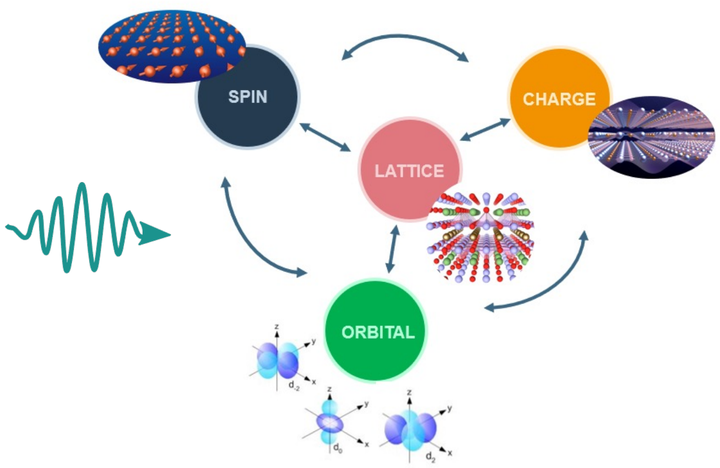
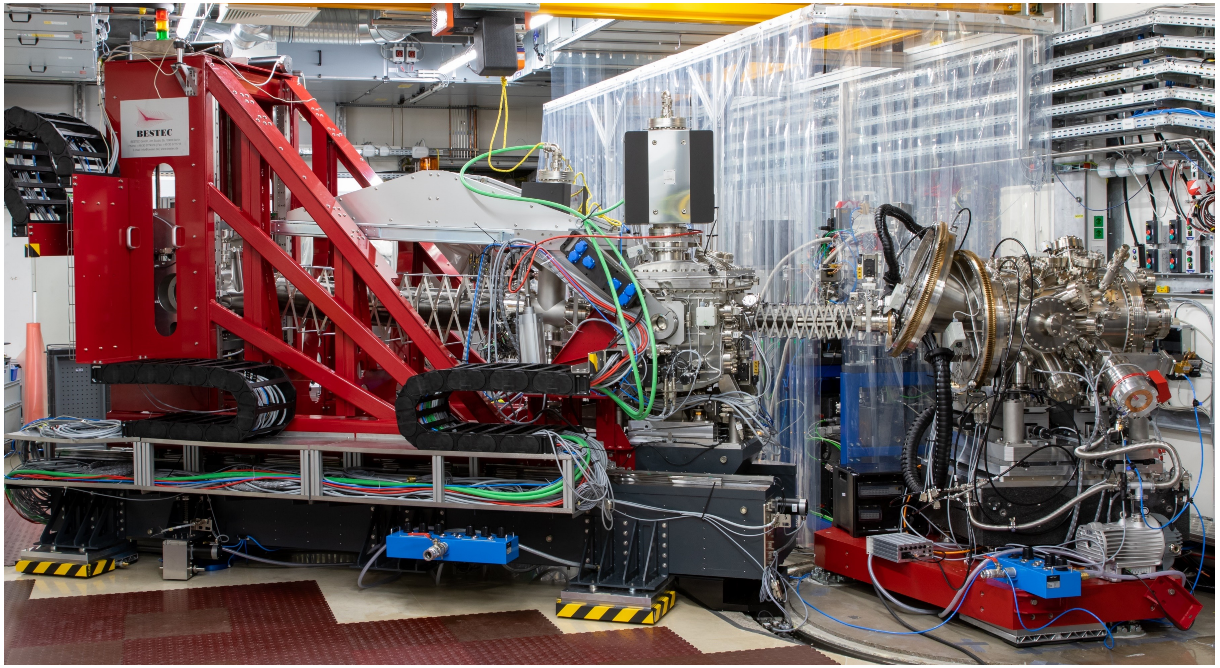
SCS instrument

European XFEL Virtual User Information Meeting, Oct. 10th, 2023
12th Call for Proposals

Andreas Scherz, SCS instrument





> Facility > Instruments > **SCS**

Scientific Instrument SCS

12th Call for User Proposals

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contact us: scs@xfel.eu

12th-Call-for-Proposals: XRD & hRIXS

SCS instrument and beam parameters

12h Call-for-Proposals, scheduled for the second half of 2024

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Online hRIXS Seminar: Information about hRIXS instrumentation

Online seminar slides for download

Provides more information about hRIXS instrumentation, performance and parameters

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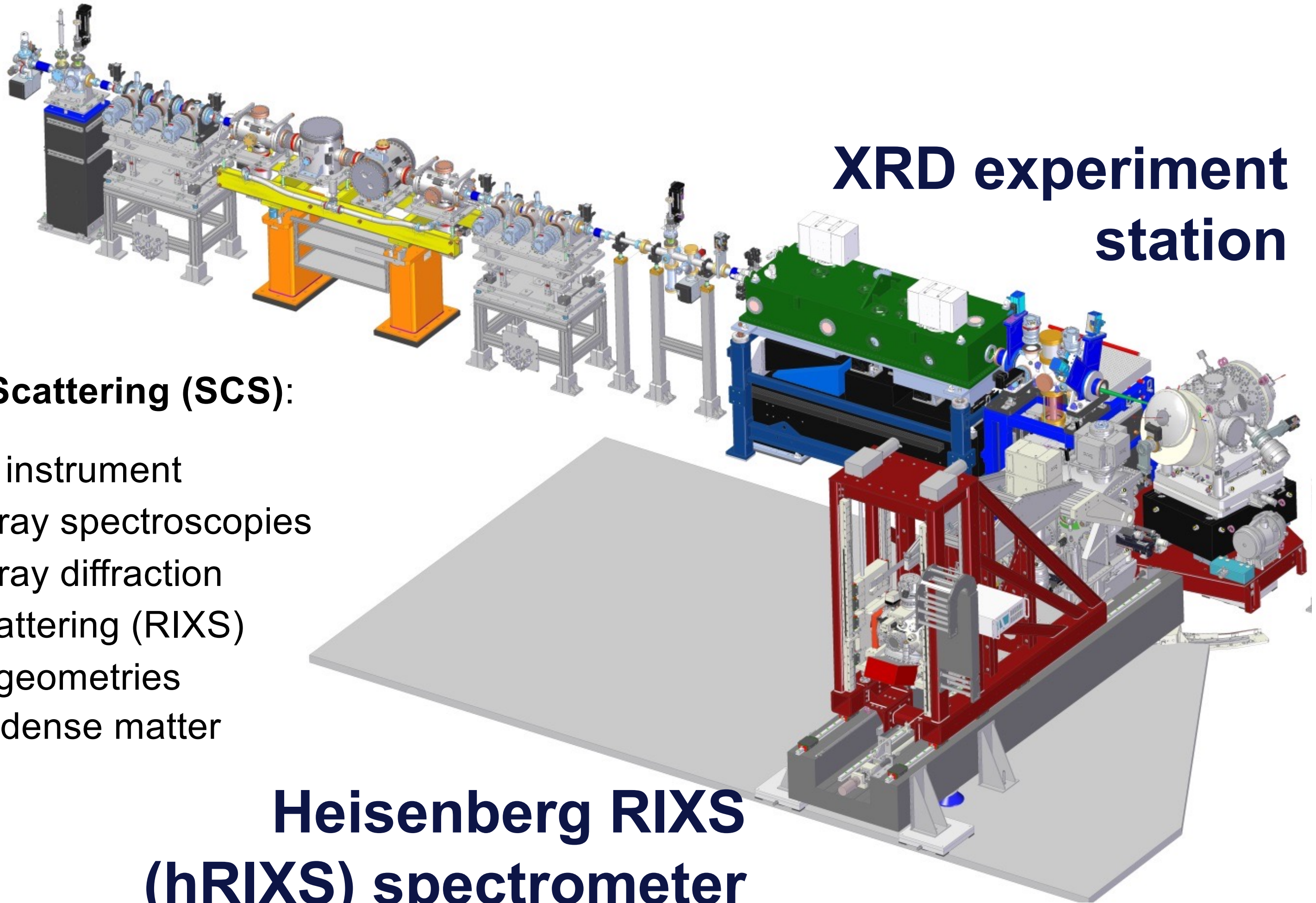
hRIXS instrumentation and information

We commissioned the hRIXS spectrometer during Spring period 2021 reaching up to 10,000 resolving power in a photon energy range between oxygen K edge and Cu L edges (0.5-1.0 keV). After a successful period of user-assisted commissioning in Februar and March of 2022, we will welcome first regular users scheduled for the second half of 2022. The XRD and CHEM experiment stations are available to users providing solid and liquid sample environments, respectively. For more information we refer to the agenda and information on the **online seminar** page, which we hosted on Oct 21st, 2021 at 5pm (CEST) to present users the outcome of the RIXS commissioning at the SCS instrument.

Scientific Instrument SCS: XRD and RIXS

SCS instrument



XRD experiment station

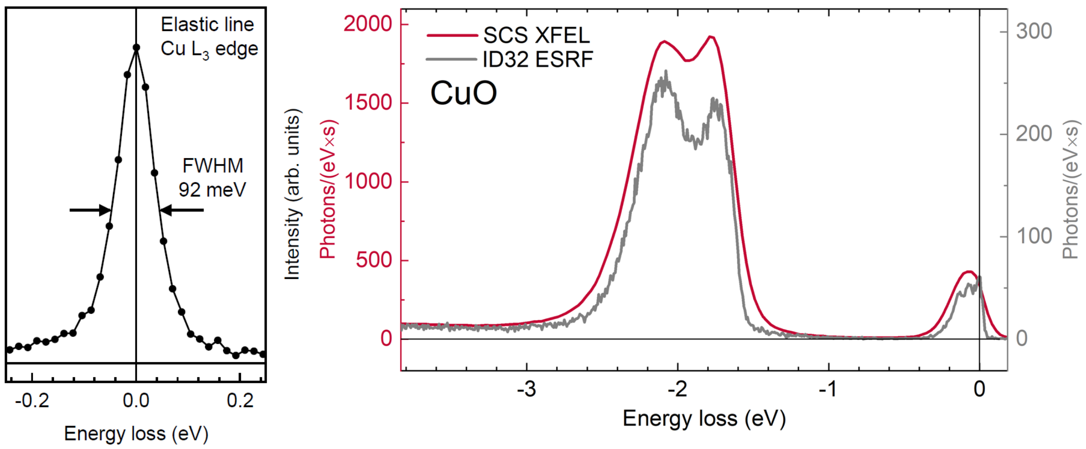
Heisenberg RIXS (hRIXS) spectrometer

Spectroscopy and Coherent Scattering (SCS):

- High-rep-rate FEL soft x-ray instrument
- Time-resolved/ non-linear x-ray spectroscopies
- Time-resolved/ non-linear x-ray diffraction
- Resonant Inelastic X-ray Scattering (RIXS)
- Reflection- / backscattering geometries
- Sample environment for condense matter samples

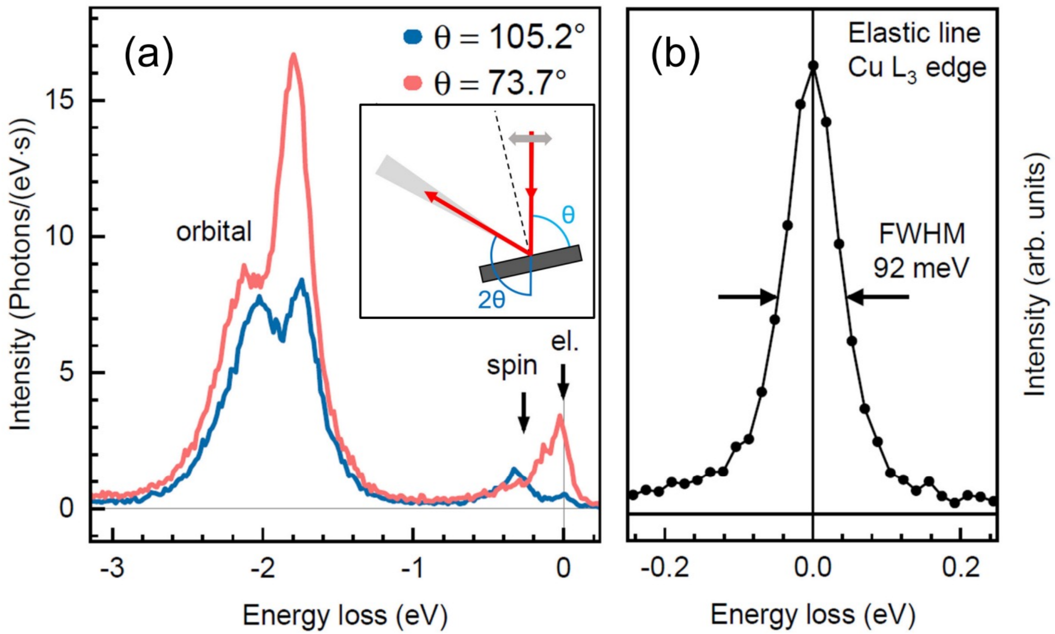
XRD experiment station and hRIXS spectrometer

hRIXS parameters	
Photon energy	0.25 (0.45 SA3) – 1.5 keV
Combined resolving power	Up to 10.000 (mono HR) 3.000 (mono LR)
Transmission	~10^{-6}
Time resolution	Limited by mono: 80-150 fs (mono HR) 30-50 fs (mono LR)
Scattering angle	65 – 145 deg Default: 125 deg

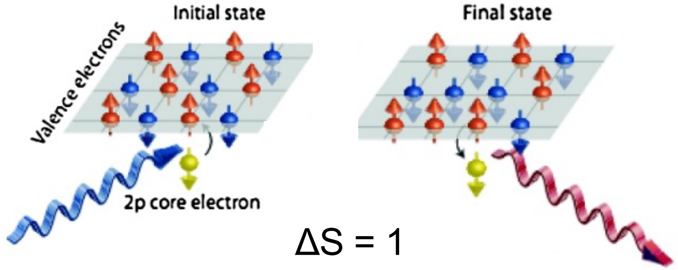


hRIXS x-ray commissioning: achieved energy resolution

Static RIXS from thin-film La_2CuO_4 at Cu L_3 edge:



Spin excitations:



L. Braicovich *et al.* *PRL* **102**, 167401(2009)

H.C. Robarts *et al.* *PRB* **103**, 224427 (2021)

Edge	Energy (eV)	Energy res. (meV)	E/ΔE
Cu L_3	930	92	10 100
Ni L_3	853	75	11 370
O K	530	49	10 400

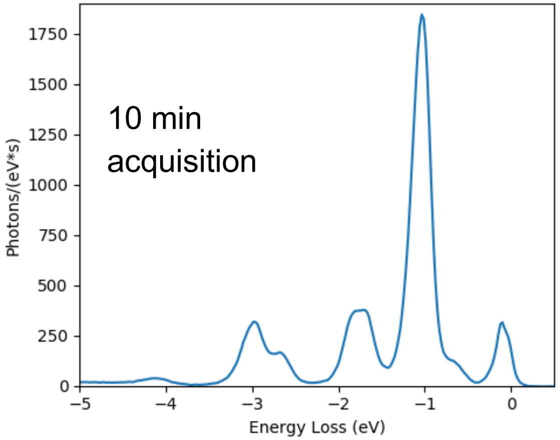
➡ Achieved combined resolving power: > 10.000

Count rates RIXS from NiO for high energy resolution

Static spectra at 1.1 MHz repetition rate:

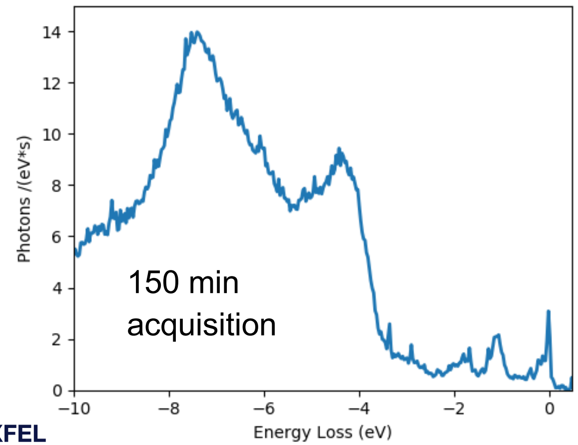
Ni L_3-edge

Incident Beam:
4,000 pulses/s
100% transmission
1.0 x 10^{13} ph/s



O K-edge

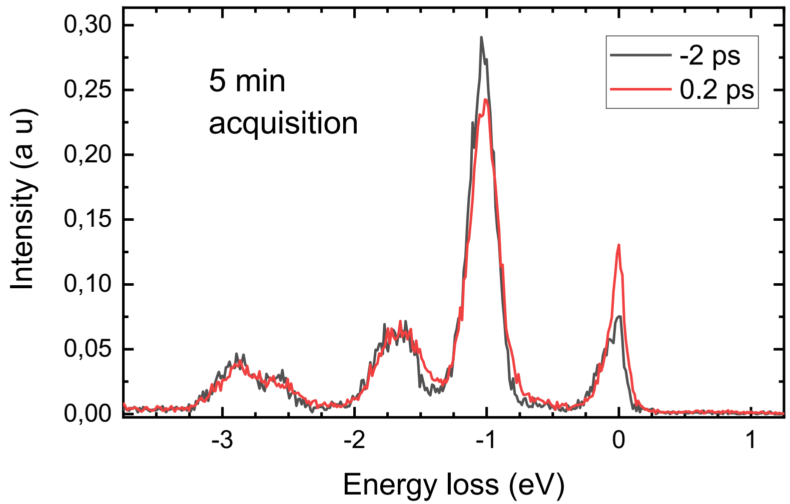
Incident Beam:
4,000 pulses/s
100% transmission
1.6 x 10^{12} ph/s



Dynamic spectra at 113 kHz repetition rate:

Ni L_3-edge

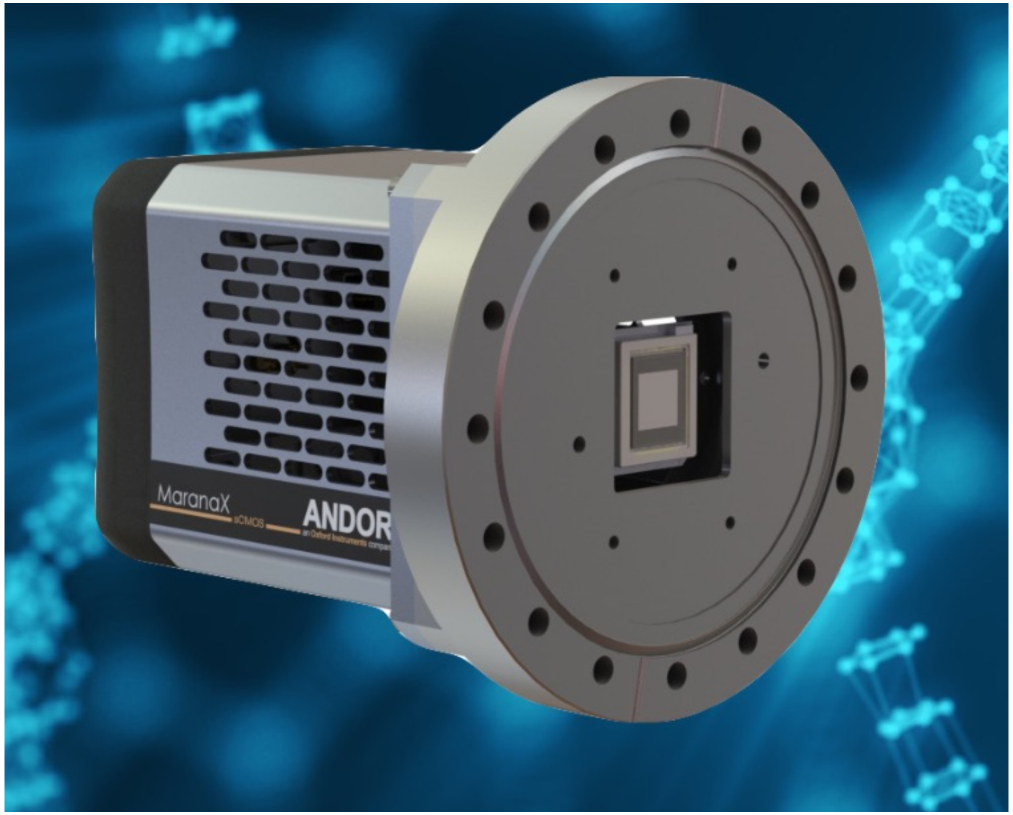
200 pulses/s
30% transmission (FEL)
266 nm pump (~10 mJ/cm²)



- La2CuO4: count rate ~ factor 10 lower
- 1.1 MHz possible for 800, 400 and 266 nm pump
- 1000 l/mm grating: 4-5 times more throughput

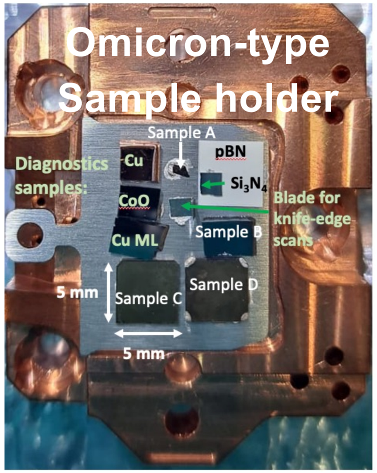
Detector upgrade for hRIXS

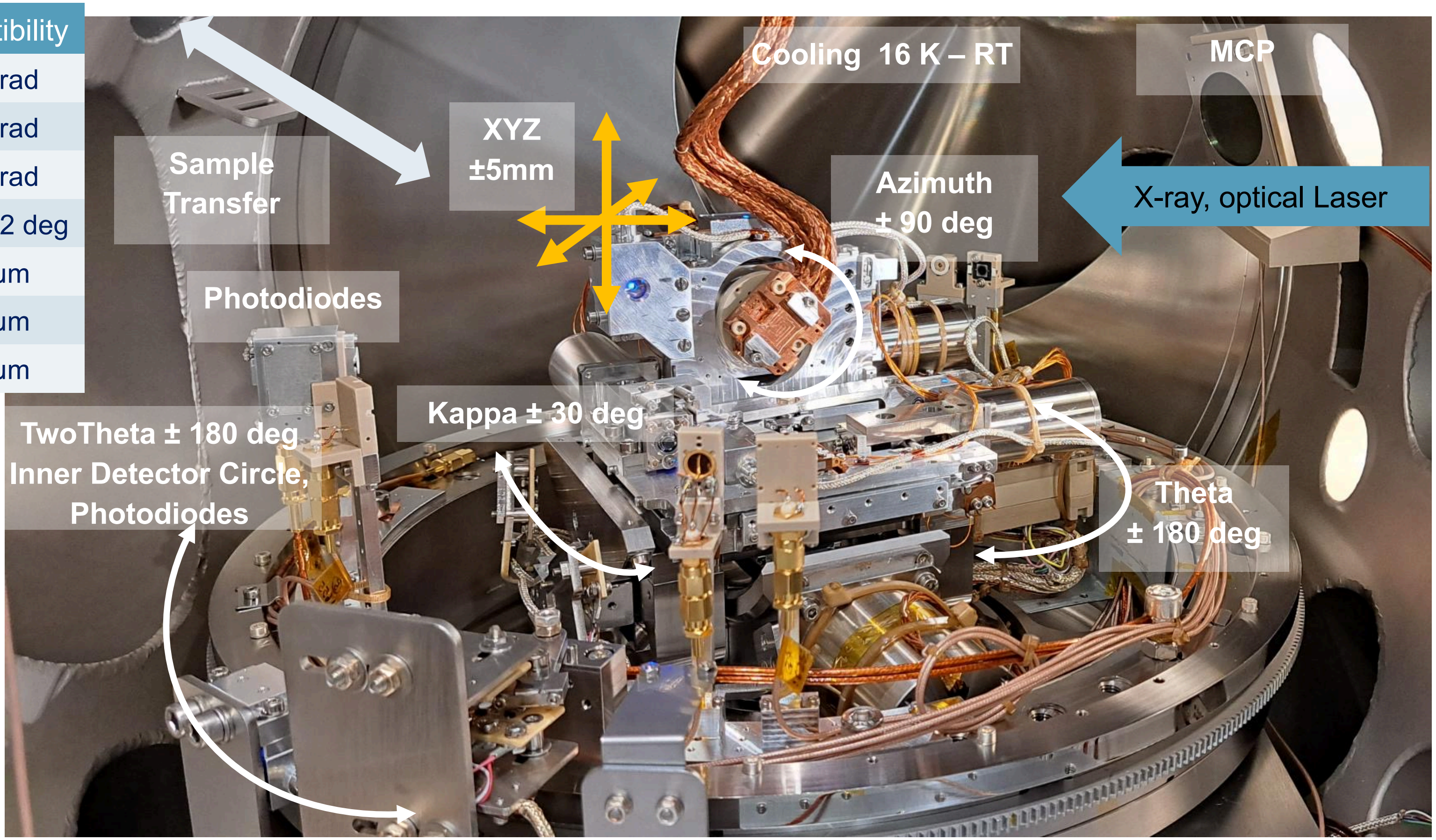
- Marana-X (available for 2024-I onwards),
  TRAIN-RESOLVED
  11µm pixel size and 48fps,
  Back-illuminated sCMOS EUV/soft X-ray camera



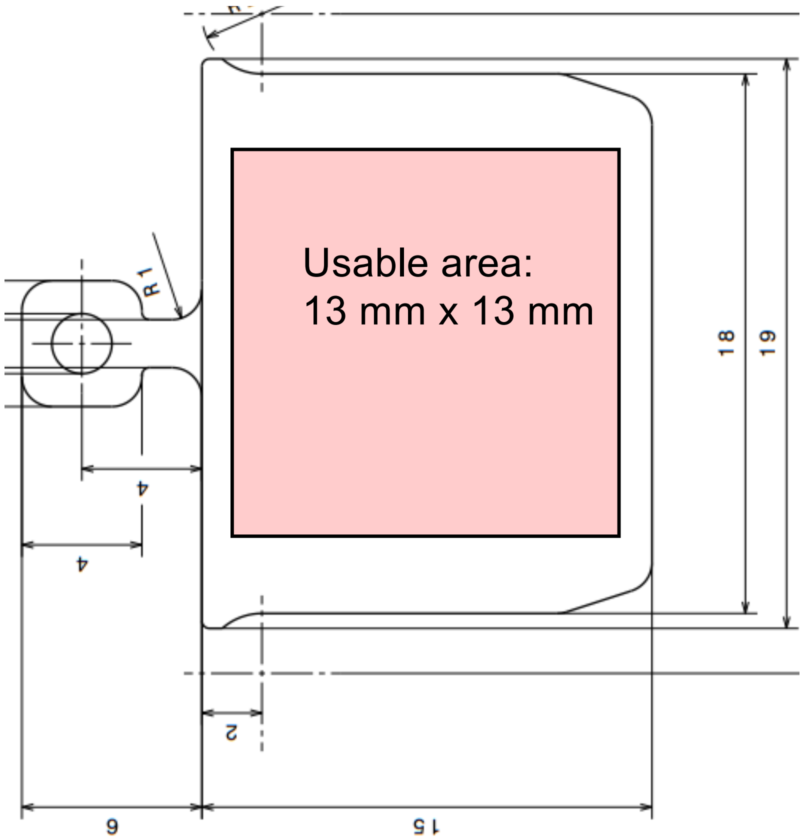
XRD inner mechanics and detectors

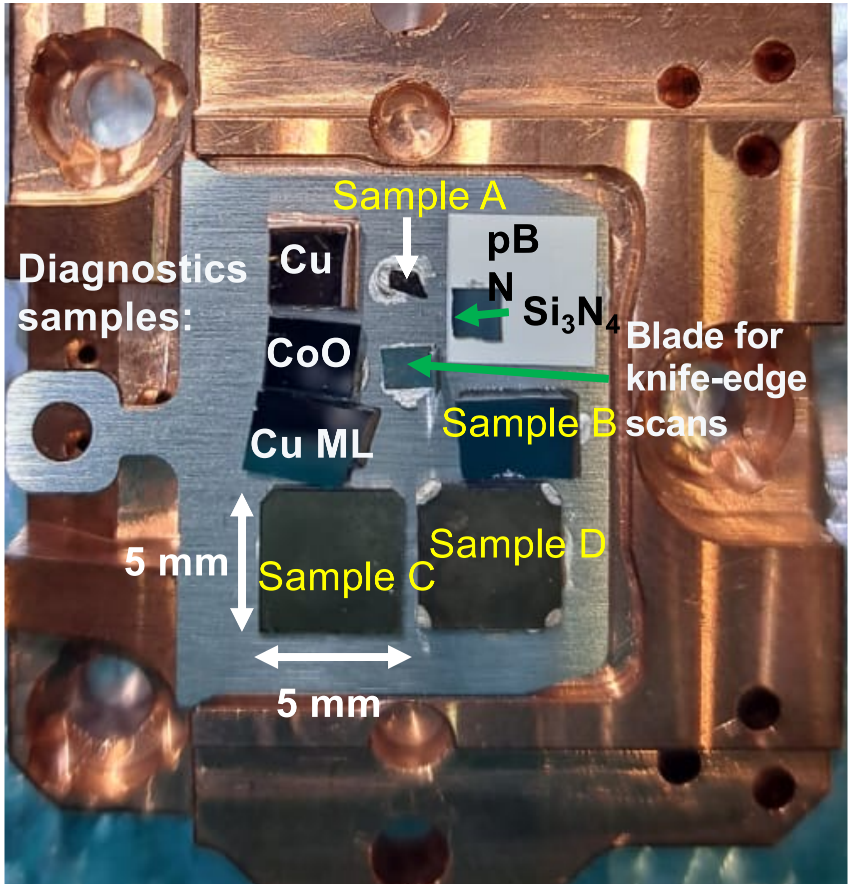
Motion	Range	Repeatibility
TwoTheta	± 180 deg	< 1 µrad
Theta	± 180 deg	< 1 µrad
Kappa	± 30 deg	< 1 µrad
Azimuth	± 90 deg	< 0.0002 deg
X	± 5 mm	0.5 µm
Y	± 5 mm	0.5 µm
Z	± 5 mm	0.5 µm



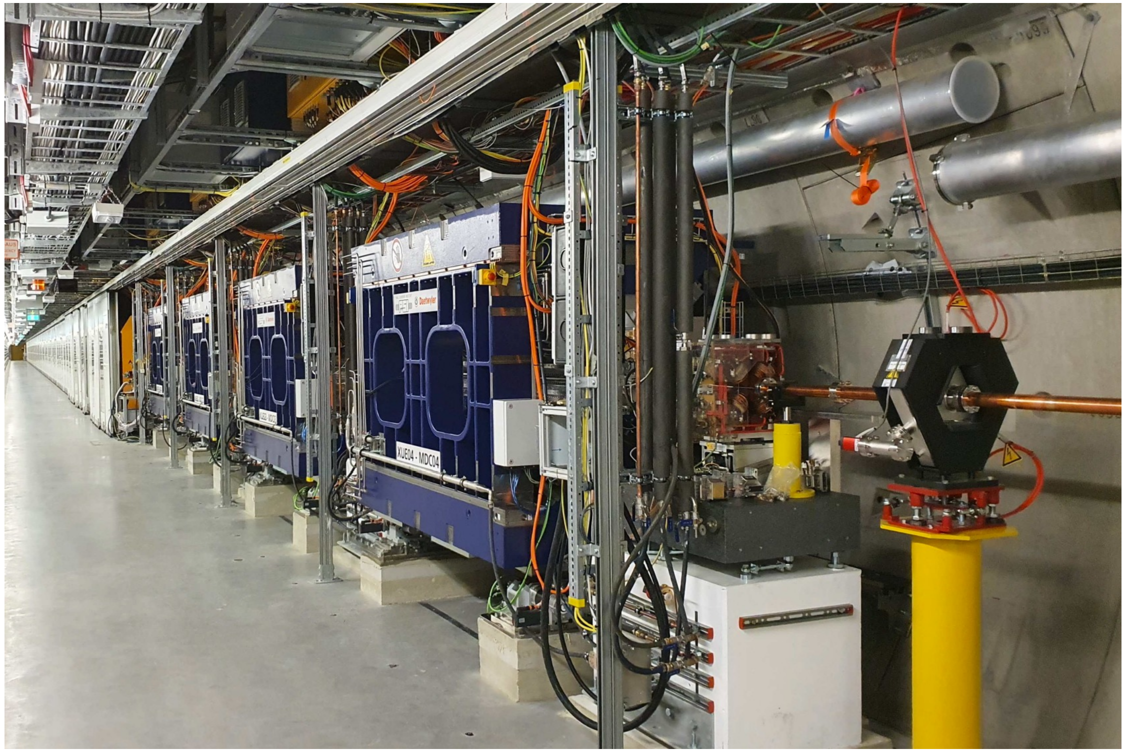


Flag-style sample holder (Omicron design)





EuXFEL APPLE-X (UE90) Variable Polarization at SA3: Linear horizontal, linear vertical, left and right circular Polarizations



- re-install foreseen in winter 2023
  -> commissioning in 2024-I

Polarization mode	**LH/LV/C+/C-**
K-Range	**9.59 – 3.38**
Photon Energy Range [keV]	
@8.5 GeV	0.163 – 1.137
@11.5 GeV	0.299 – 2.082
@14 GeV	0.443 – 3.085
@16.5 GeV	0.615 – 4.286
@17.5 GeV	0.692 – 4.821

Optical laser parameters

Optical laser system	SASE3 PP laser	
Center wavelength	800 nm	
Pulse duration	15 or 50 fs	
Repetition rate and Pulse energy	2 mJ @ 113 kHz, 800 nm 0.2 mJ @ 1.13 MHz, 800 nm	Possibly also 564kHz mode. Inquire for details
Wavelength tunability	Conversions from 800 nm / 50 fs: SHG (400 nm) , THG (266 nm), OPA: wavelength between 350 nm and 2.5 microns Please inquire for details on pulse energies	
Spot size	~100 µm	
Polarization	Linear and circular	
Operation	Burst mode synchronized to FEL with jitter <50 fs	

- Second and third harmonic generation from 800nm, 50fs to 400nm and 266nm
- 113 kHz
  - 800nm, 2 mJ/pulse
  - 400nm, 350 µJ/pulse
  - 266nm, 75 µJ/pulse
- 1.1 MHz
  - 800nm, 200 µJ/pulse
  - 400nm, 30 µJ/pulse, (typically use 25% of this)
  - 266nm, 1.5 µJ/pulse (aim for 20 µJ/pulse)

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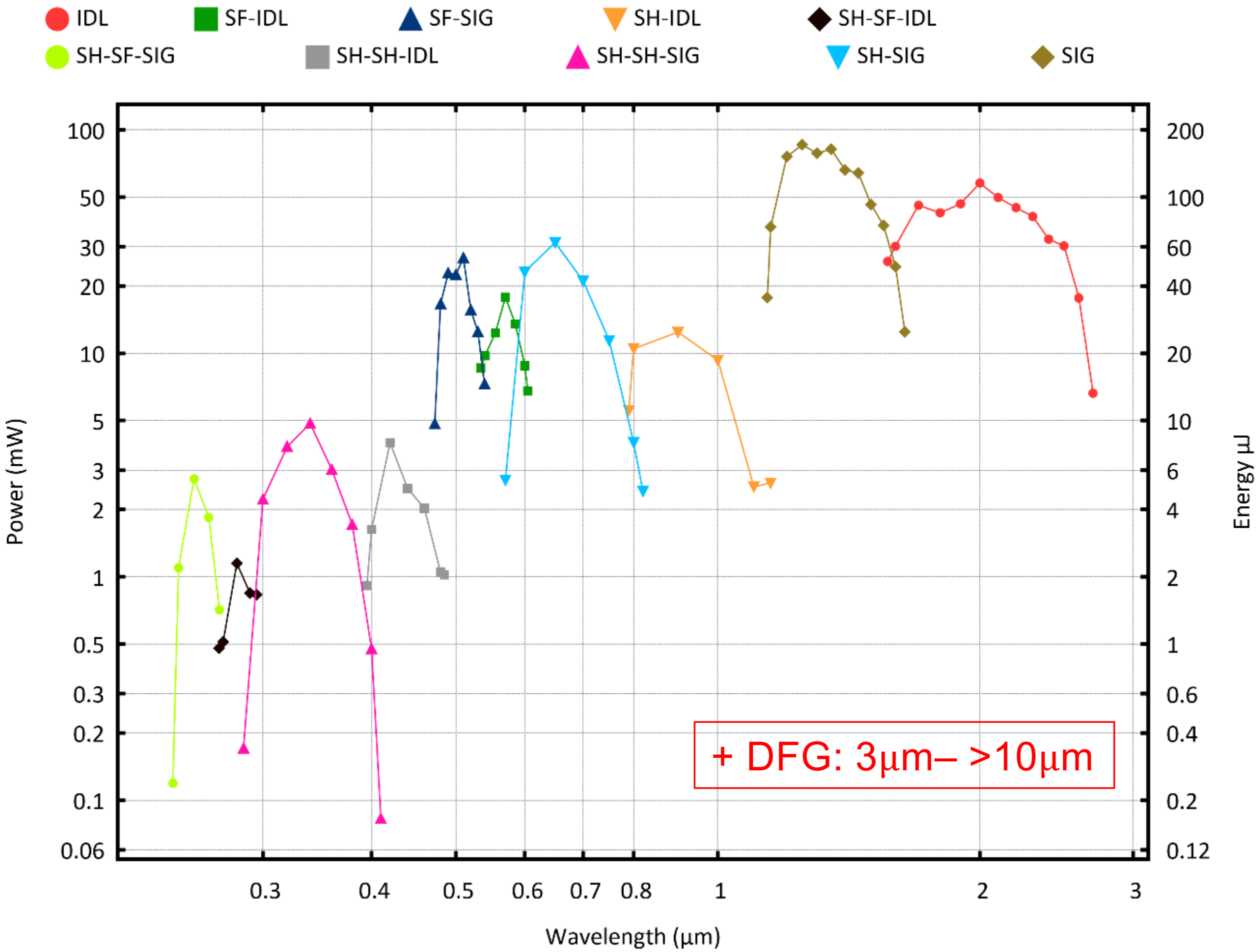
PP laser information

Frequency Conversion 1: SHG and THG

- Second and third harmonic generation from 800nm, 50fs to 400nm and 266nm
- 113 kHz
  - 800nm, 2 mJ/pulse
  - 400nm, 350 µJ/pulse
  - 266nm, 75 µJ/pulse
- 1.1 MHz
  - 800nm, 200 µJ/pulse
  - 400nm, 30 µJ/pulse, (typically use 25% of this)
  - 266nm, 1.5 µJ/pulse (aim for 20 µJ/pulse)

Frequency Conversion 1: SHG and THG

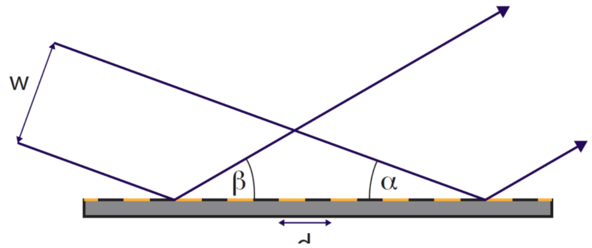
- OPA (Light Conversion Topas)
  - Wide range of wavelengths allows e.g resonant pumping, above or below band gaps, …
  - Repetition rate 113kHz, 50 fs, (1.1MHz, 50fs)
  - User experiments so far: UV (320nm), visible (550nm, 633nm), NIR (1300nm), IR (2500nm)



Additional Information (Q&A session)

Monochromator settings SCS beamline:

The use of monochromator leads to pulse stretching.
Resolution has to be compromised for time resolution.



Time delay: $\Delta\tau_{rms} = \frac{1}{c} w_{rms} d_0 \lambda$

Low-resolution grating

LR grating	
Line density	50 l/mm
Resolving power	3.000 (1st order)
Pulse stretching	30-50 fs
X-ray pulse energy	up to 30 μJ

→ Moderate combined energy resolution
→ High temporal resolution

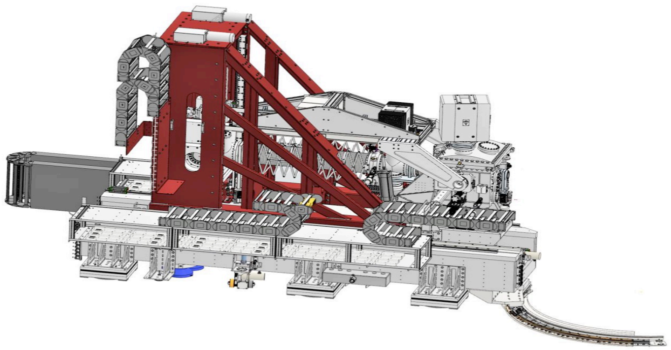
High-resolution grating

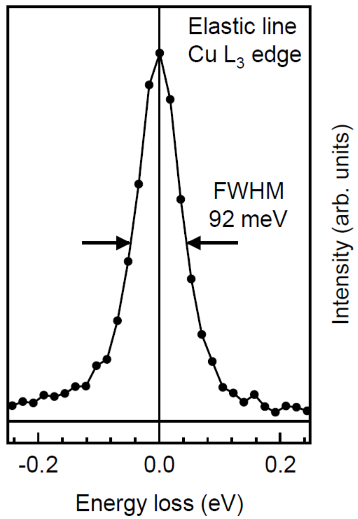
HR grating	
Line density	150 l/mm
Resolving power	Up to 10.000 (1st order)
Pulse stretching	80-150 fs
X-ray pulse energy	up to 5 μJ

→ High combined energy resolution
→ Moderate temporal resolution

Gerasimova, et al., *JSR*, *29*, 1299–1308 (2022).

hRIXS parameters





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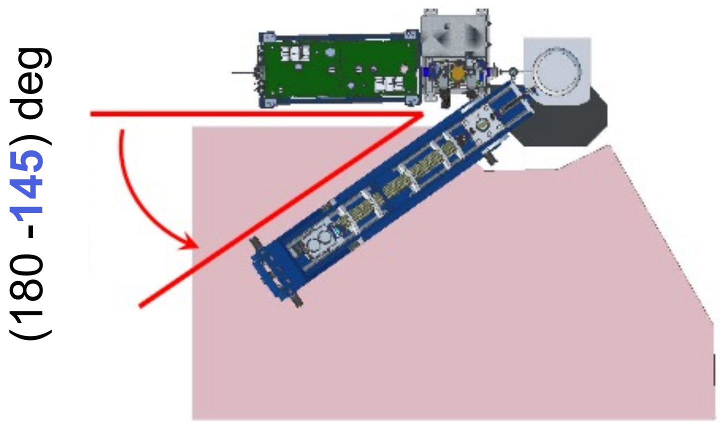
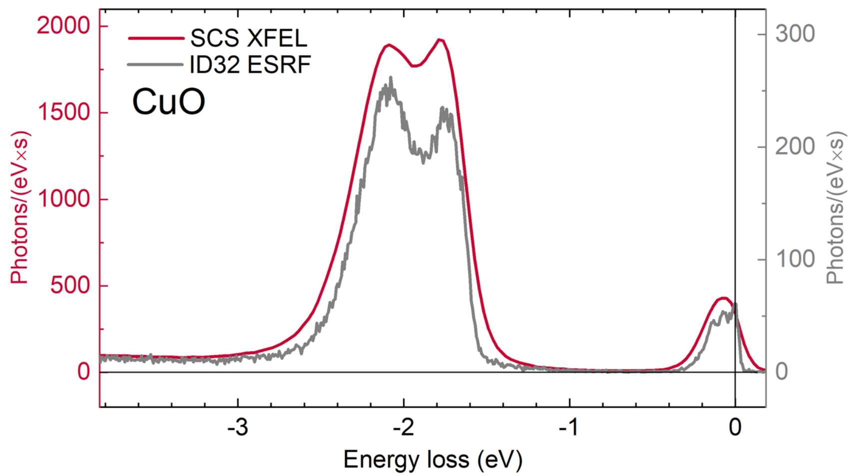




Energy resolution: three working points

- There are two working points for the monochromator:

(A) High transmission grating

Low Resolution (LR) grating:	
Line density	50 l/mm
Resolving power	**3.000** (1st order)
Pulse stretching	**30-50 fs**
X-ray pulse energy	up to 30 µJ

→ High throughput, lower pulse stretching
→ Energy resolution limited by the mono

(B) High resolution grating

High Resolution (HR) grating:	
Line density	150 l/mm
Resolving power	**> 10.000** (1st order)
Pulse stretching	**80-150 fs**
X-ray pulse energy	up to 5 µJ

- Can be used with:

a) High-resolution RIXS grating (3000 l/mm)
- Resolving power >10.000, Transmission > 3%

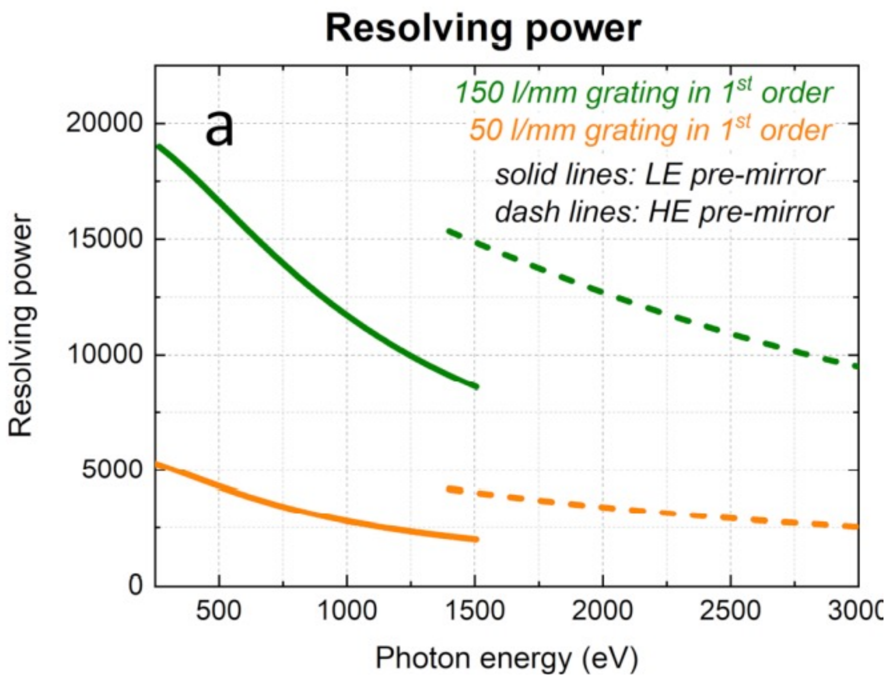
→ Energy resolution limited by the mono

b) High-transmission RIXS grating (1000 l/mm)
- Resolving power <10.000, Transmission > 12%

→ Expected combined resolving power of 6,000 – 7,000

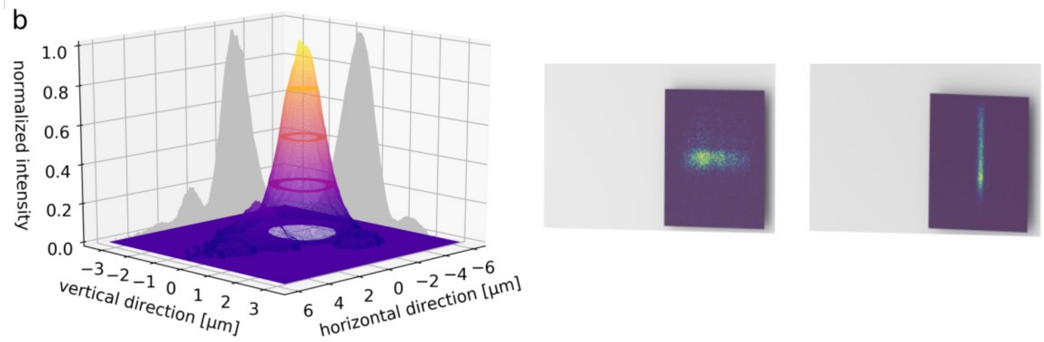
SCS instrument: photon energy, resolving power and beam size

- Two monochromator gratings:



N. Gerasimova et al., J. Synchrotron Rad. 29, 1299 (2022)

- Variable beam size due to bendable KB mirrors:
  - beam width from 1 µm - 1 mm
  - symmetric or line shape

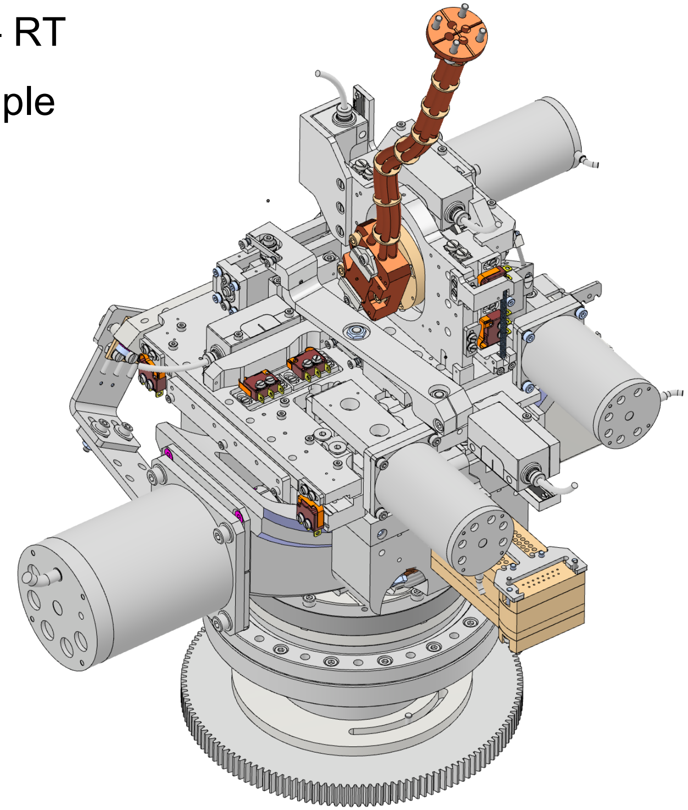


G. Mercurio et al., Opt. Express 30, 20980 (2020)

XRD setup: sample environment

- UHV ($p < 10^{-9}$ mbar)
- Cryogenic temperatures: 16 K – RT
- 6 degrees of motion for the sample

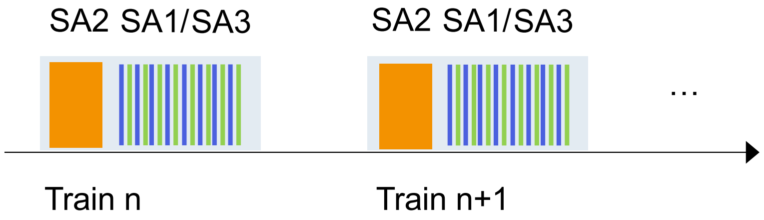
Motion	Range
Azimuth	± 90 deg
X	± 5 mm
Y	± 5 mm
Z	± 5 mm
Kappa (tilt)	± 30 deg
Theta	± 180 deg
TwoTheta	± 180 deg



FEL pulse pattern

- Pulse train at 10 Hz, Burst mode with 400 μs for SCS, Repetition rate variable up to 1.1 MHz
- PP laser: also burst mode (the same pattern as FEL)

Interleaved mode with SA1:



Repetition rate of up to 1.1 MHz for SCS