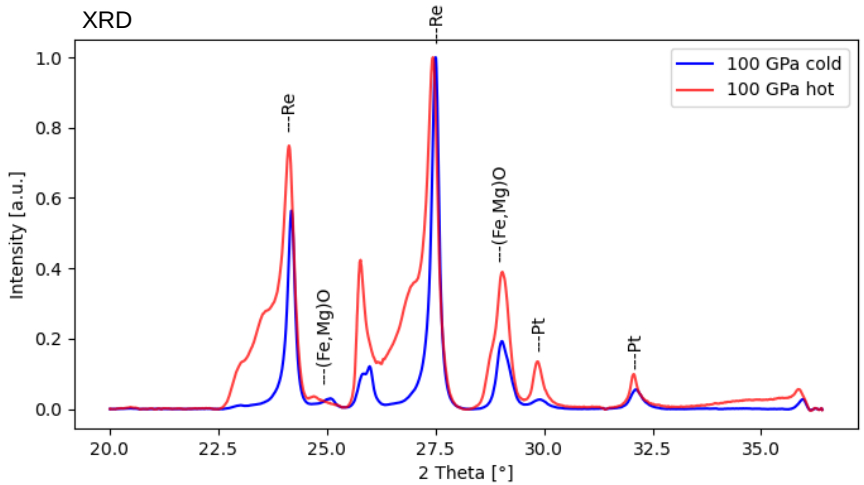
Example: Spin state of (Fe,Mg)O at pT conditions of the Earth's core

Courtesy J. Kaa



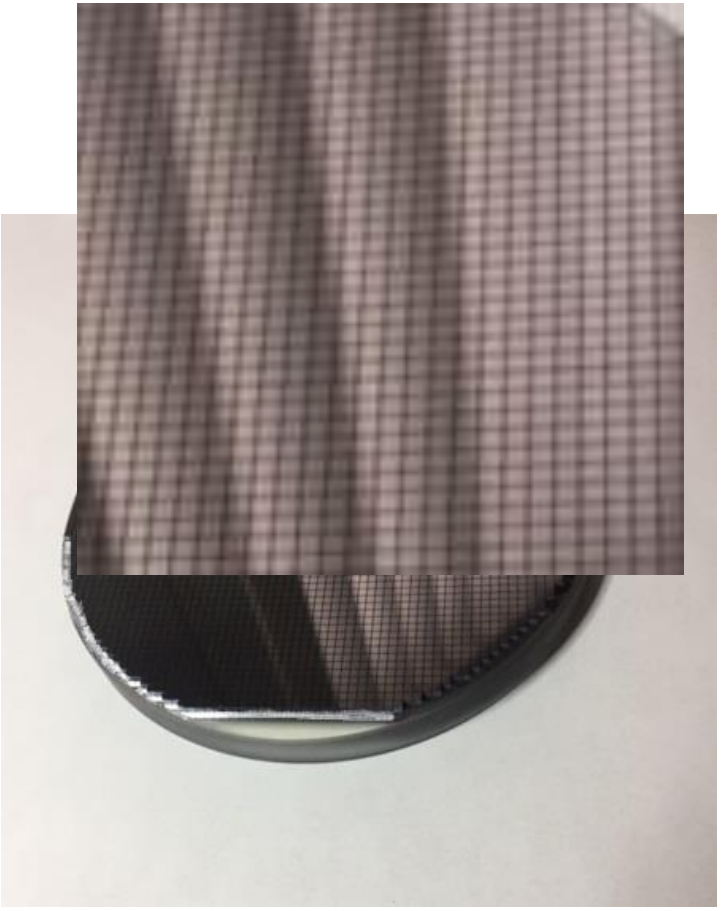
- Kβ fluorescence from $(Fe_{0.5},Mg_{0.5})O$ at ~**100 GPa**
- Pulsed X-ray heating up to 1800 K
- Low-spin to High-spin change due to pressure loss

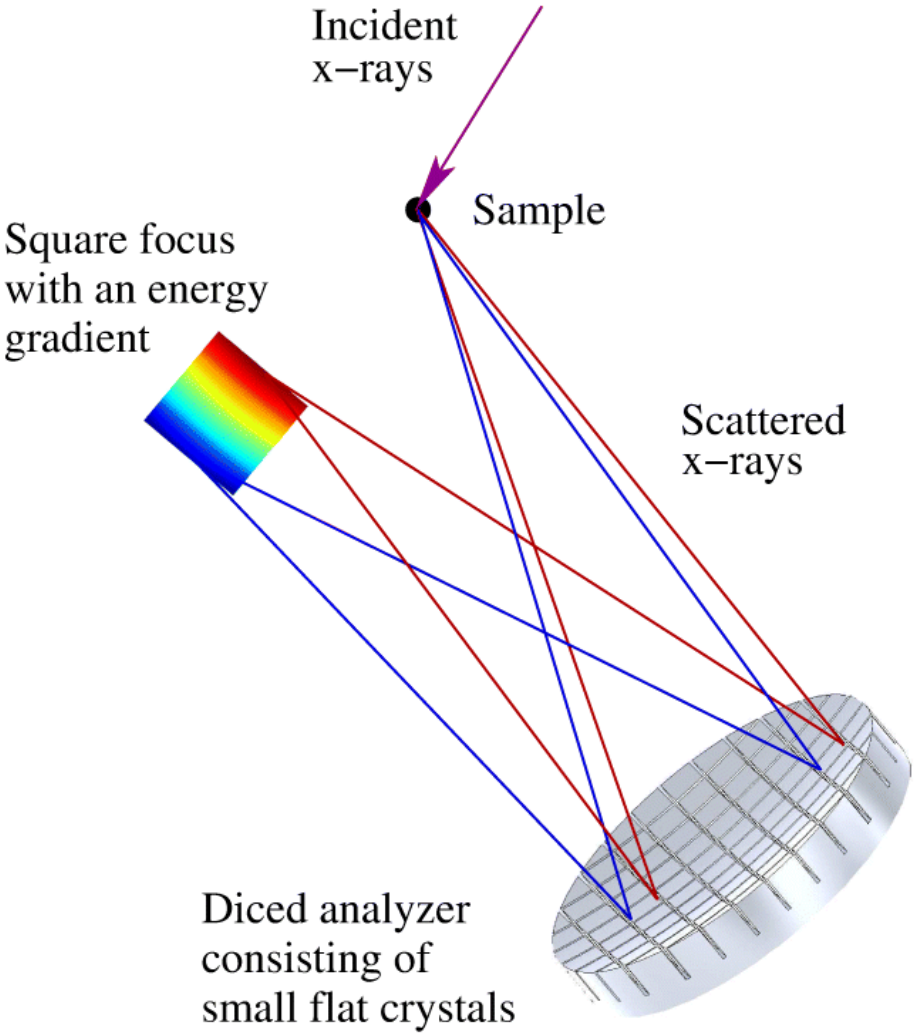




Lin et al 2007: doi: 10.1126/science.1144997#

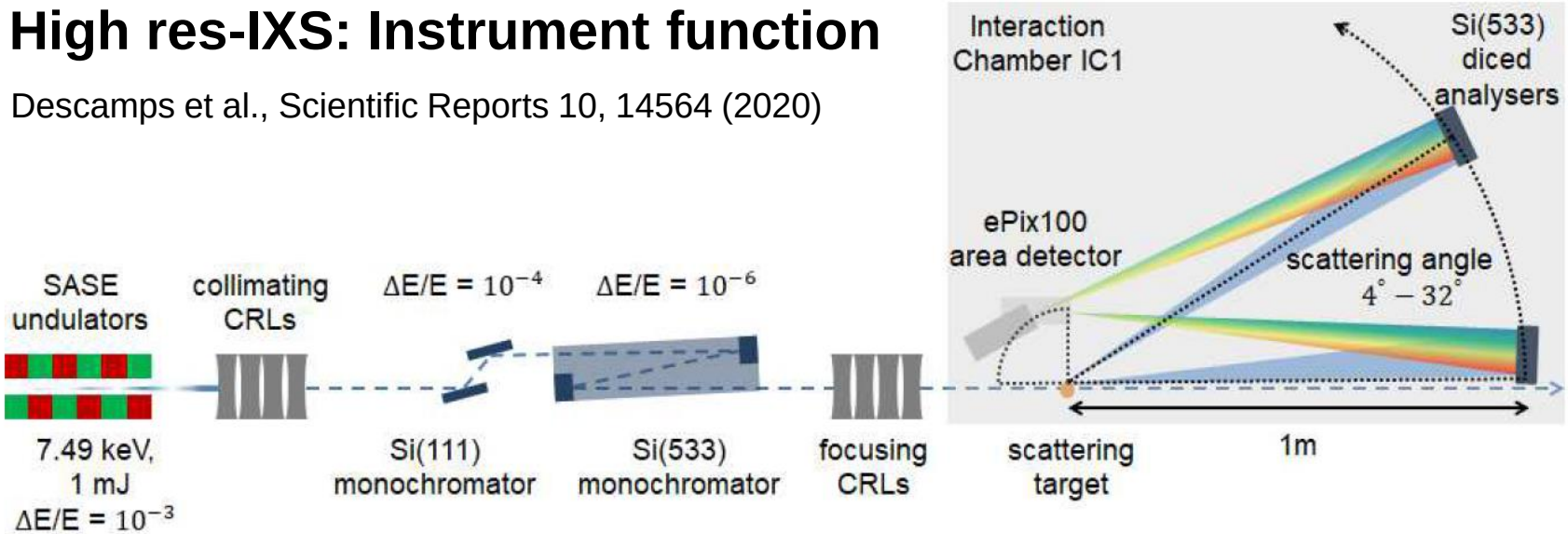
Diced analyzer crystals





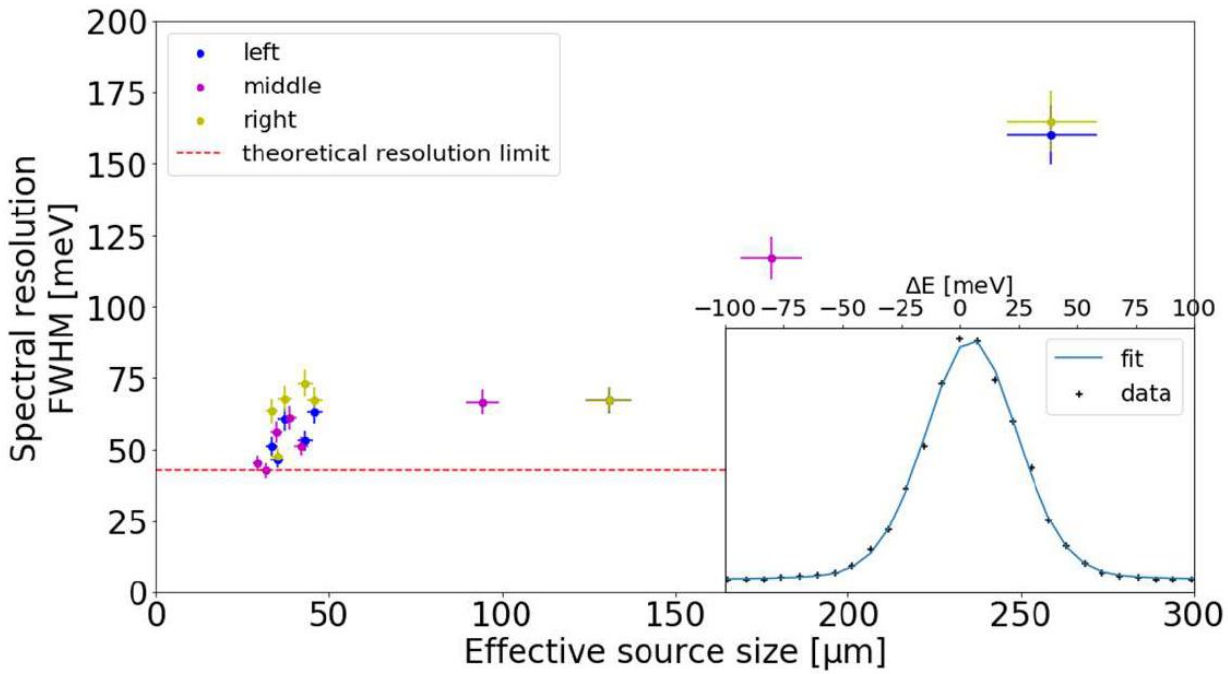
High res-IXS: Instrument function

Descamps et al., Scientific Reports 10, 14564 (2020)

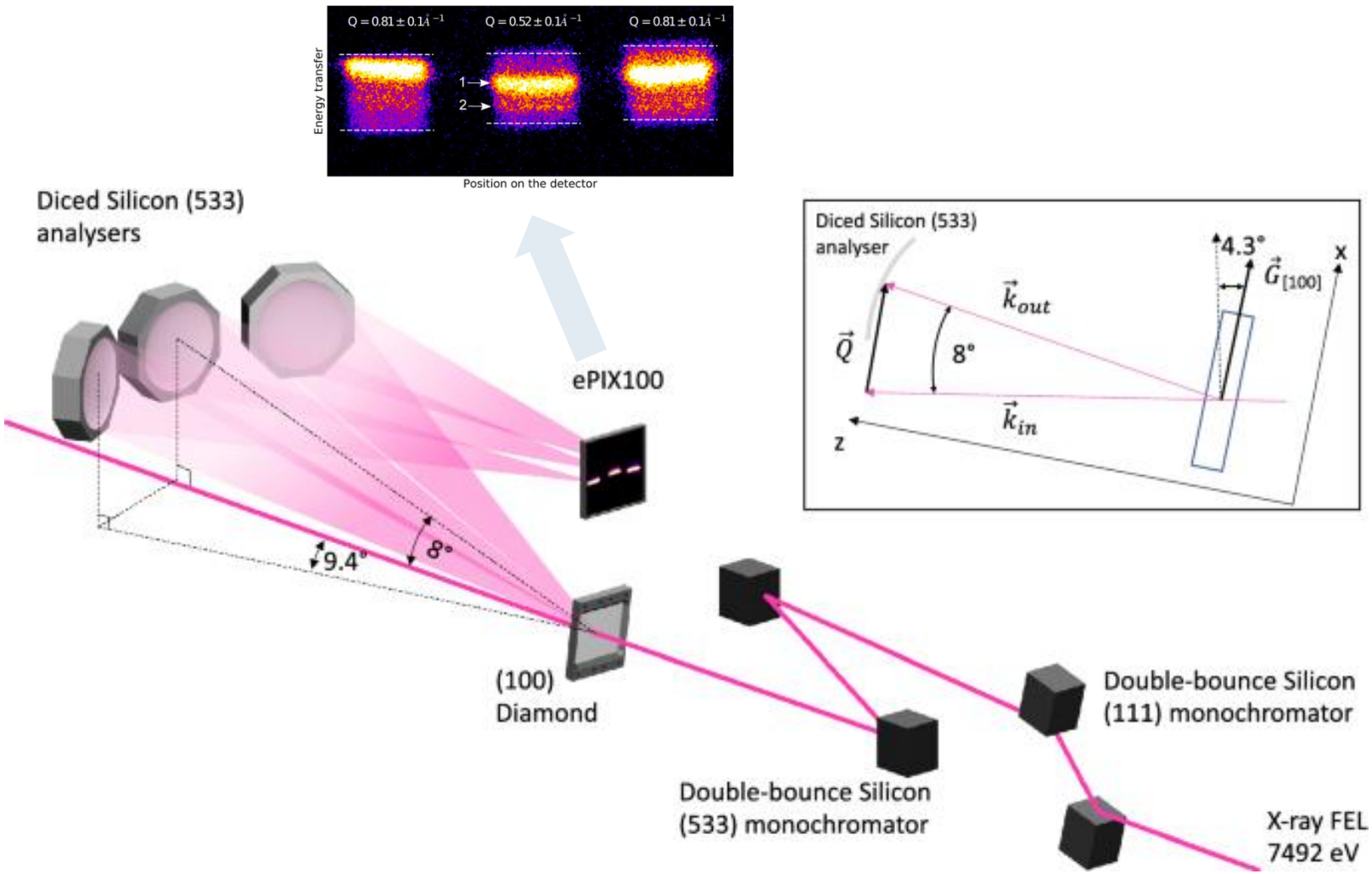


Thin samples yield close-to design spectral resolution

45 meV

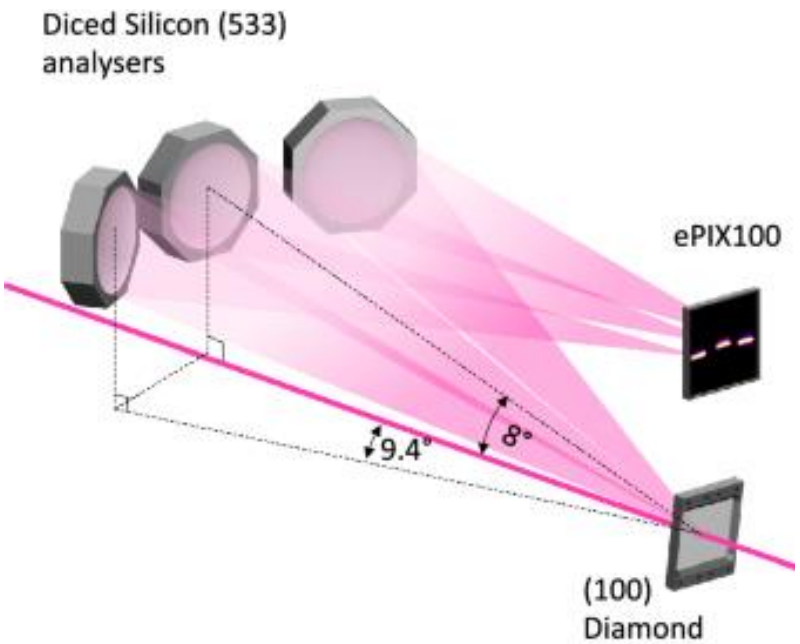


meV-IXS: measure instrument function, and then phonon dispersion from single crystal diamond

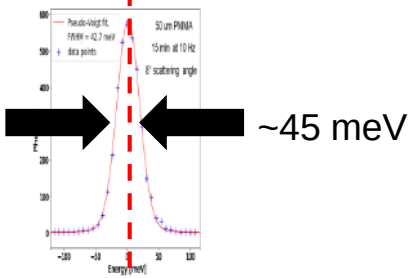


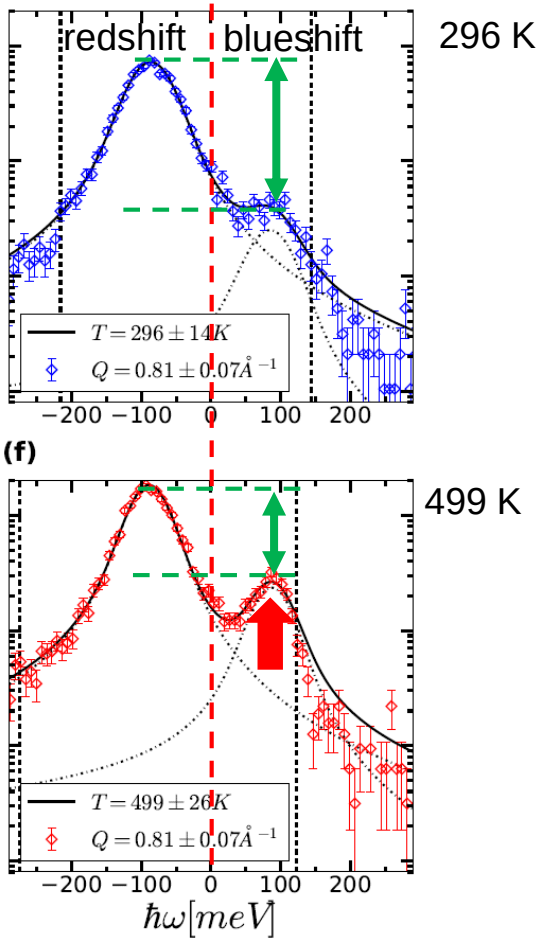
Descamps et al., Scientific Reports 10, 14564 (2020)

meV-inelastic scattering at HED



Instrument resolution (elastic)

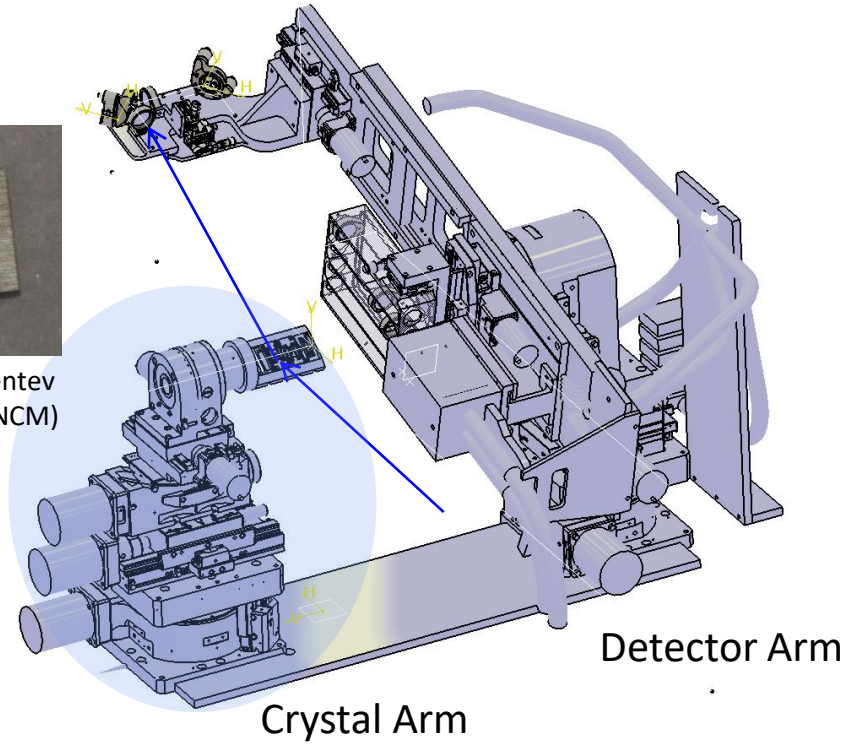


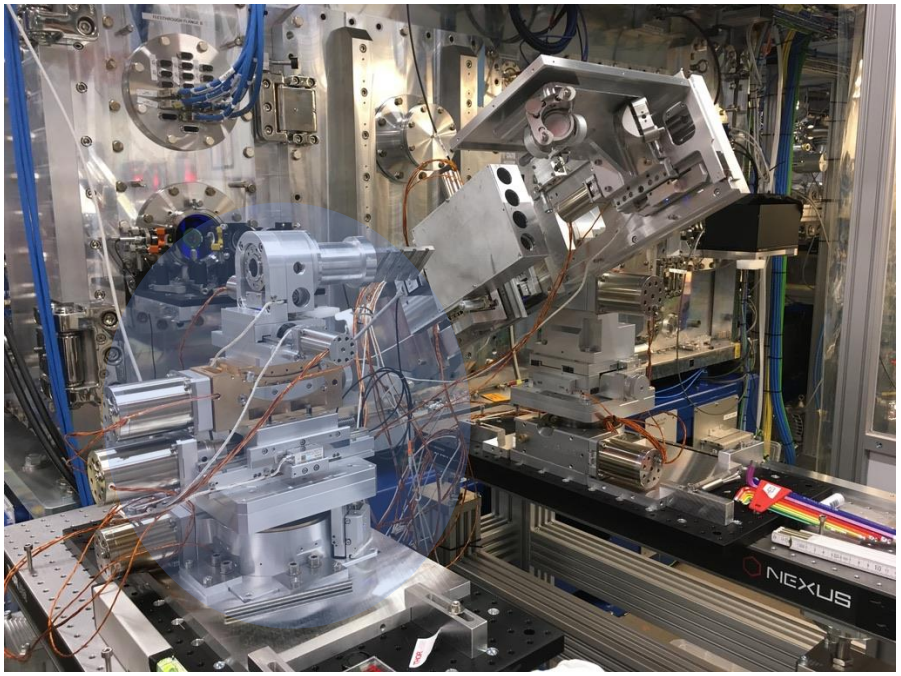


The CNRS spectrometer at HED

- Compact and vacuum compatible design to work in and out IC1 at HED
- From 5 to 25keV
- Energy resolution ~ 0.1 – 0.7eV at 7.12keV
- Multiple crystals and easy modifications (C* 110 and C* 111 100mm Radius of curvature, Si 111, 110 and 100 membranes with 50-100mm radius of curvature
- Full rotation of the arm to allow matching with upstream spectrometers

© S. Terentev
(FSBI TISNCM)

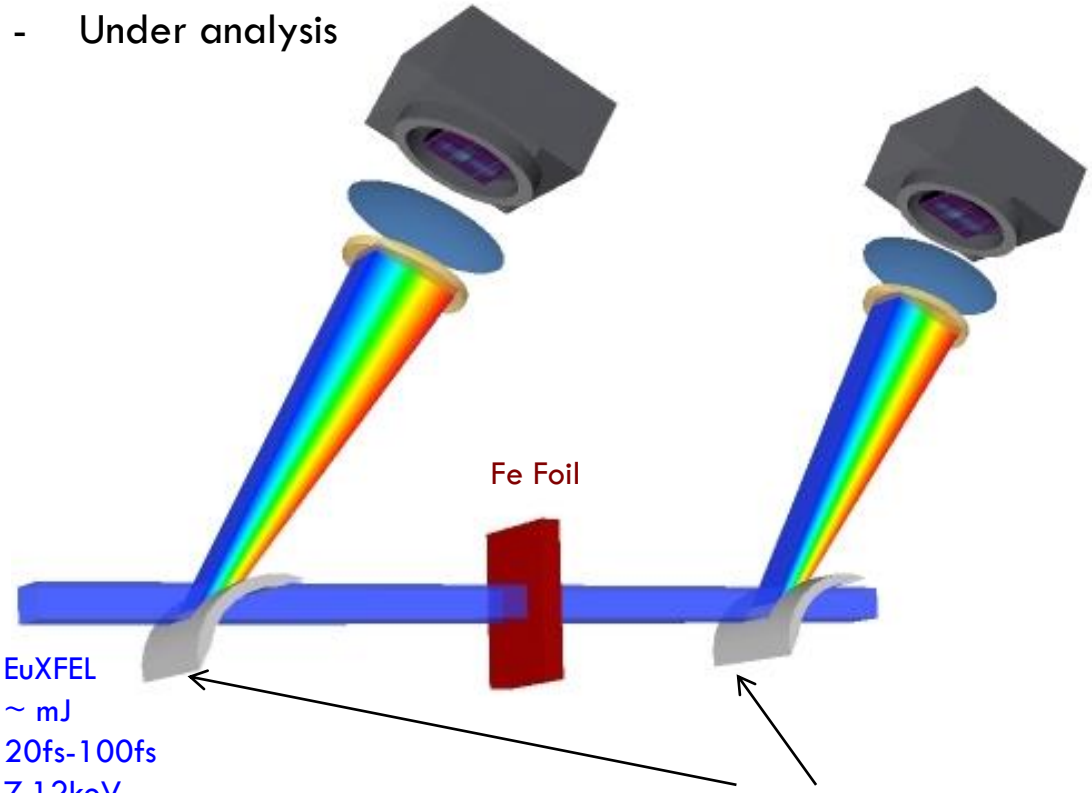




XANES Commissioning at HED

November 2021

- At 7.12 keV Fe K-edge
- Using HIREX 2 and HED-FLEX spectrometers in addition to the CNRS sepctrometer
- Tests for different configurations (focusing, collimated)
- Under analysis



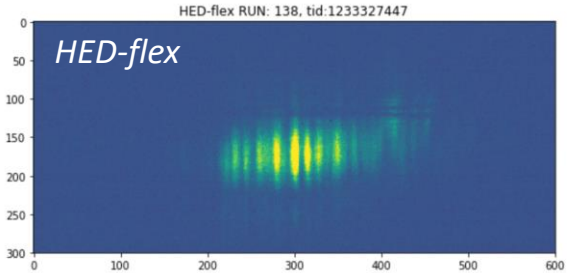
2 identical spectrometers
HIREX 2 & CNRS
CNRS & FLEX

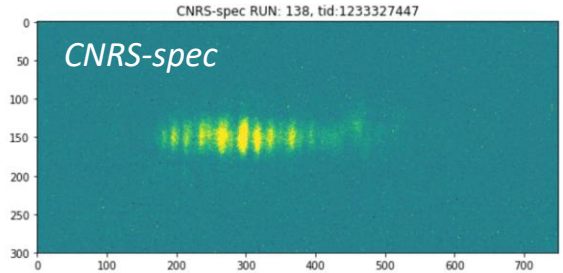
- 3 single shot identical spectrometers: Hirex 2 + CNRS and HED-FLEX at the HED endstation
- Correlation between spectrometers can be observed by the extinction of the signal of the 2nd spectrometer

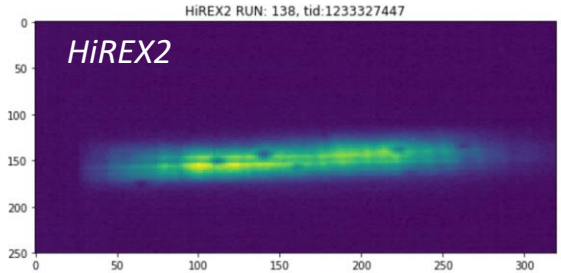
M. Harmand et al. Arxiv 2020

***M. Harmand**, F. Dorchies, J. Pintor*
***M. Makita, K. Appel**, C. Baehtz, L. Wollenweber, K. Buakor, C. Strohm, N. Kujala, R. Gautam, T. Michelat*
And the HED and support teams

Correlation between 3 spectrometers

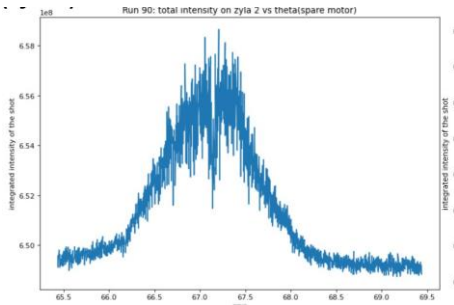


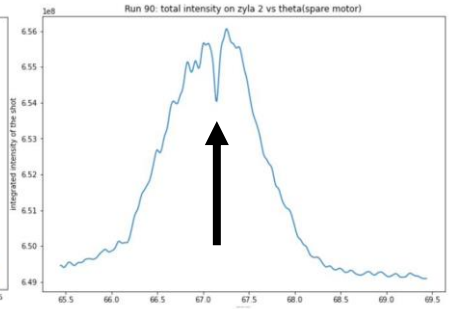


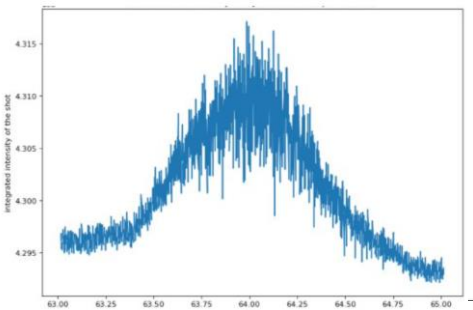


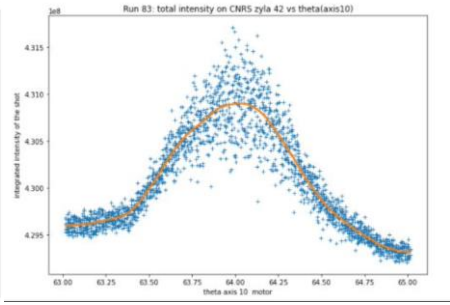
Extinction angle observed at ~ 67.14 deg on HED-FLEX

No clear extinction ➔ weak correlation





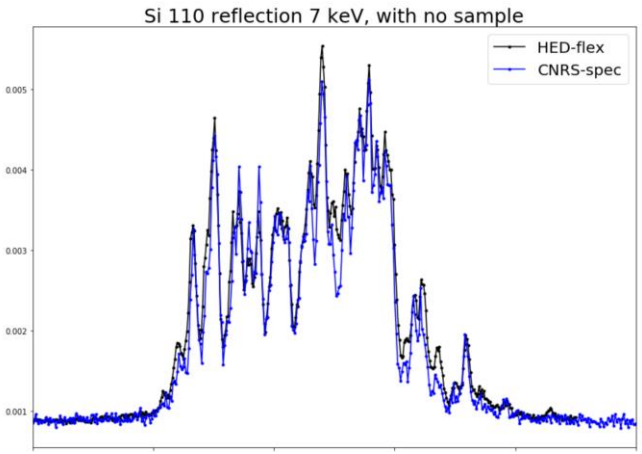


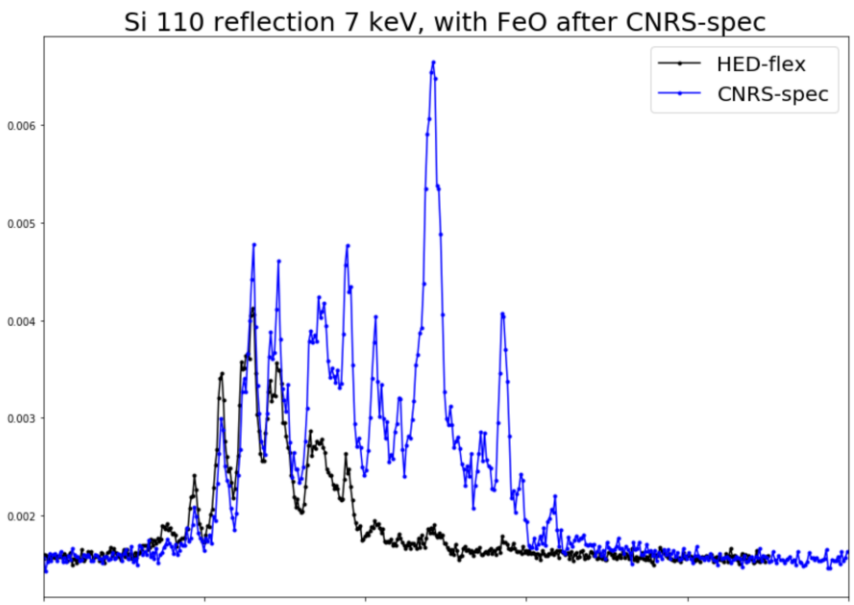


- Appearance of extinction angle corresponds to spectra-correlation ➔ possible for XANES
- no/weak correlation indicates strong wavefront modification between the two spectrometers

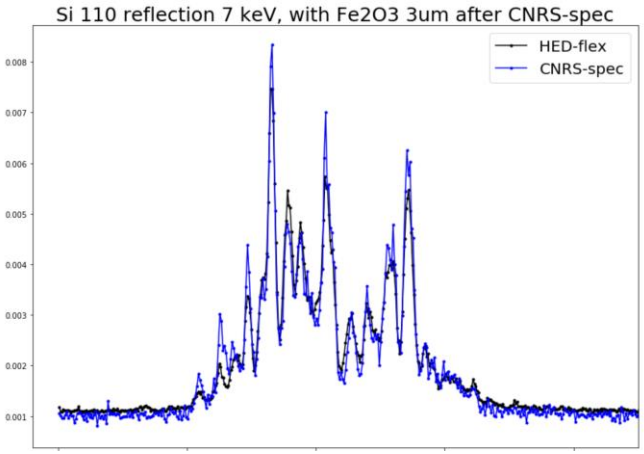
Single-shot spectra: first impressions

- Single-shot SASE FEL pulse correlation
  → generally in very good agreement
- **Absorption edge confirmed in single-shot: FeO**
- Under-investigation: Fe, Fe2O3, Fe3O4,…



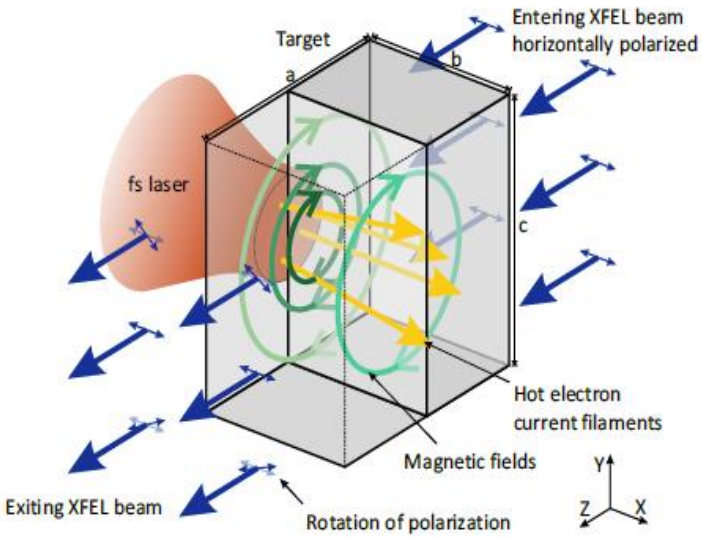


High eV ← 7.1 keV → Low eV



Goals for the upcoming years

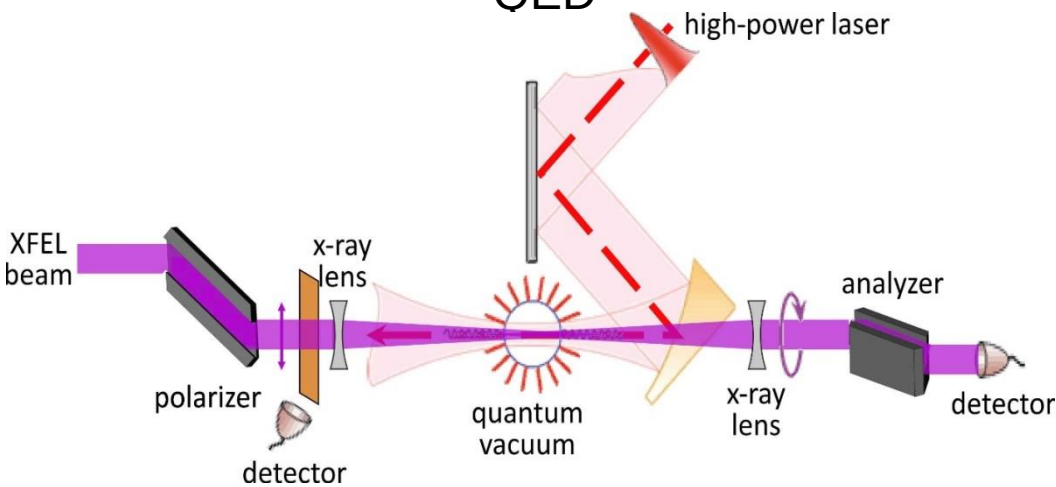
Measurement of **magnetic fields** in solid-density plasma via Faraday rotation



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



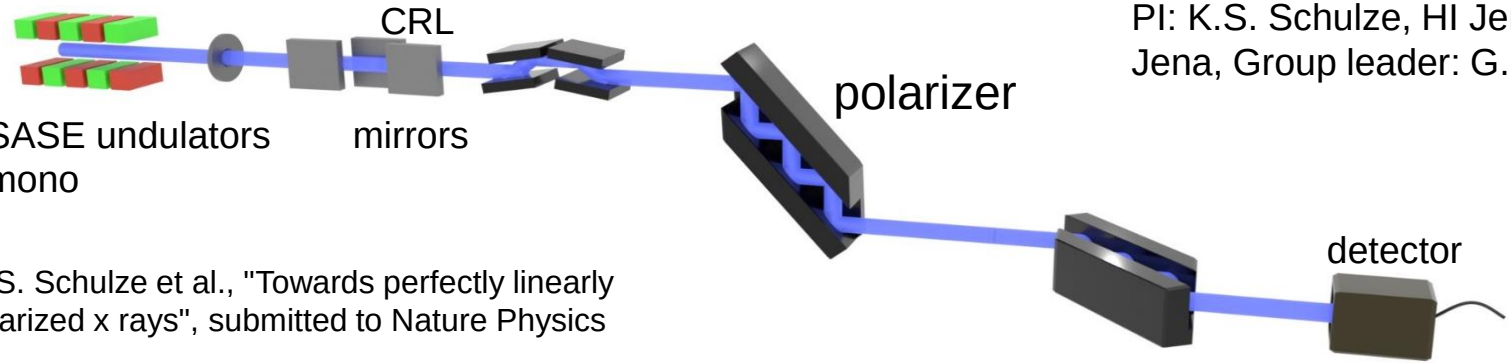
ellipticity of 10^{-13}…10^{-12} expected @ 300 TW

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)

High-purity X-ray polarimetry

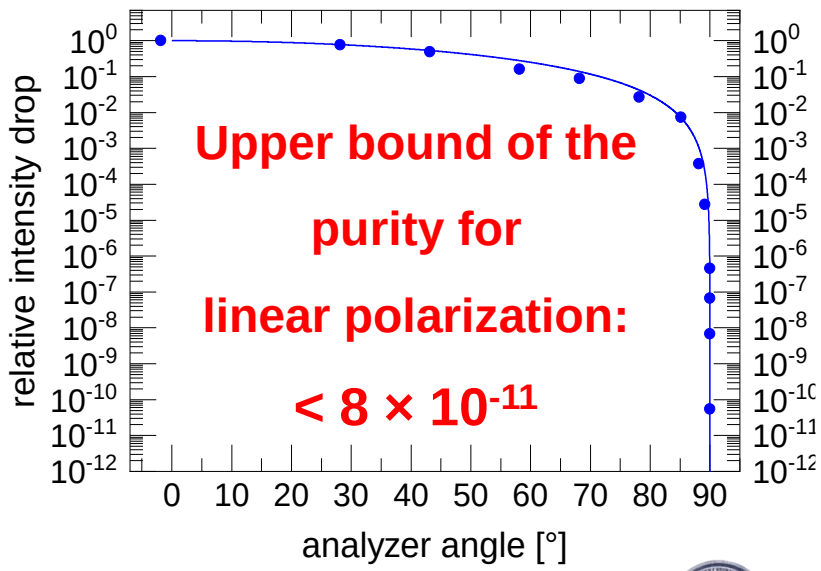
HED beamtime #2194, May 2019

PI: K.S. Schulze, HI Jena & FSU Jena, Group leader: G.G. Paulus

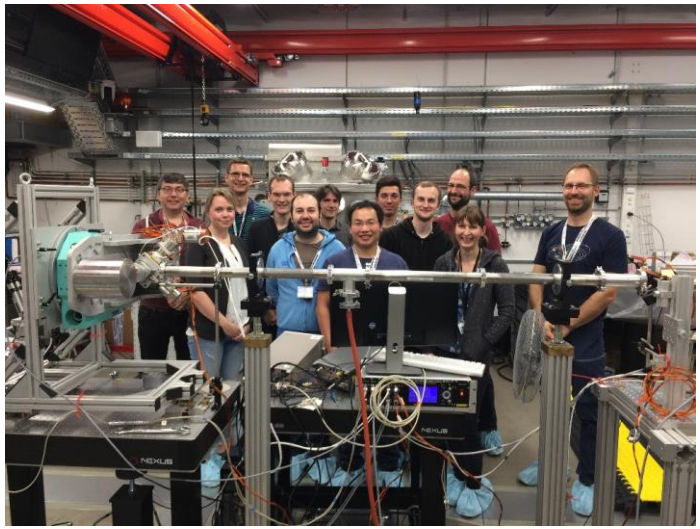


K. S. Schulze et al., "Towards perfectly linearly polarized x rays", submitted to Nature Physics

The highest ever measured polarization purity of x-rays was achieved.



10^{-13} should be possible, once seeding is available



European XFEL FRIEDRICH-SCHILLER-UNIVERSITÄT JENA HI JENA Helmholtz Institute Jena HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF DESY European XFEL

Towards harder x-rays

- Up to 24 keV is available already (seeded up to 13+ keV)
- 200 – 300 µJ were achieved at SASE2 in fall 2021 **at 30 keV**

- Super-conducting undulator „**after burner**“
  - planned at SASE 2 from 2027+
  - Requires updates for focusing, diagnostics, and detectors (high-Z).

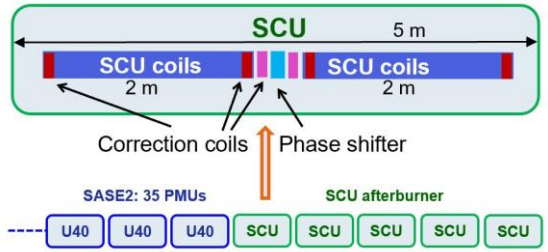
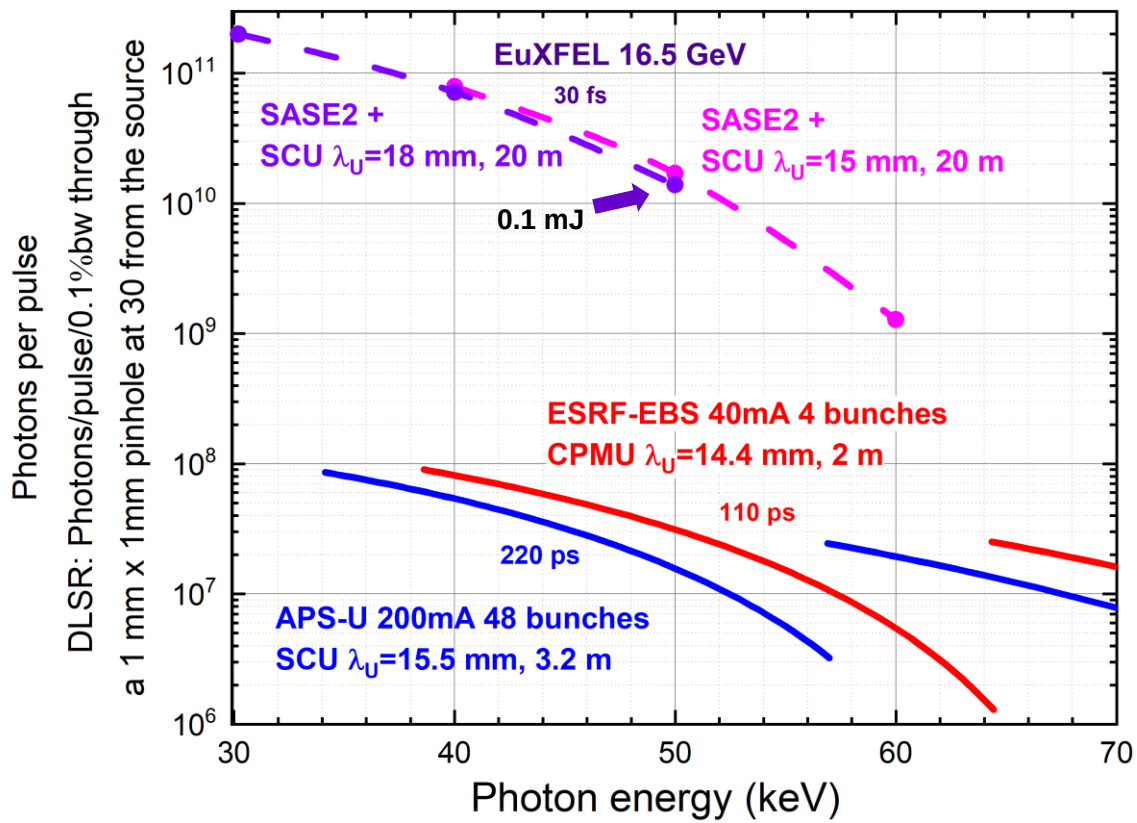


Figure provided by S. Casalbuoni, European XFEL



Instrument papers

- General overview of the HED instrument
  - Zastrau, Appel, Baehtz et al., J. Synchrotron Rad. (2021). 28, 1393–1416
- Details and performance of the HAPG von-Hamos spectrometers
  - Preston et al., Journal of Instrumentation, Volume 15 (2020)
- Design and performance of the meV high resolution setup
  - Wollenweber et al., Review of Scientific Instruments 92, 013101 (2021)
- The experimental platform for XRD from Diamond Anvil Cells
  - Liermann et al., J. Synchrotron Rad. (2021). 28, 688-706
- ReLaX: the HiBEF high-intensity short-pulse laser driver:
  - Laso Garcia et al., High Power Laser Science and Engineering, 1.5 (2021)
- Design and performance of the SAXS mirror:
  - Smid, Baehtz, Pelka et al., Review of Scientific Instruments 91, 123501 (2020)
- New frontiers in extreme conditions science at synchrotrons and free electron lasers
  - Cerantola et al., K. *Phys.: Condens. Matter* **33** 274003 (2021)

2022 Users' Meeting | HED XFEL - Google Suche

https://www.google.com/search?client=firefox-b-d&q=HED+XFEL

HED XFEL

rexx-HR | MyRexx | p4t | Adlatos | Alfresco | TTFeLog | XFEL Status | xfel elog | XFELMdC | EXFLgateway | HED Confl | HIBEF | Google verwende

Google

HED XFEL

Alle | Bilder | News | Videos | Maps | Mehr | Suchfilter

Ungefähr 14 900 Ergebnisse (0,36 Sekunden)

Tipp: Begrenze die Suche auf **deutschsprachige** Ergebnisse. Du kannst deine Suchsprache in den Einstellungen ändern.

https://www.xfel.eu › index_eng ▾ Diese Seite übersetzen

Scientific Instrument HED - European XFEL

The High Energy Density (**HED**) scientific instrument is a new, unique platform for experiments combining hard X-ray FEL radiation and ...

https://www.xfel.eu › index_eng ▾ Diese Seite übersetzen

HED/HIBEF group members - European XFEL

The joint HED and HIBEF groups. Members of the HiBEF project group "Bau und ...

Summary

- SASE lasing, fully tunable 5-24 keV and beyond
- Seeding < 1 eV bandwidth
- two colors SASE two pulses, with < 300 fs delay
- Monochromators Si(111), Si(533)
- HAPG von-Hamos for XES, IXS - 2.7 eV spectral resolution
- Silicon von-Hamos for XES from DAC - 1 eV spectral resolution
- Diced analyzers, meV IXS, 45 meV spectral resolution
- XANES
- High-purity polarimetry
- 30 keV, and superconducting afterburner in 2027+