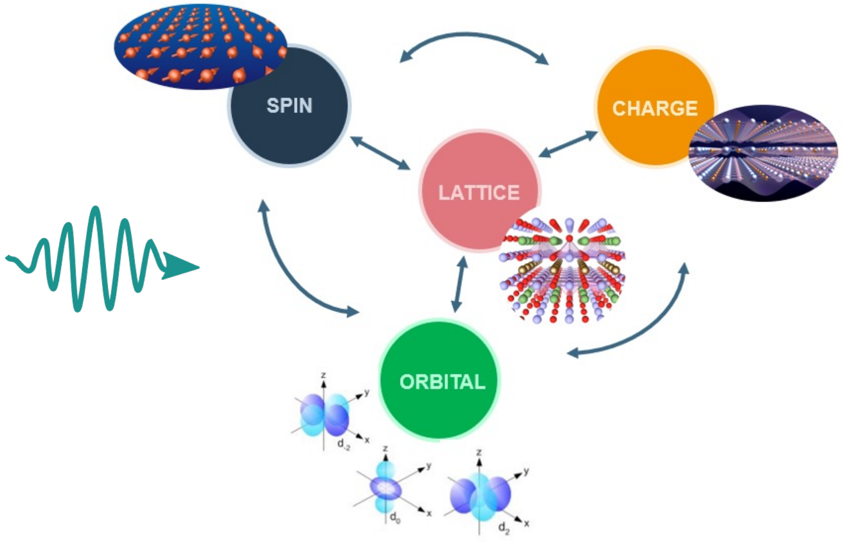
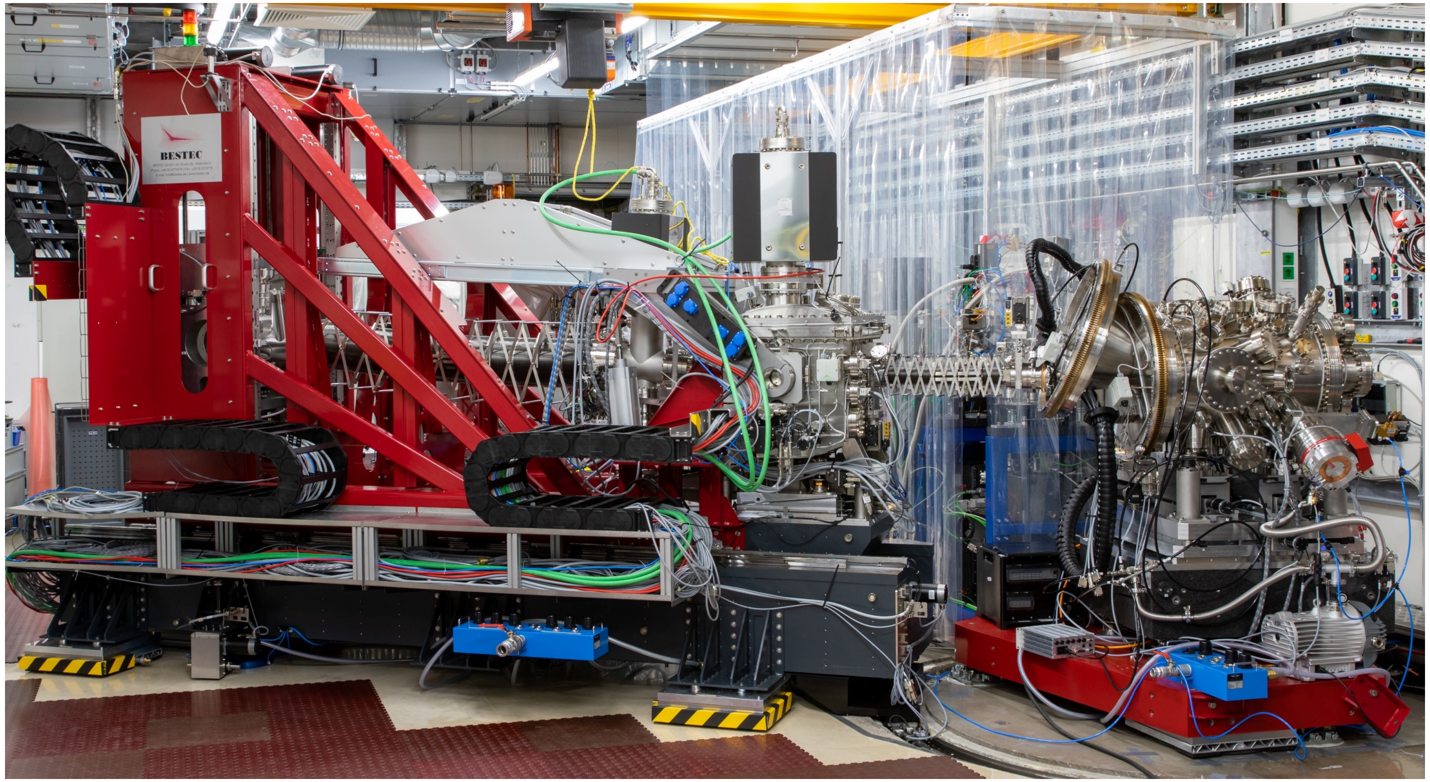
SCS instrument

European XFEL Virtual User Information Meeting, Nov. 10th 2022
10th Call for Proposals

Andreas Scherz, SCS instrument





Scientific Instrument SCS

10th Call for User Proposals

We are happy to accept proposals, scheduled for the second half of 2023, addressing ultrafast solid state material dynamics exploiting the XRD experiment station and the hRIXS spectrometer for x-ray diffraction, reflection and resonant inelastic X-ray scattering experiments. Detailed parameters can be found below. Please note that the FFT experiment station and CHEM station are not included in this call.

contact us: scs@xfel.eu

https://www.xfel.eu/facility/instruments/scs

10th-Call-for-Proposals: XRD & hRIXS

SCS instrument and beam parameters

10th Call-for-Proposals, scheduled for the second half of 2023

DOWNLOAD

Online hRIXS Seminar: Information about hRIXS instrumentation

Online seminar slides for download

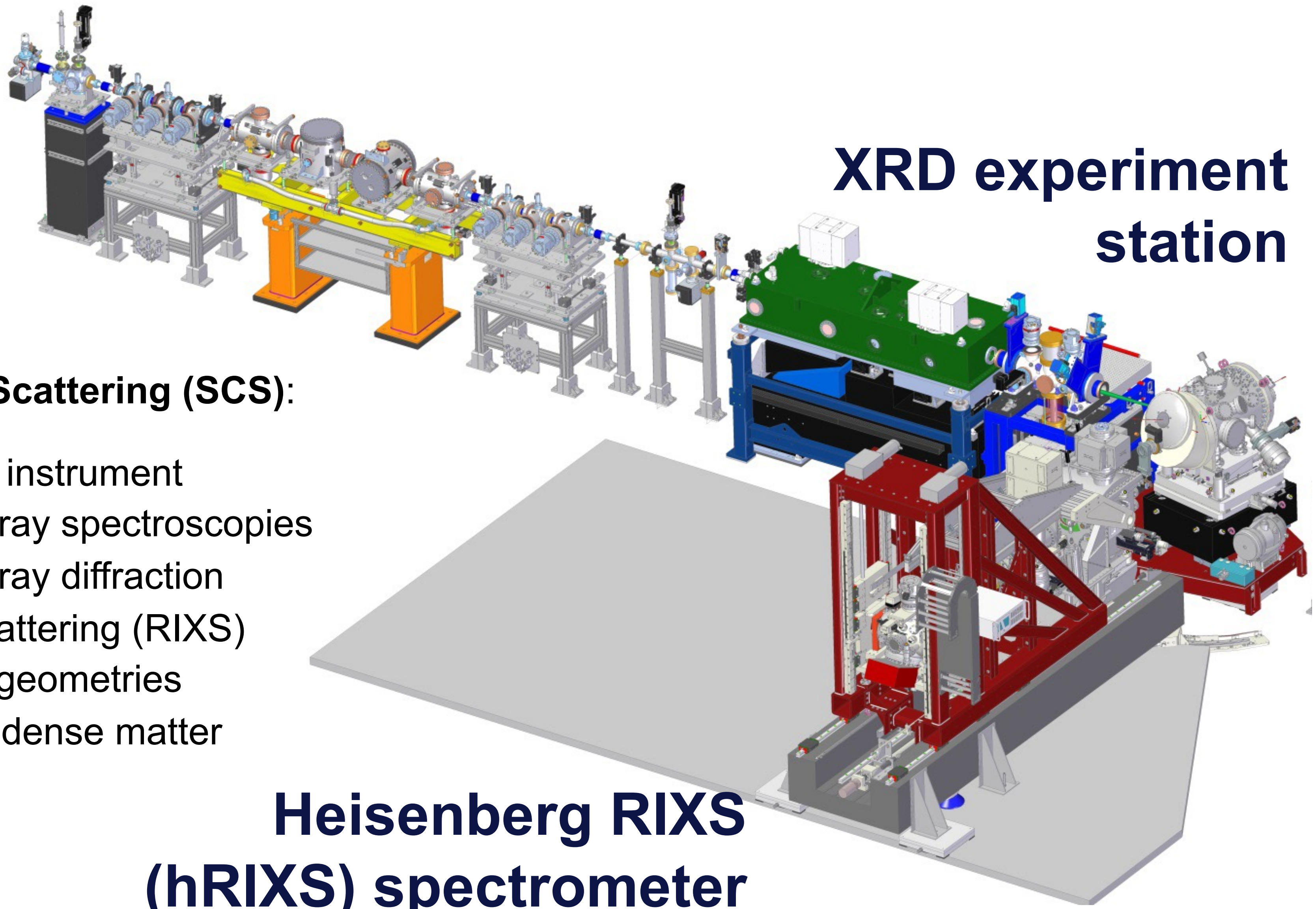
Provides more information about hRIXS instrumentation, performance and parameters

DOWNLOAD

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-assiste… commissioning in Februar and March of 2022, we will welcome first regular users scheduled f… second half of 2022. The XRD and CHEM experiment … liquid sample environments, respectively. For …mation on the **online seminar** page, which we … esent users the outcome of the RIXS commissioning at the SCS instrument.

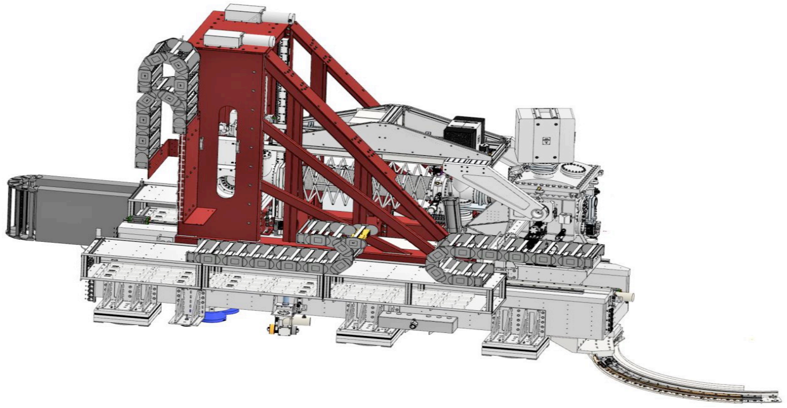
Scientific Instrument SCS: XRD and RIXS

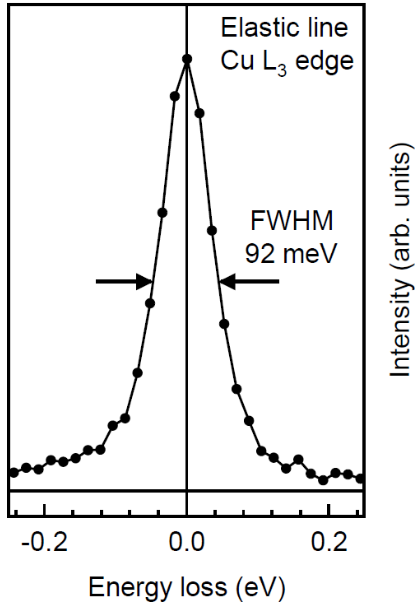


Spectroscopy and Coherent Scattering (SCS):

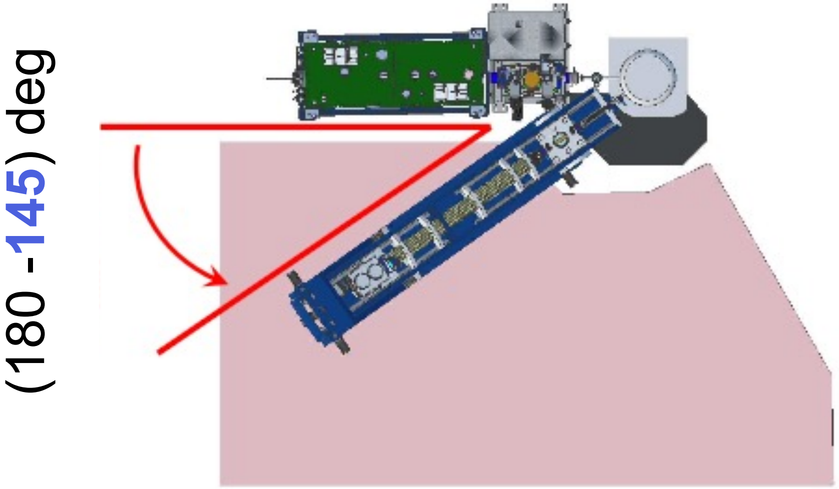
- High-rep-rate FEL soft x-ray instrument
- Time-resolved/ non-linear x-ray spectroscopies
- Time-resolved/ non-linear x-ray diffraction
- Resonant Inelastic X-ray Scattering (RIXS)
- Reflection- / backscattering geometries
- Sample environment for condense matter samples

hRIXS parameters





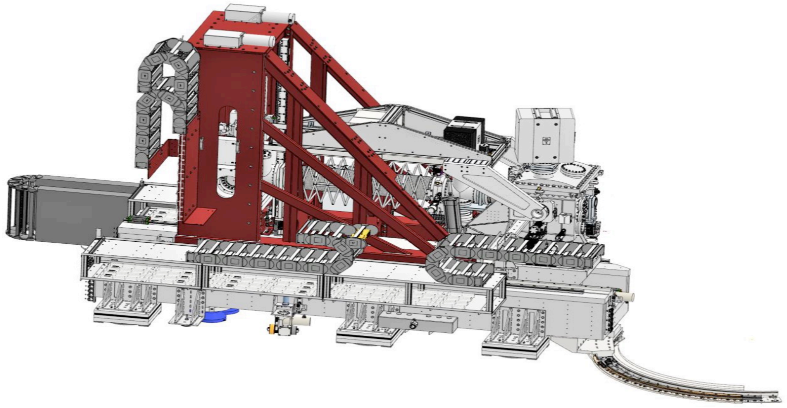
hRIXS parameters	
Photon energy	0.25 (0.45 SA3) – 1.5 keV
Combined resolving power	Up to 10.000 (mono HR) 3.000 (mono LR)
Transmission	~10^{-6}
Time resolution	Limited by mono: 80-150 fs (mono HR) 30-50 fs (mono LR)
Scattering angle	65 – 145 deg Default: 125 deg

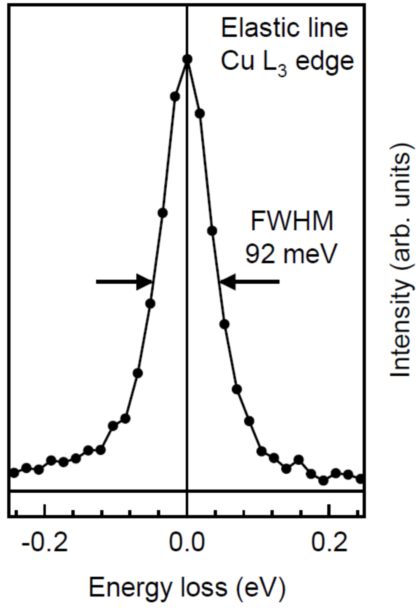


Performance comparable to state-of-the-art synchrotron instruments

- High energy resolution and high time resolution
- pump-probe experiments at 1 MHz repetition rate, ~80fs X-ray pulses @ Cu L3 edge and 10,000 resolving power

hRIXS parameters





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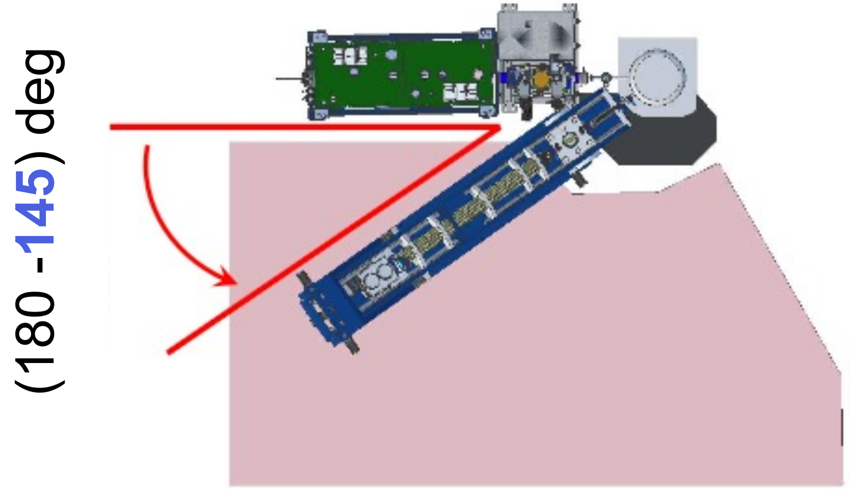
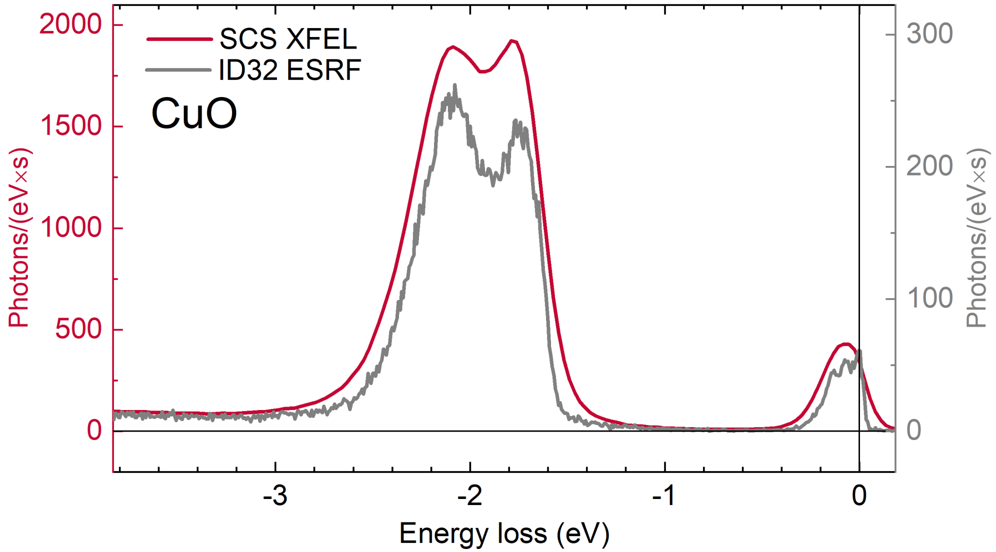


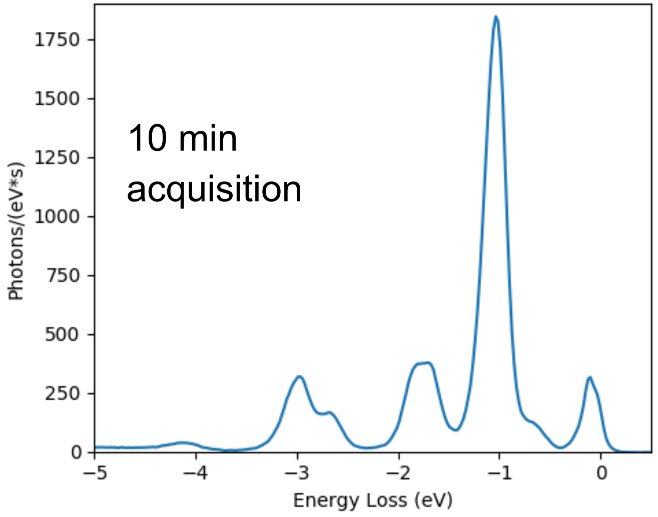


Count rates RIXS from NiO for high energy resolution

Static spectra at 1.1 MHz repetition rate:

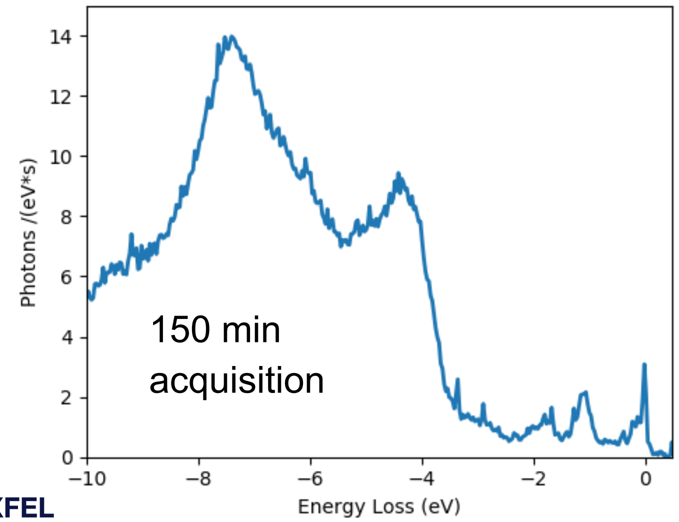
Ni L_3-edge

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



O K-edge

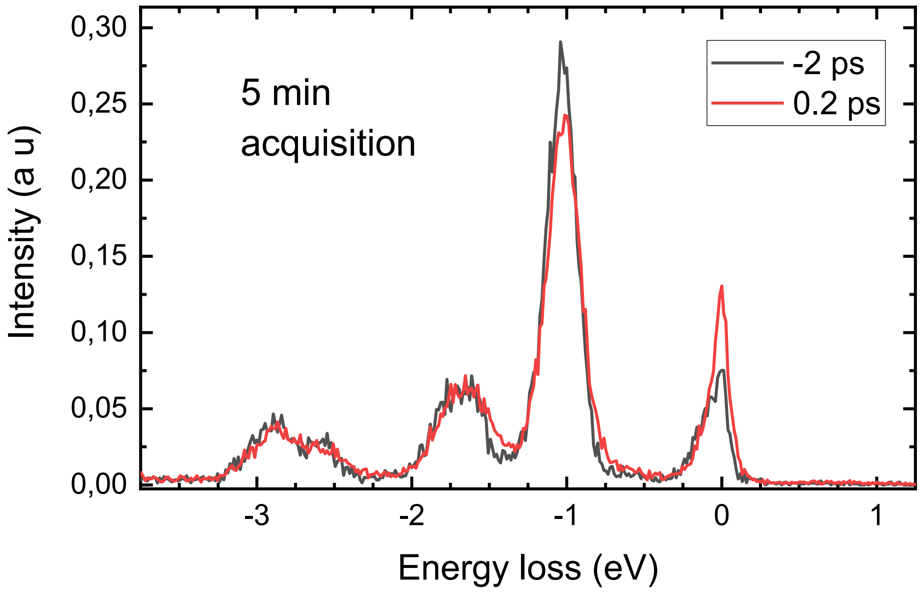
Incident Beam:
4,000 pulses/s
100% transmission
1.6 x 10^{12} ph/s



Dynamic spectra at 113 kHz repetition rate:

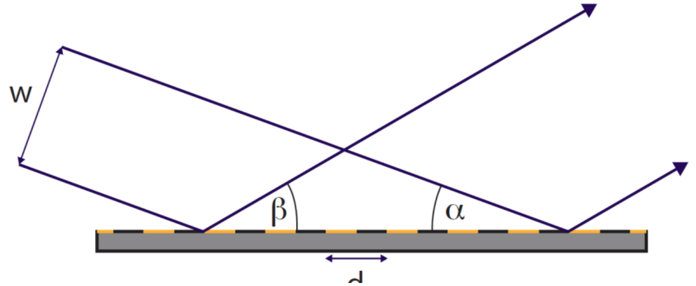
Ni L_3-edge

200 pulses/s
30% transmission (FEL)
266 nm pump (~10 mJ/cm^2)



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

Monochromator settings SCS beamline:



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

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

Low-resolution grating

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

→ Moderate combined energy resolution
→ High temporal resolution

High-resolution grating

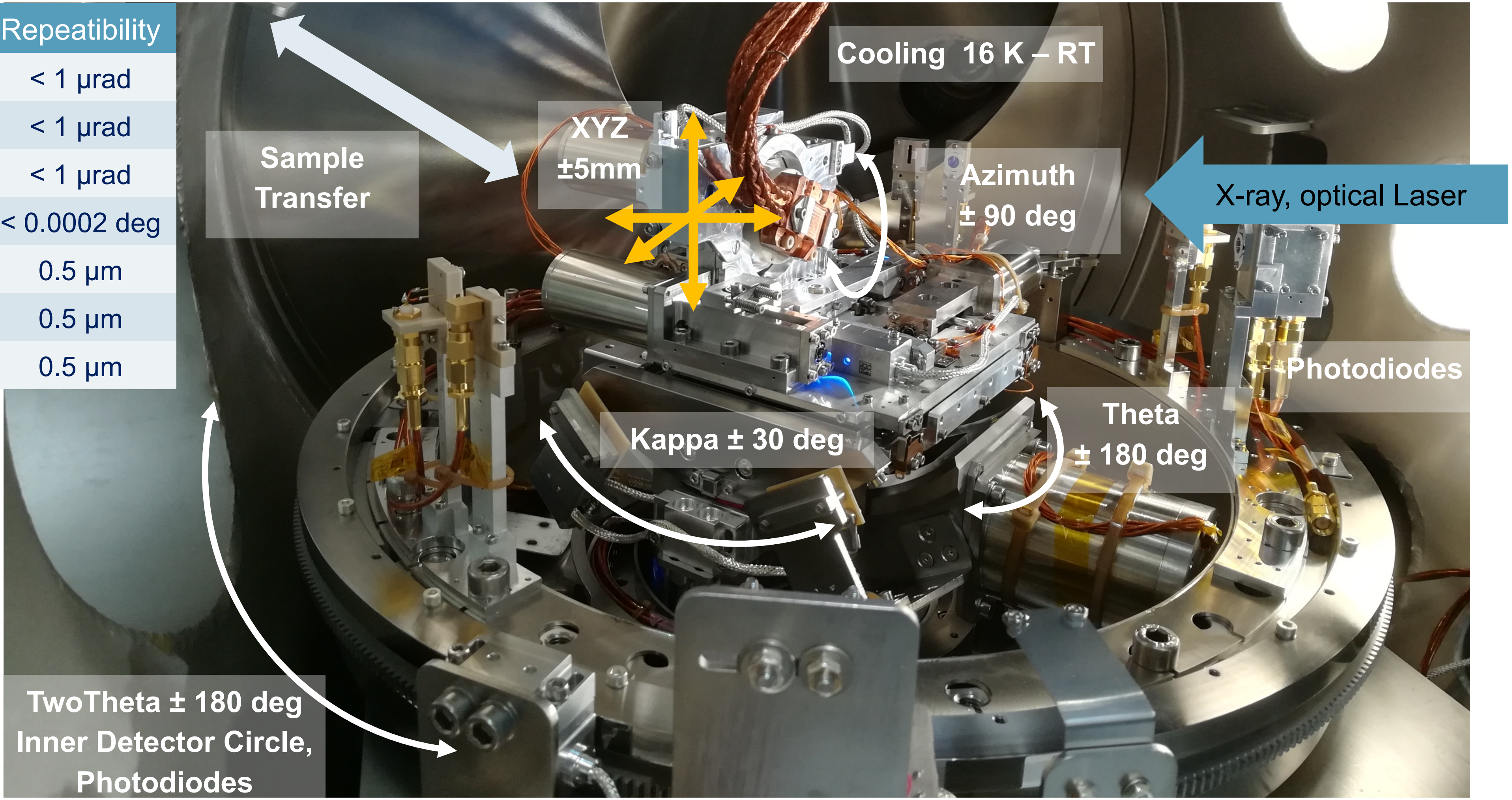
HR grating	
Line density	150 l/mm
Resolving power	Up to 10.000 (1^{st} order)
Pulse stretching	80-150 fs
X-ray pulse energy	up to 5 μJ

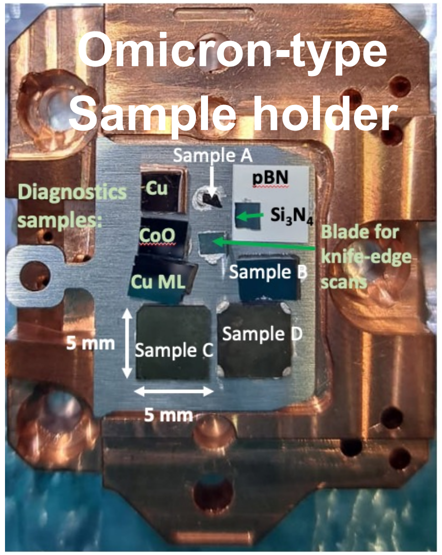
→ High combined energy resolution
→ Moderate temporal resolution

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

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





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)

PP laser information (Q&A session)

PP Laser Operating Points

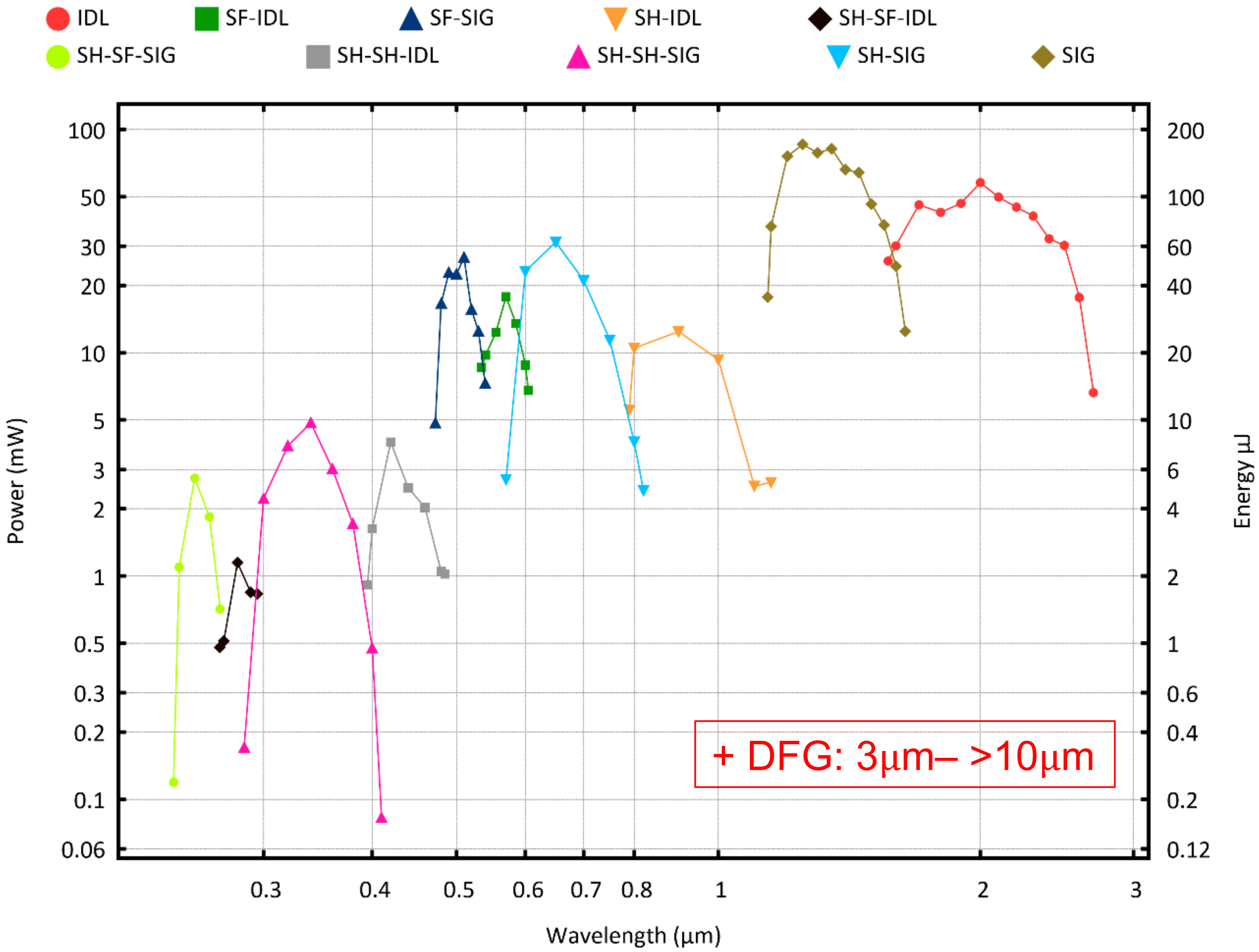
				800 nm	1030 nm
Mode	**F_rep / MHz**	**Δt / ns**	**F_eff / kHz**	**E_pulse / mJ**	**E_pulse / mJ**
1	4.5	222	27	0.05	1
2	1.1	1000	6	0.2	4
3	0.226	5000	1.2	1	20
4	**0.113**	**10000**	**0.6**	**2**	**40**
5	0.5	2000	3	?	?
		Pulse duration		15 fs or 50 fs	<1ps or 400 fs

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)

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%

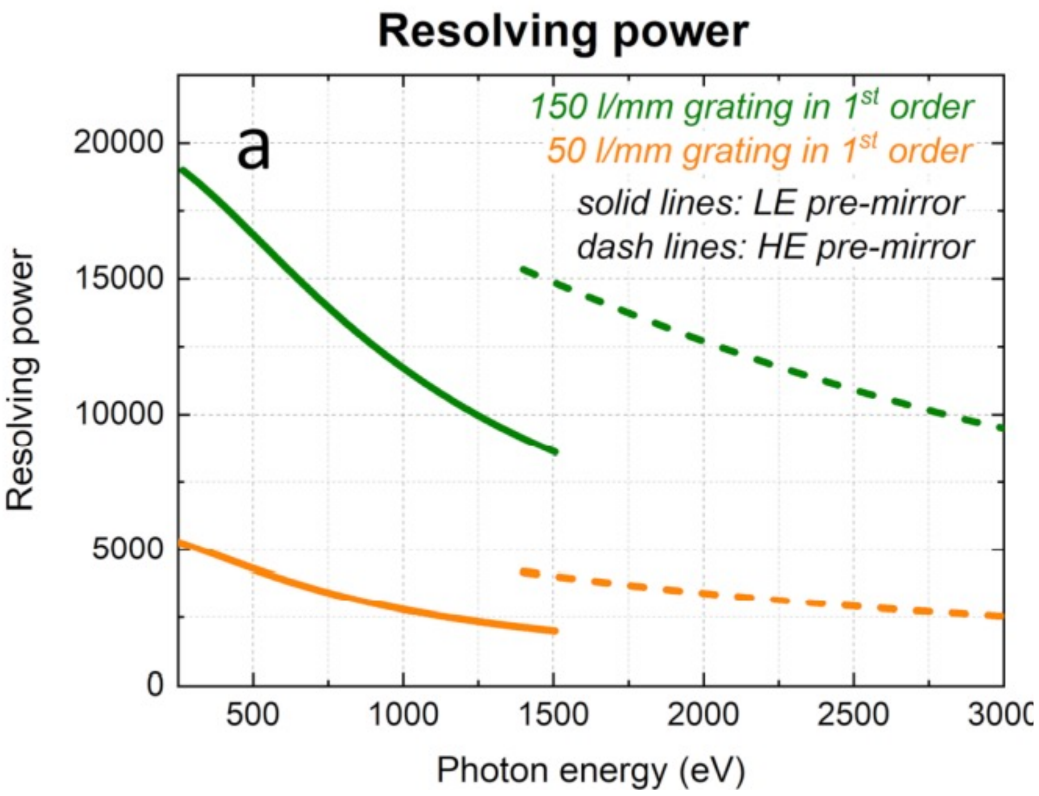
→ Energy resolution limited by the mono

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

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

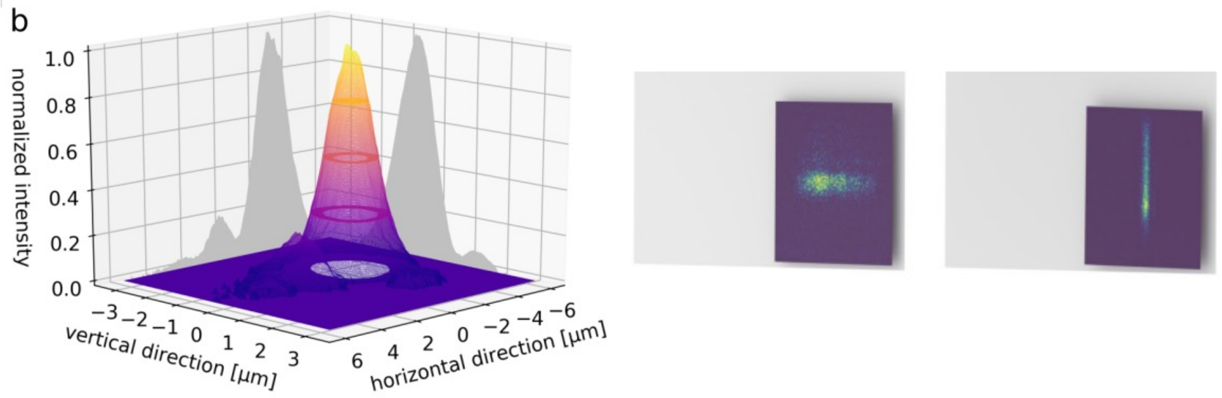
SCS instrument: photon energy, resolving power and beam size

- 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



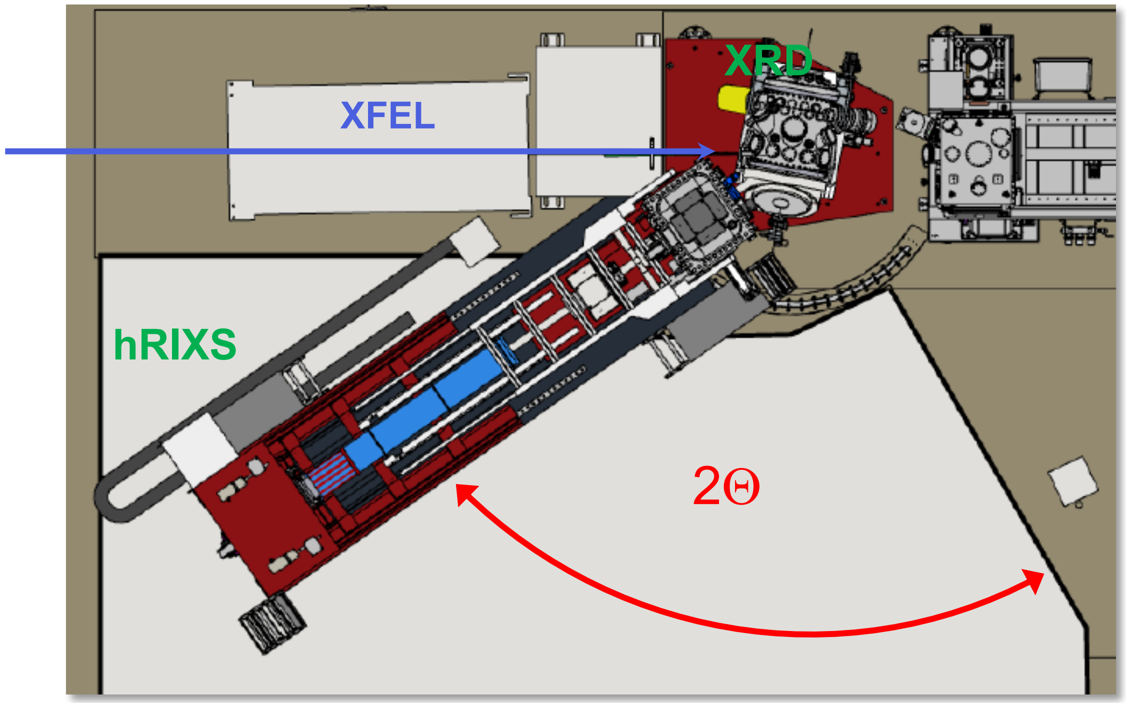
G. Mercurio et al., Opt. Express 30, 20980 (2020)

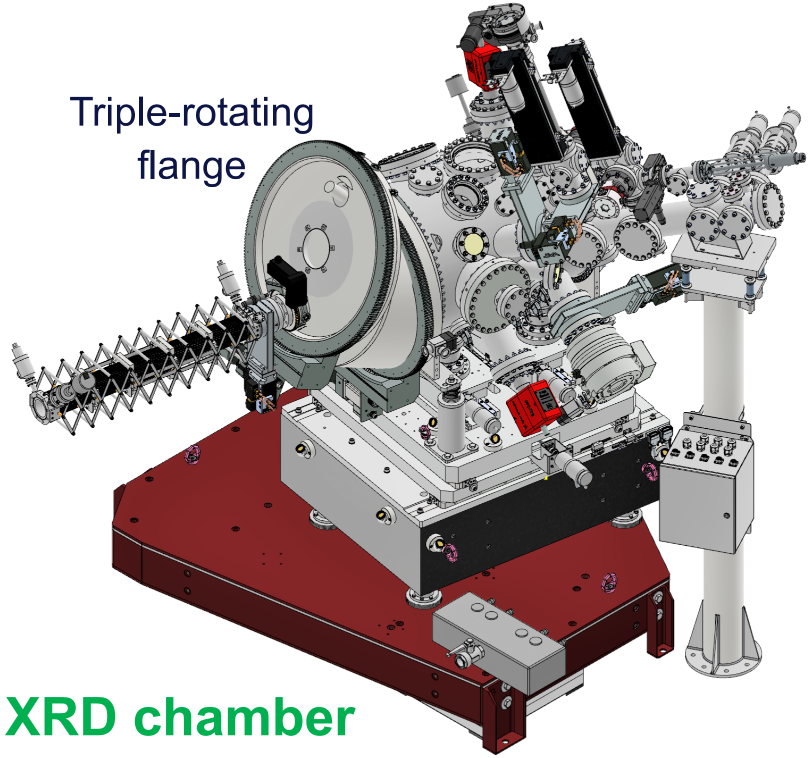
XRD baseline SCS setup for momentum-resolved RIXS and x-ray diffraction

- Continuous change of scattering angle: 65 deg ≤ 2Θ ≤ 145 deg

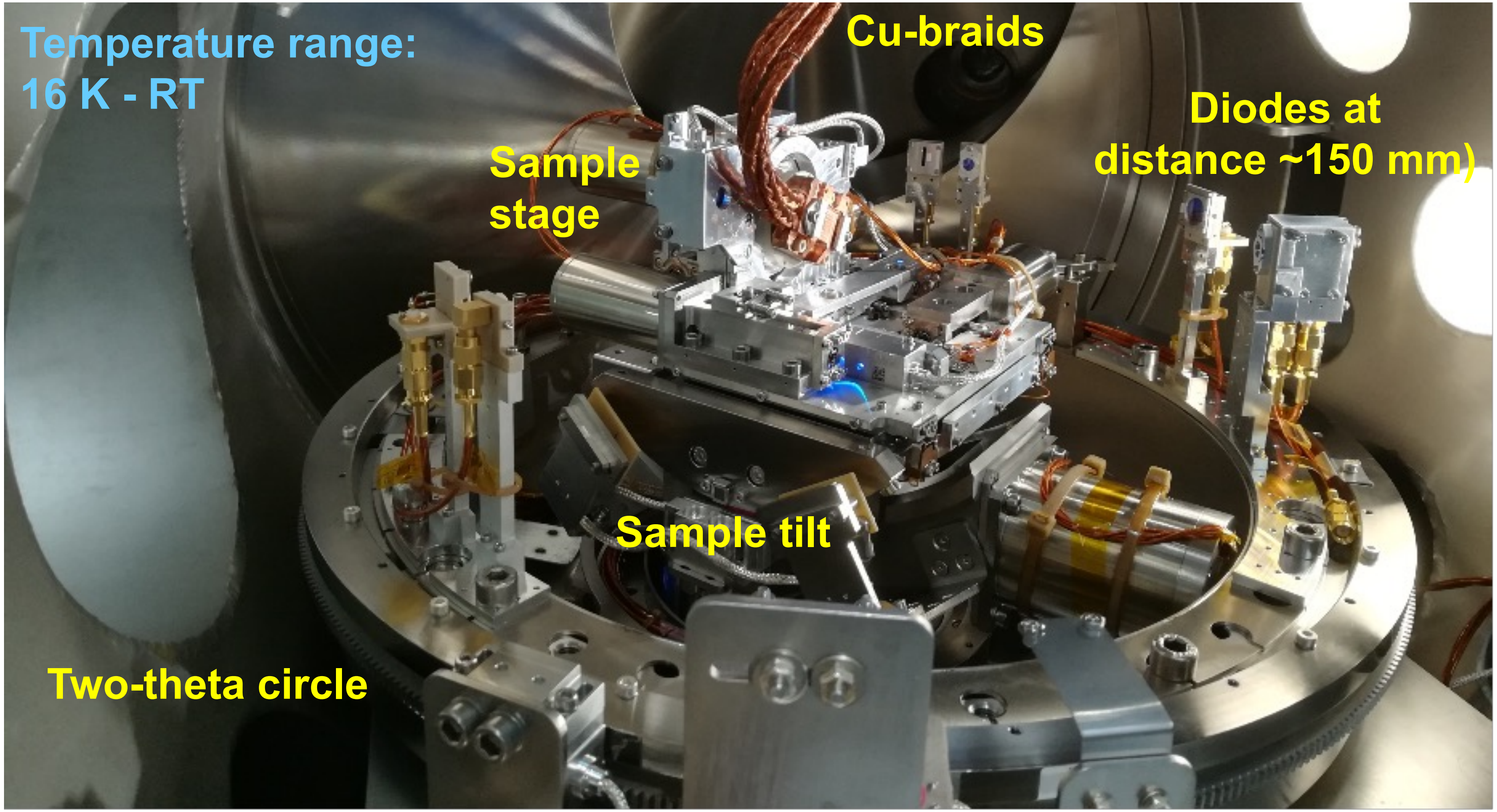
→ Mechanical motion just commissioned

→ No experience yet whether re-alignment of hRIXS is required (after changing 2Θ)





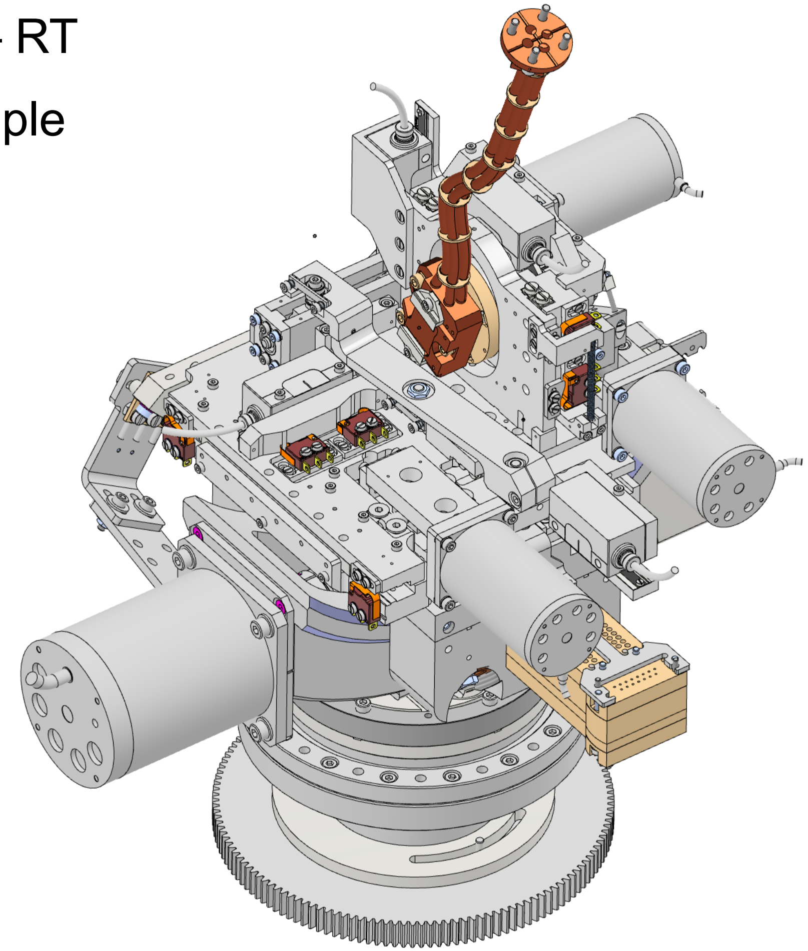
XRD setup: sample stage and in-vacuum diffractometer



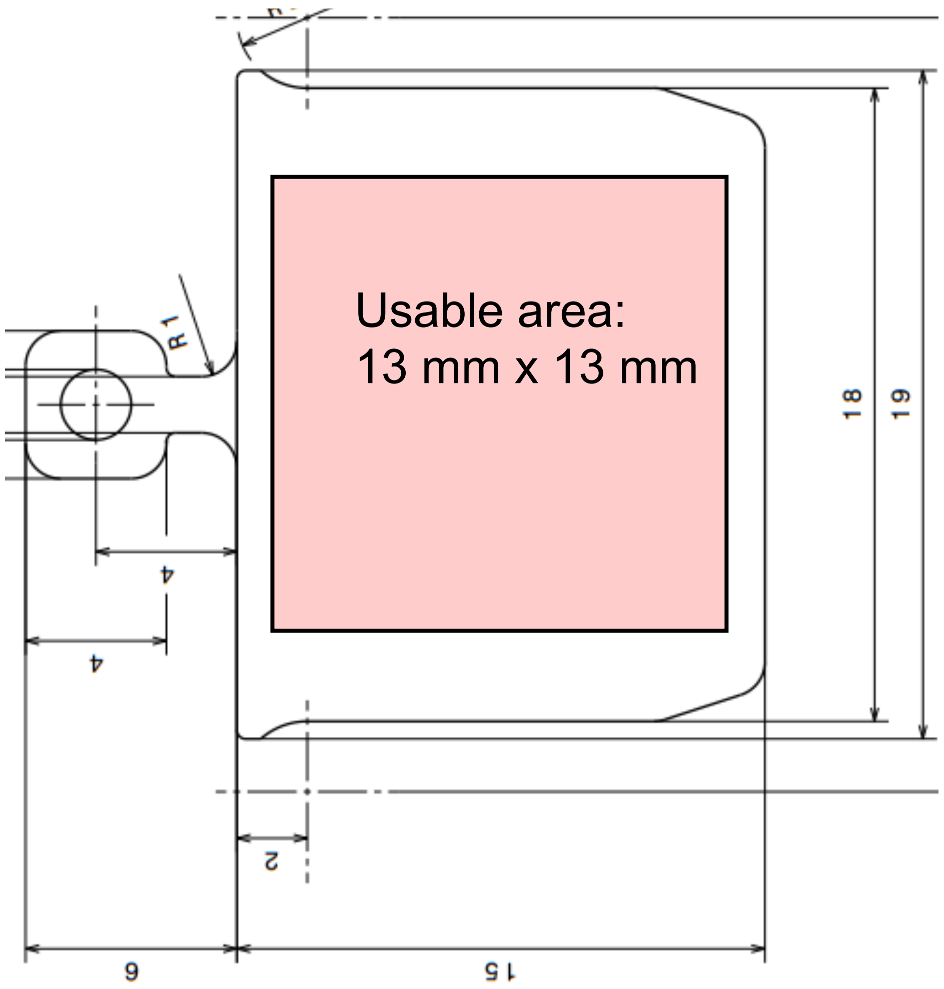
XRD setup: sample environment

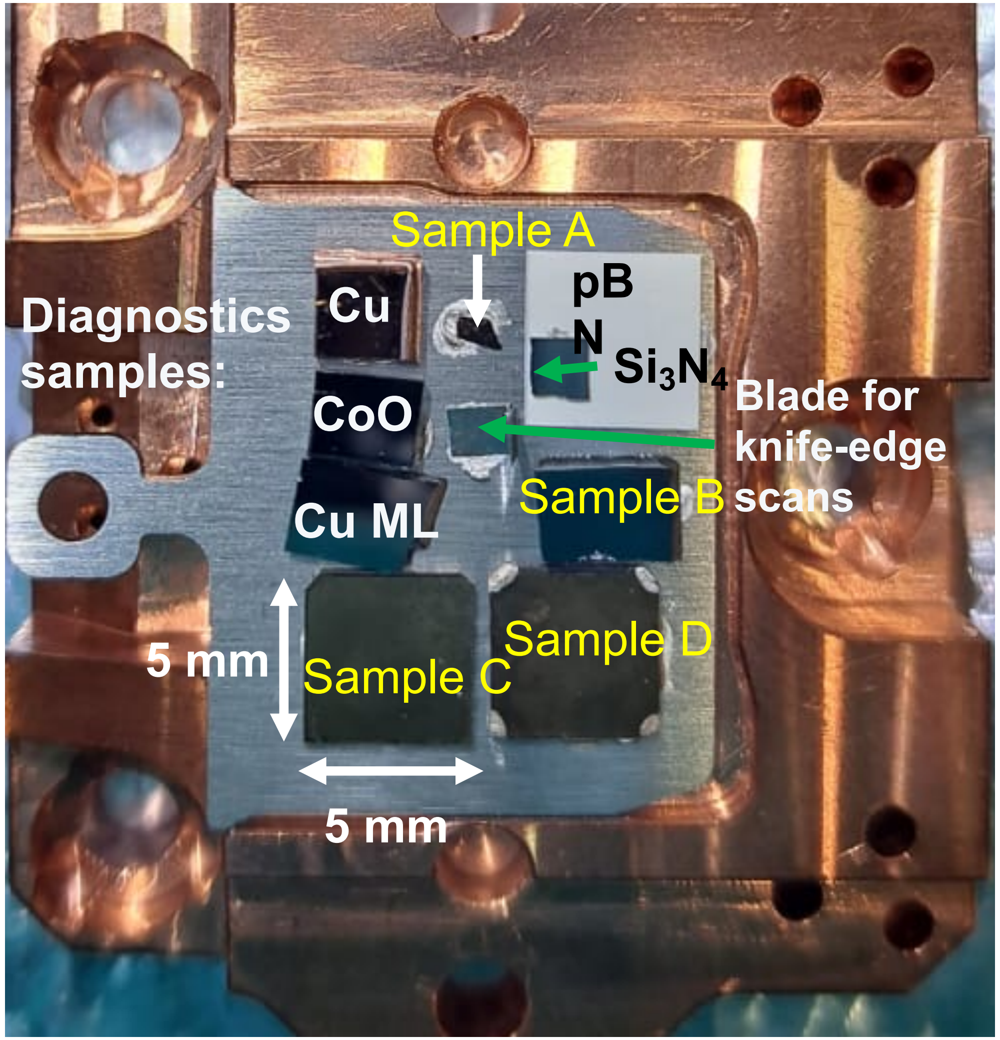
- UHV ($p < 10^{-9}$ mbar)
- Cryogenic temperatures: 16 K – RT
- 6 degrees of motion for the sample

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



Flag-style sample holder (Omicron design)



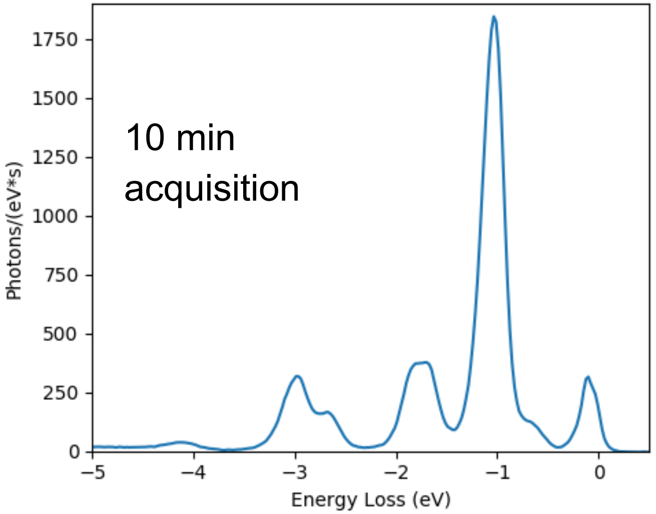


Count rates RIXS from NiO for high-energy-resolution mode

Static spectra at 1.1 MHz repetition rate:

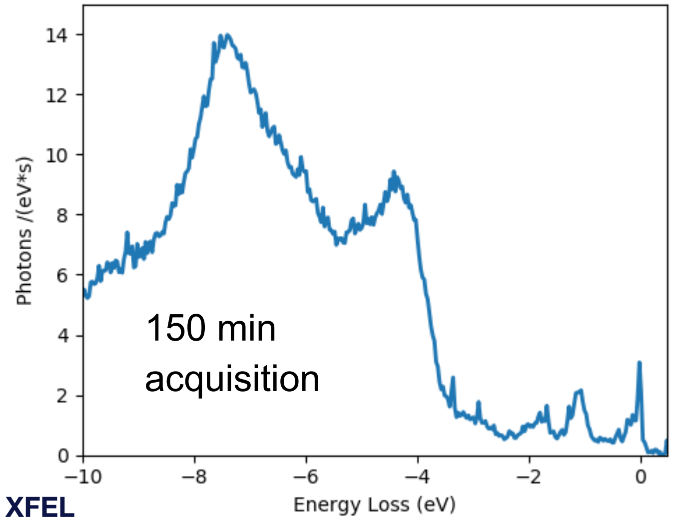
Ni L_3-edge

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:

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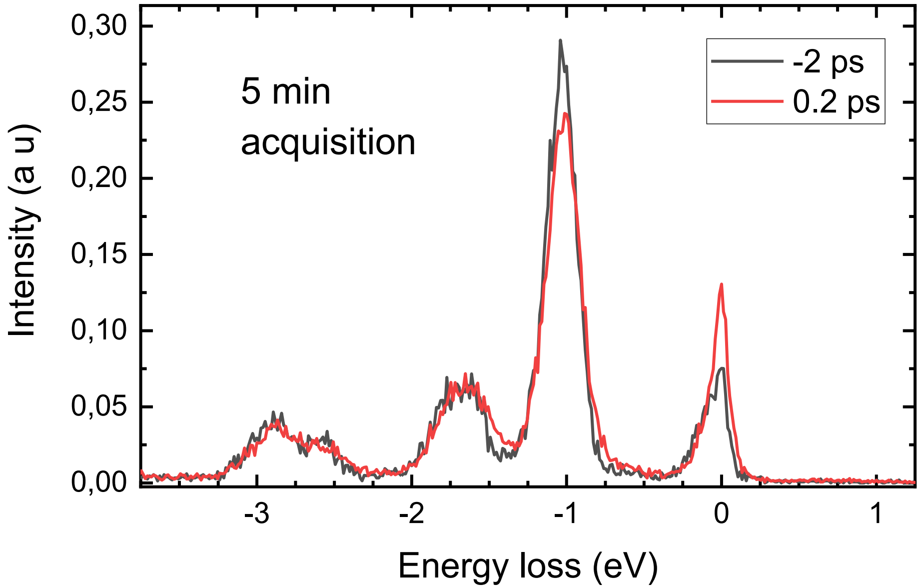
200 pulses/s
30% transmission (FEL)
266 nm pump (~10 mJ/cm^2)

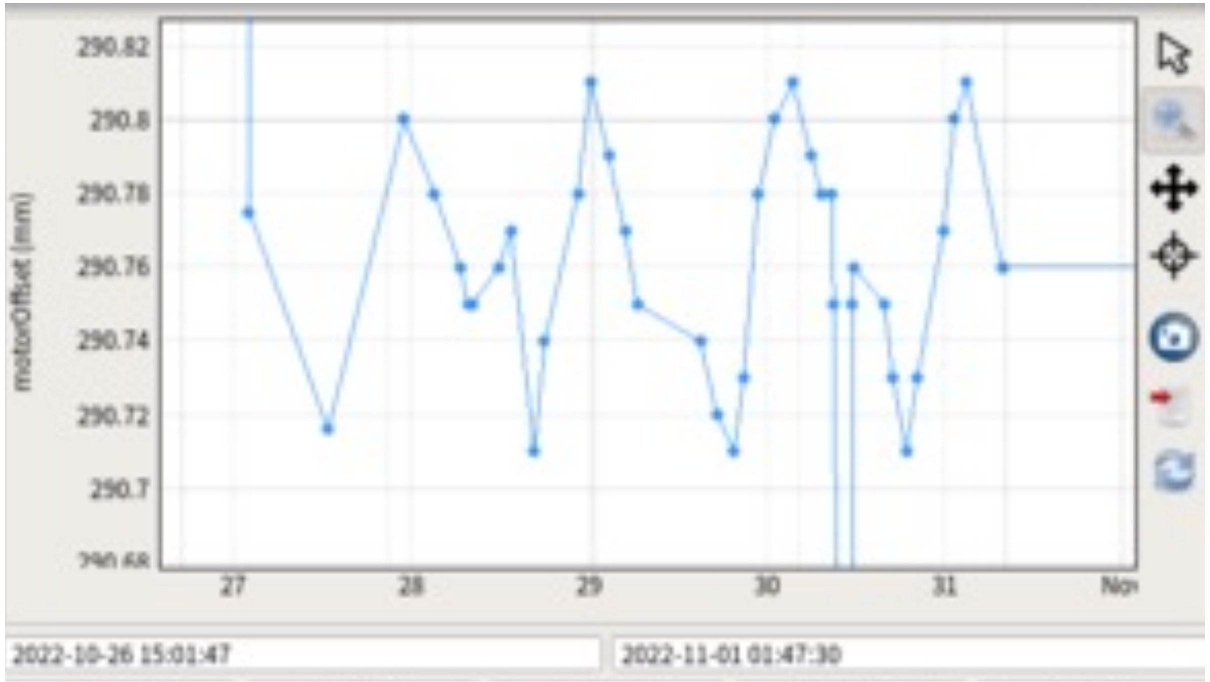


- La2CuO4: count rate ~ factor 10 lower
- 1.1 MHz possible for 800 nm or 400 nm pump
- 1000 l/mm grating: 4-5 times more throughput

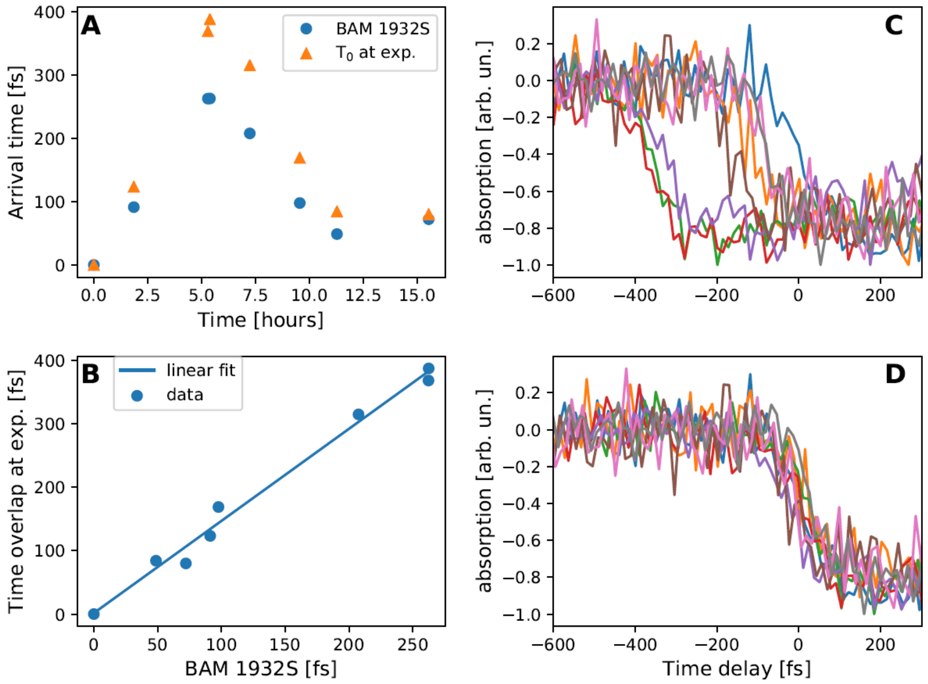
Timing stability during UAC experiment, February 2021

- Short time scales (up to 10 min): size of the inter-train jitter is ~15 fs
- Long time scales (hours): dominant is a periodic drift with amplitude of ~600 fs, due to tidal change of ground water level

Time-zero from XAS on sample, over days:



→ It is possible to correct for the periodic drift, using Bunch Arrival Monitor (BAM) feedback, reduction down to ~50 fs (over 16 h)

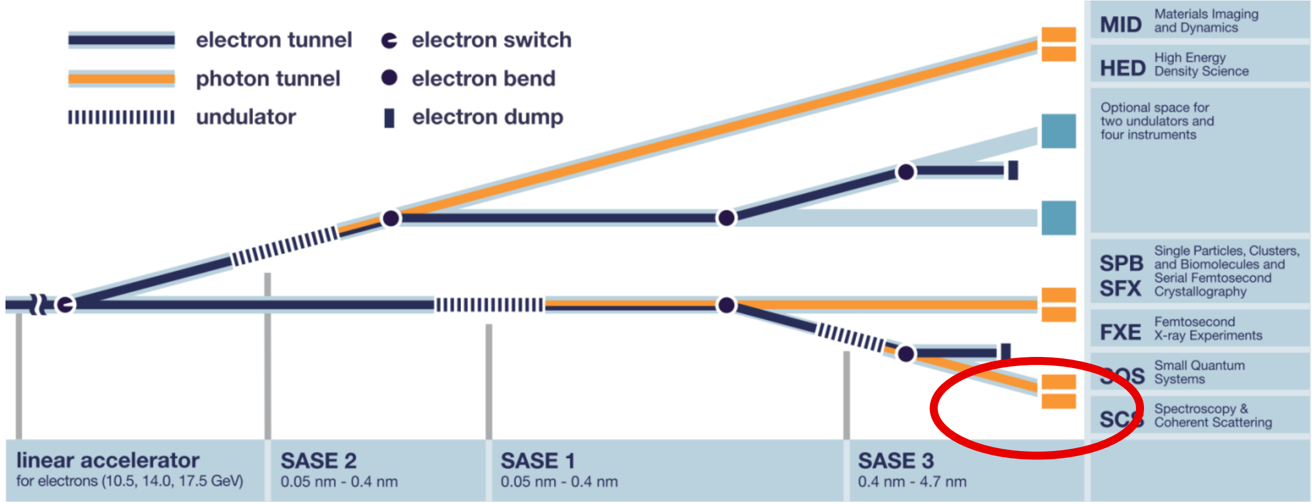


FEL pulse pattern

- 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)

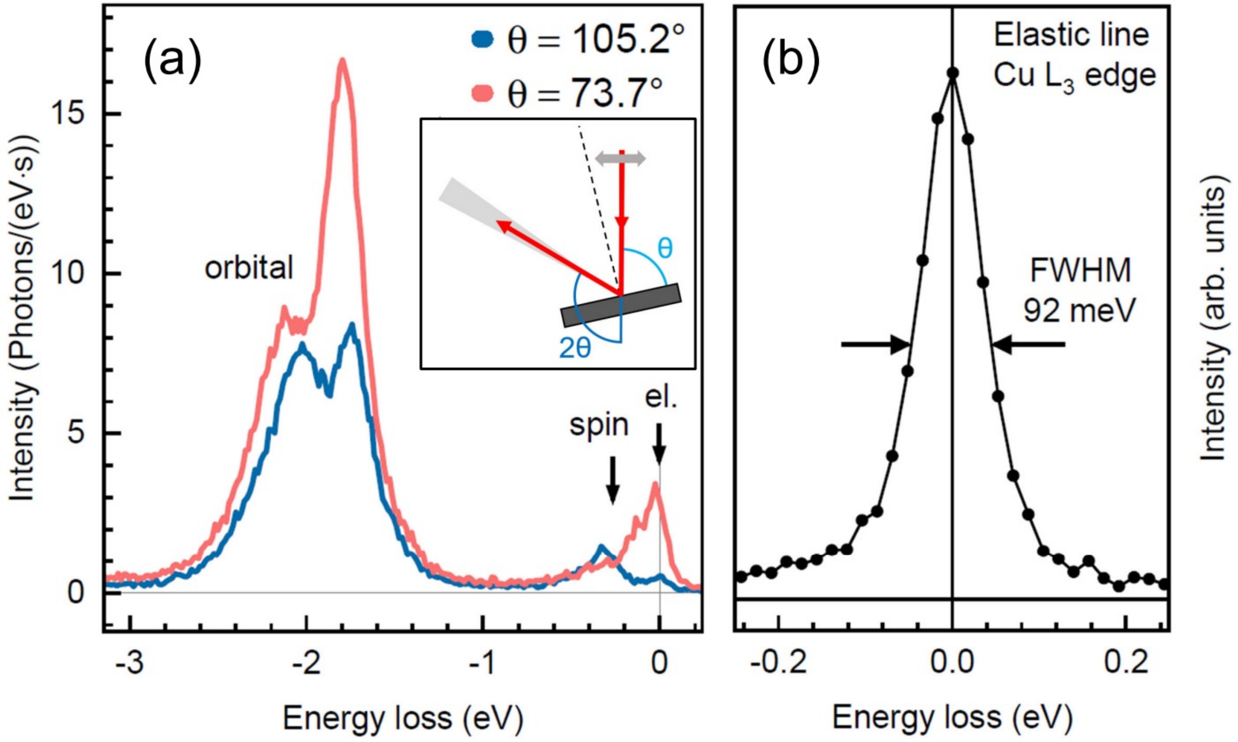
Interleaved mode with SA1:

Repetition rate of up to 1.1 MHz for SCS

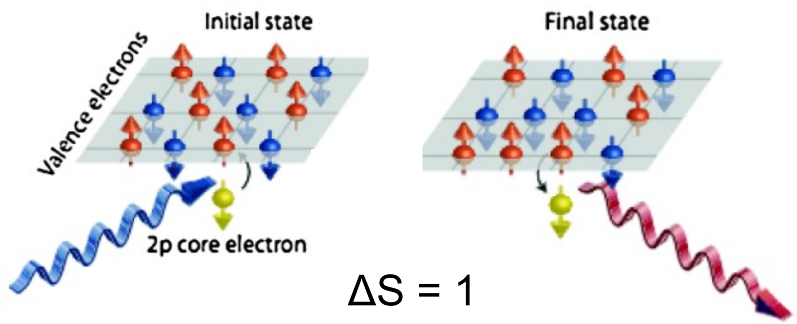


hRIXS x-ray commissioning: achieved energy resolution

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	84	10 200
O K	530	49	10 400

➡ Achieved combined resolving power: > 10.000