PG beamlines: Status and Plans

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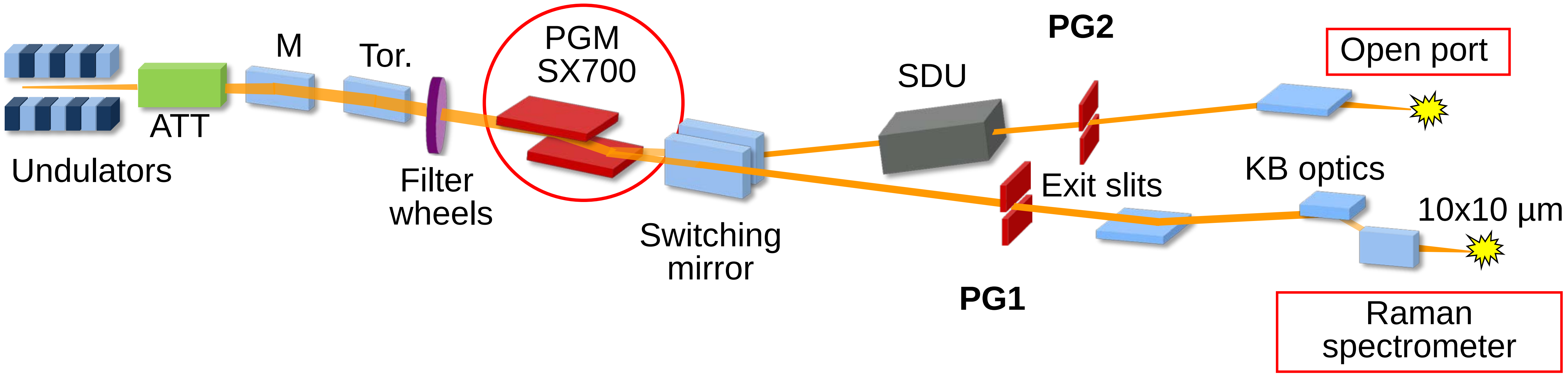
Hamburg, 19.02.2019

Outline

- **High – resolution XAS at PG2**
  - PG beamline
  - XAS concept
  - High resolution XAS at PG2
  - Time–resolved XAS measurements at FLASH
- **Time-resolved high resolution RIXS at PG1**
  - RIXS concept
  - Spectrometer design
  - Pump-probe measurments
- **Future perspectives**

PG beamline

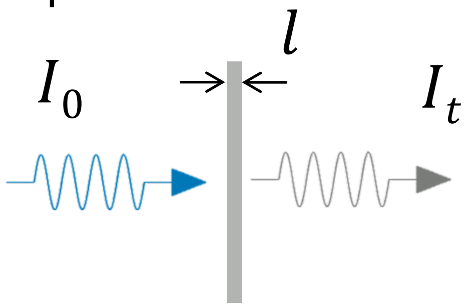


- 50 – 250 eV + higher harmonics
- High flux (~1E10 ph/pulse) / High resolution (E/ΔE ~ 12000)
- Short FEL pulses (< 100 fs to 2 ps)

X-ray Absorption Spectroscopy

Incident photon flux

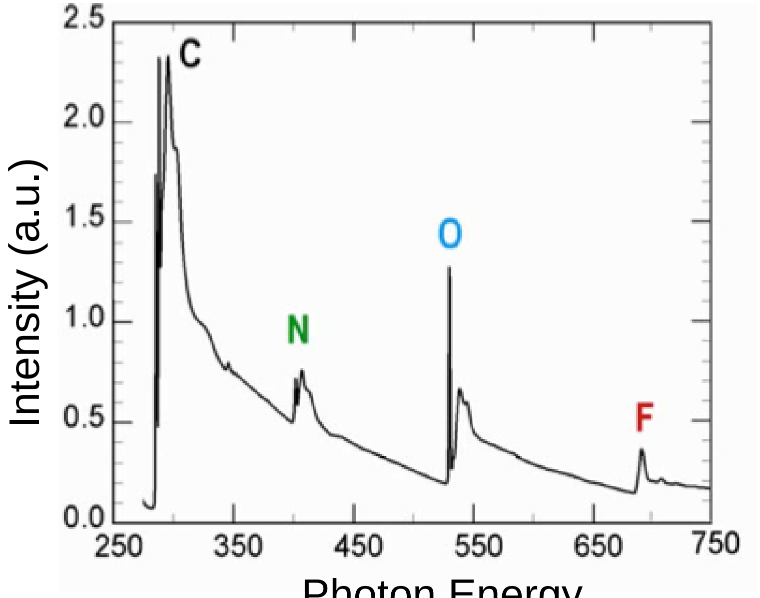
Transmitted flux



$$I_t = I_0 e^{-\mu l}$$

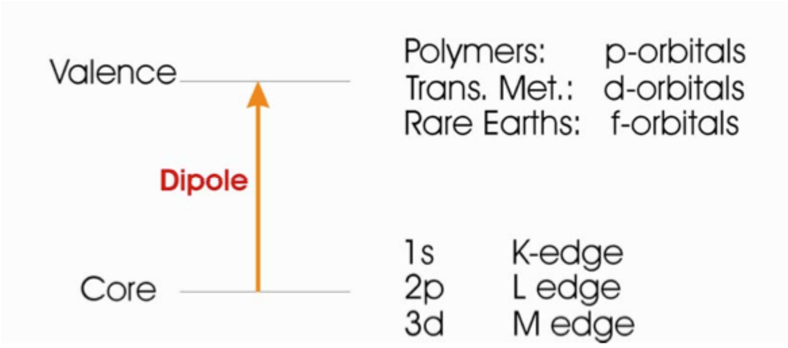
$$\mu \approx \frac{pZ^4}{AE^3}$$

Near edge x-ray absorption fine structure spectroscopy



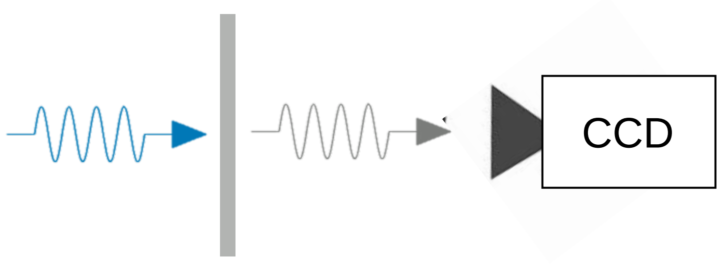
- Element specific sensitivity and contrast
- Absorption gives information about energy levels of electrons in atoms
- Spectrum is sensitive to bonding enviroment of absorbing atom, molecular orientation, polarization, etc.

Energy levels



X-ray Absorption Detection

Transmission detection with Photodiode/CCD



XAS in soft X-ray range at FELs challenging for several reasons:

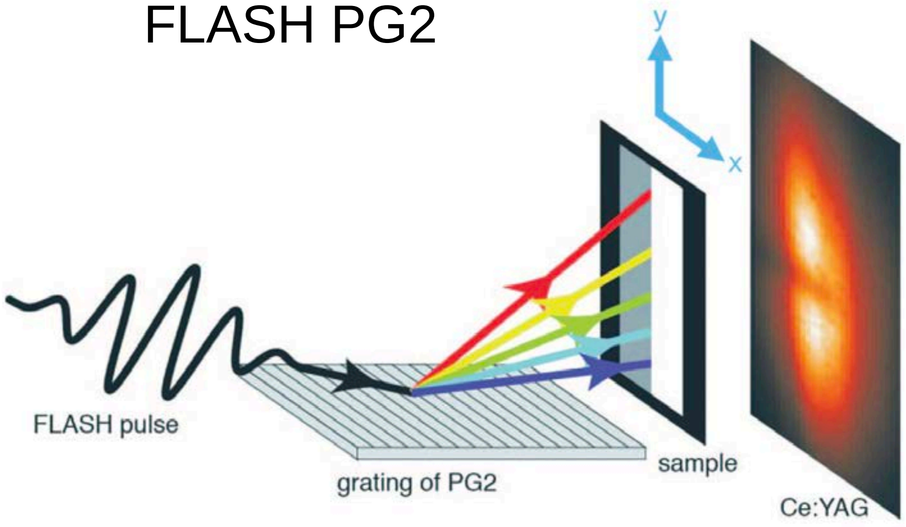
- Very high temporal & spatial density of X-rays (detector linearity/saturation problem)
- Strong intensity fluctuations in SASE spectrum (even enhanced behind monochromator)

→ Normalization method needed to measure small changes in absorption

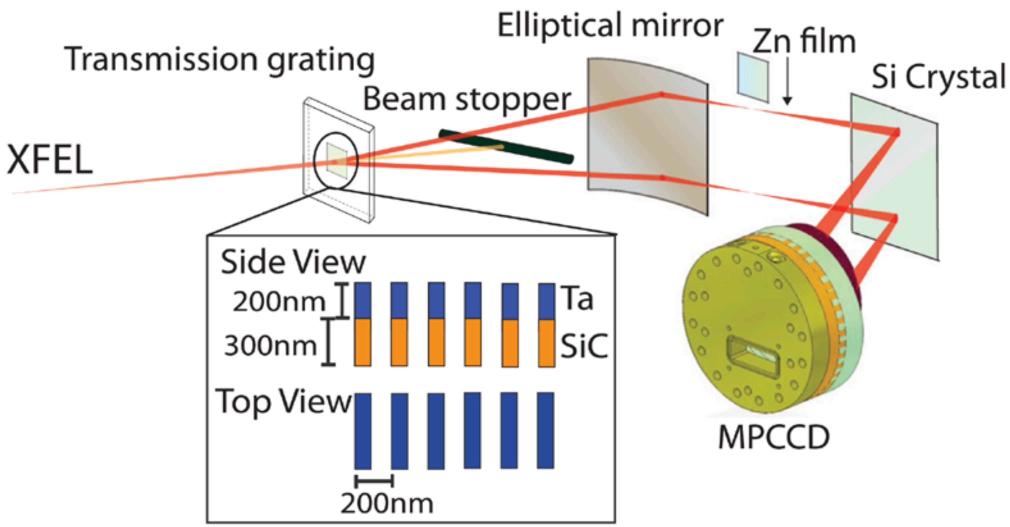
Divided beams to cope with fluctuations in SASE spectrum

Previous approaches

FLASH PG2



SACLA



- Divergence and dispersion produces large beam
- Sample divides beam just in front of YAG-crystal

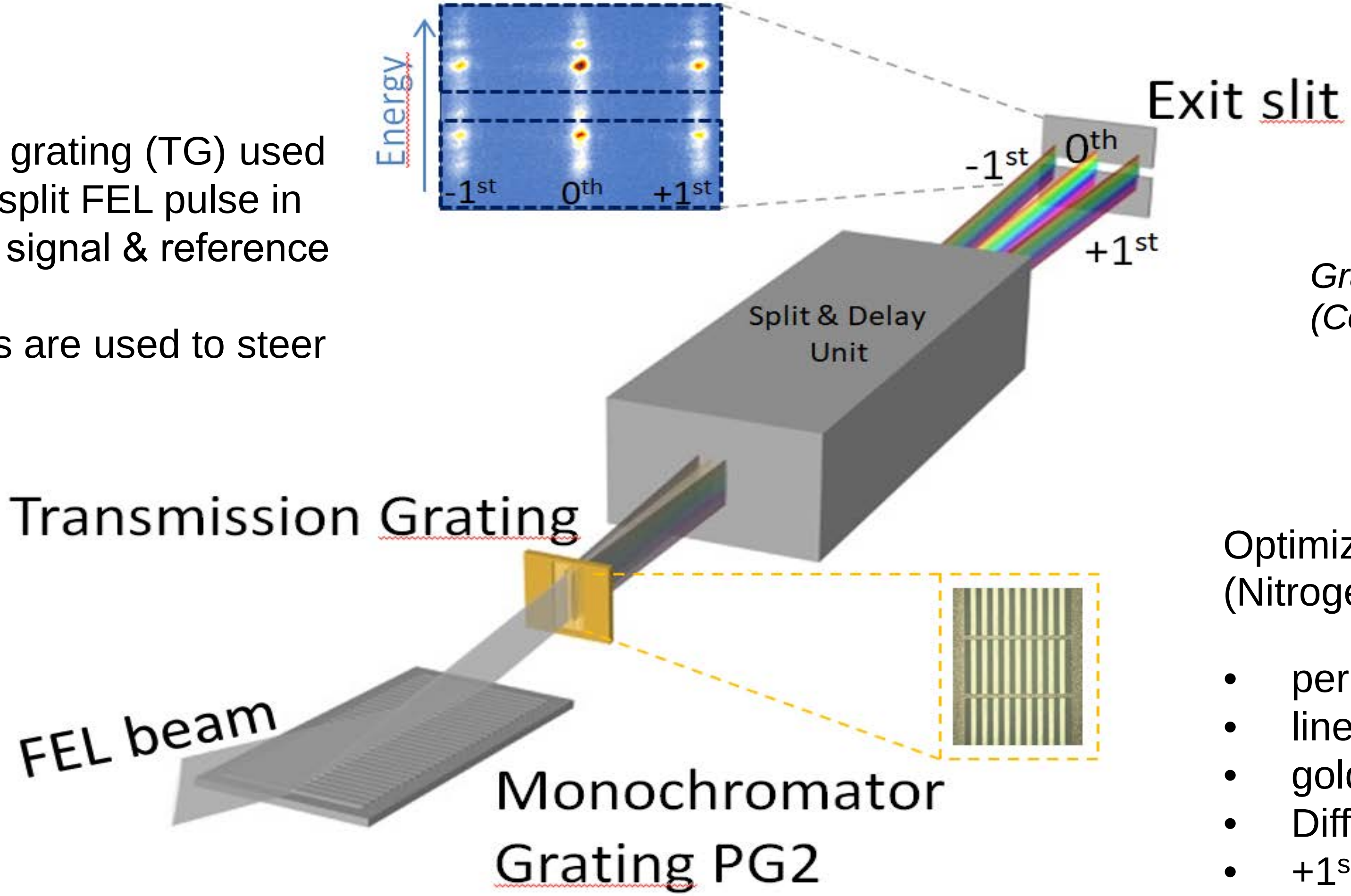
- Transmission grating to split beam via wavefront division
- Spectrometer behind to achieve energy dispersion

D. P. Bernstein, et al., Appl. Phys. Lett. 95 , 134102 (2009)

Tetsuo Katayama, et al., Appl. Phys. Lett. 103 , 131105 (2013)

New high resolution XAS setup at PG2

- Diffractive transmission grating (TG) used as amplitude splitter to split FEL pulse in two identical copies → signal & reference beam.
- Split & Delay Unit optics are used to steer the beams



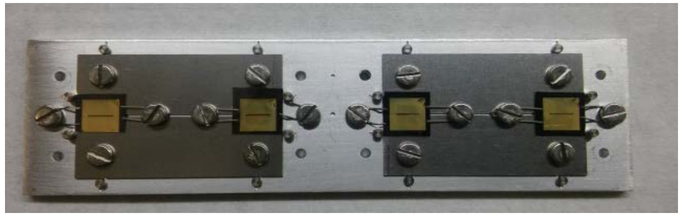
Grating Design by PSI (Contact: Christian David)

PAUL SCHERRER INSTITUT PSI

Optimized for 133 eV / 400 eV (Nitrogen K-edge)

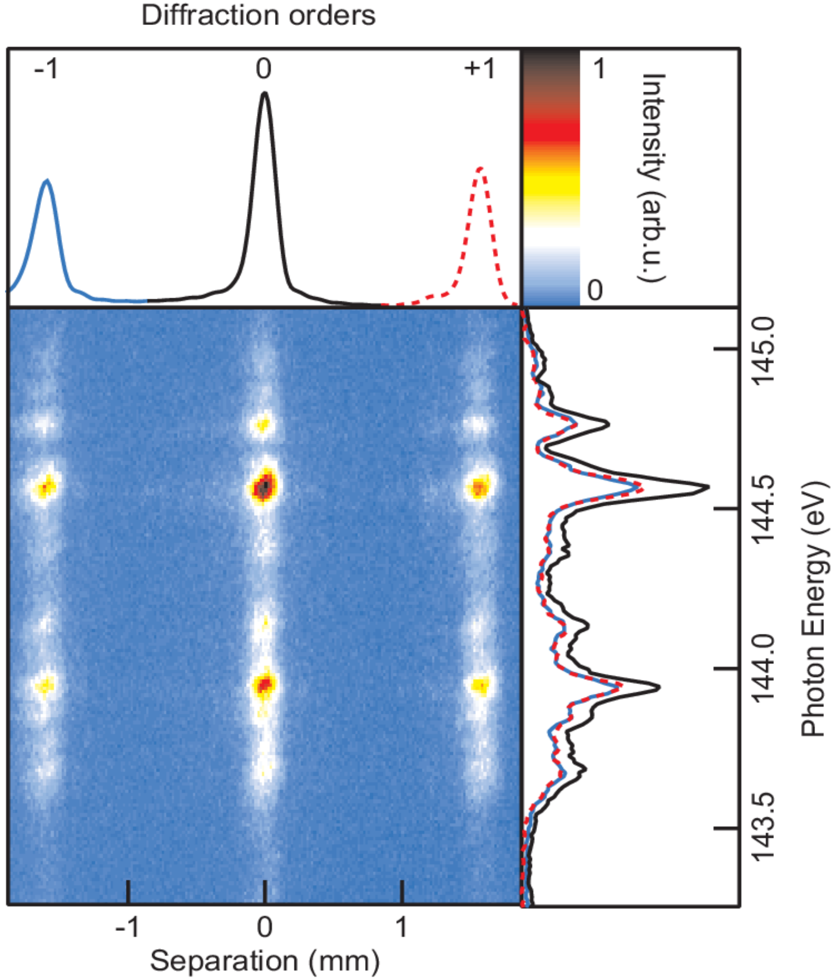
- period 34 µm
- line width 17 µm
- gold thickness 100 nm
- Diffraction efficiency ~ 25 %
- +1st/-1st order equal intensity

Grating holder

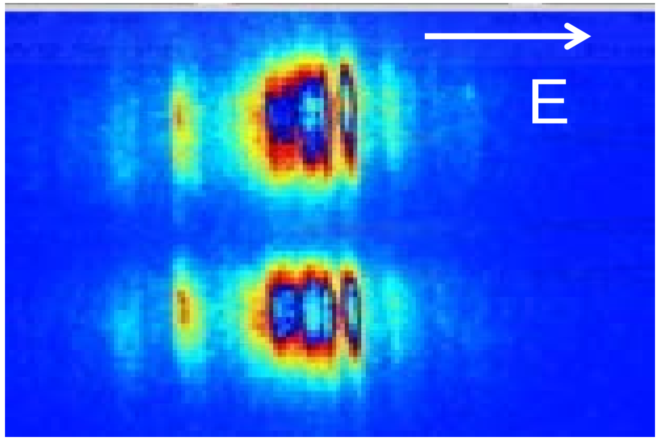


Correlation of signal & reference beam

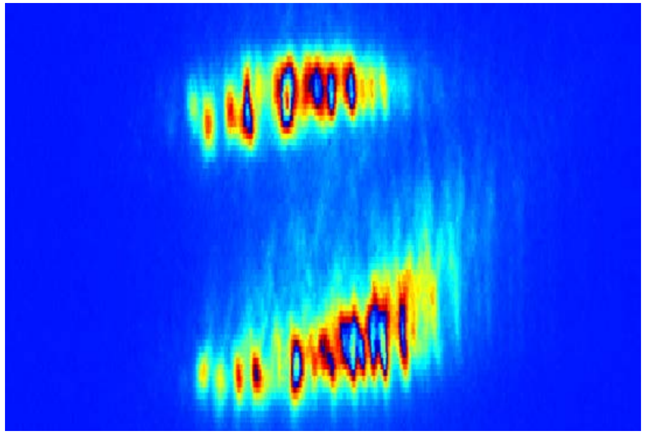
Single shot SASE spectra measured at monochromator exit slit



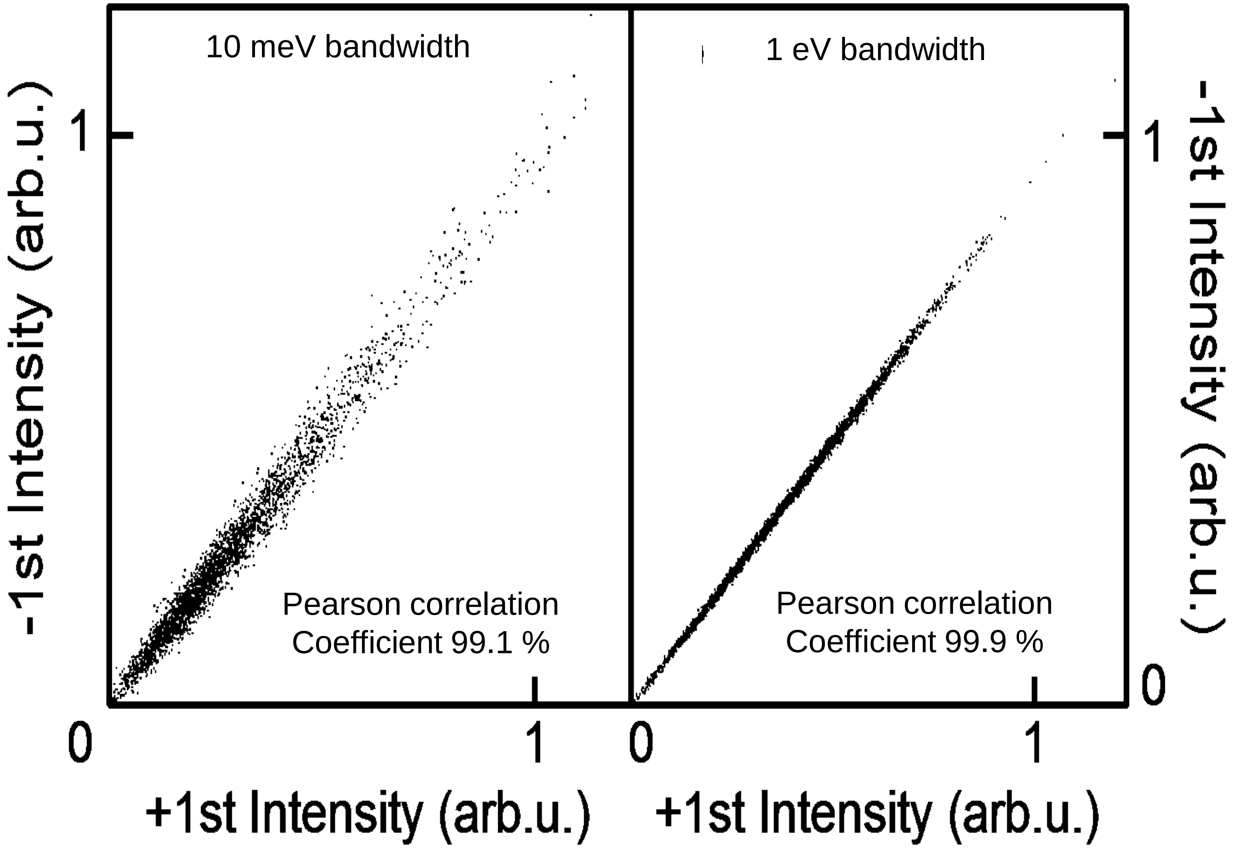
Transmission Grating

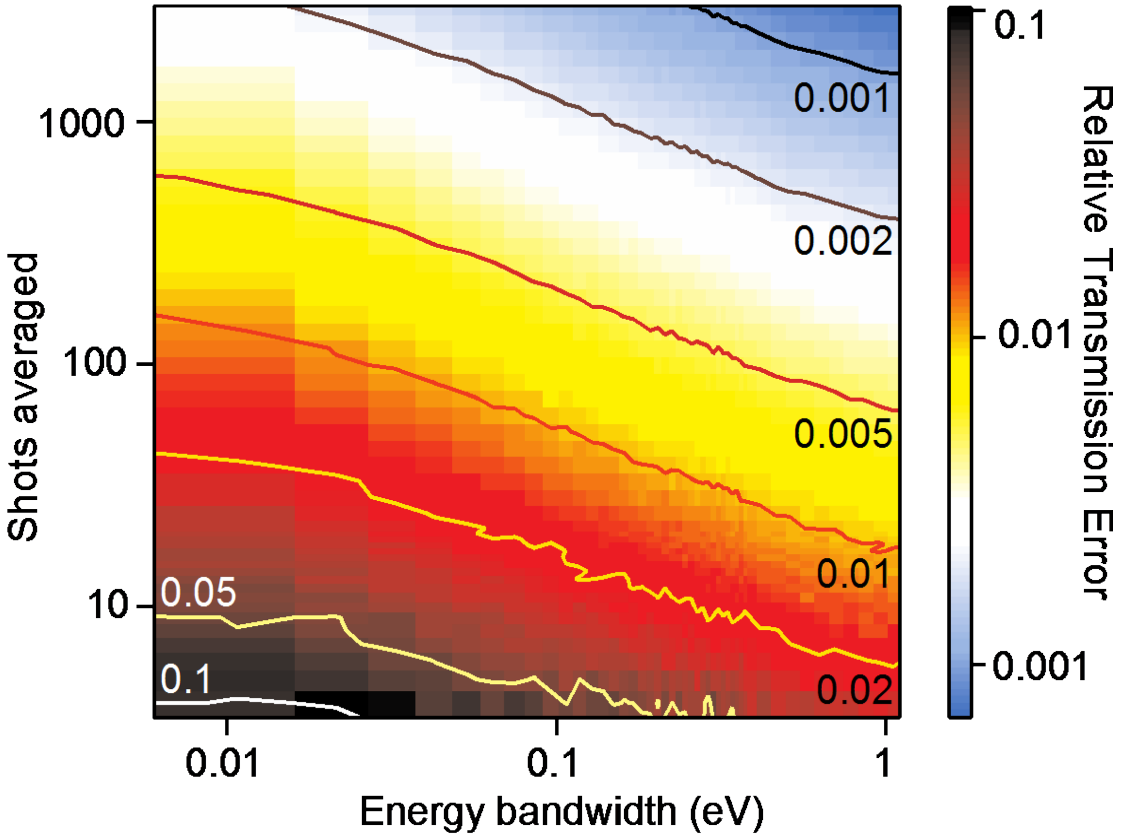


Split & Delay Unit (Amplitude division)



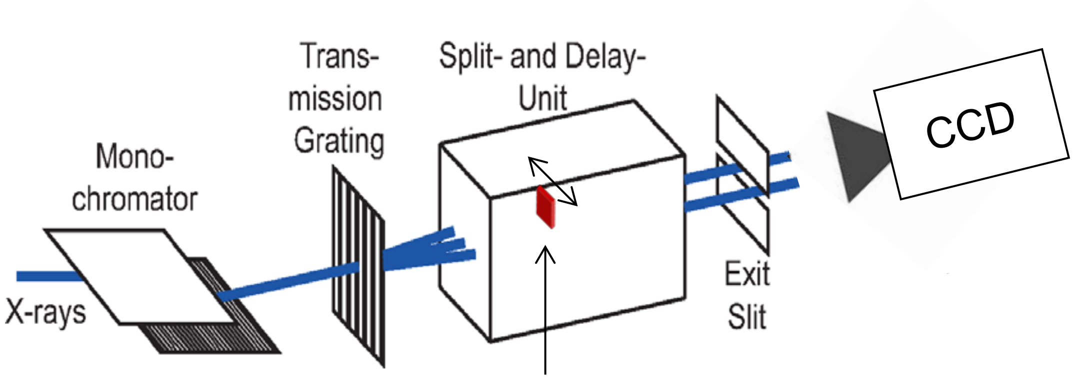
Intensity correlation & Sensitivity to absorption changes





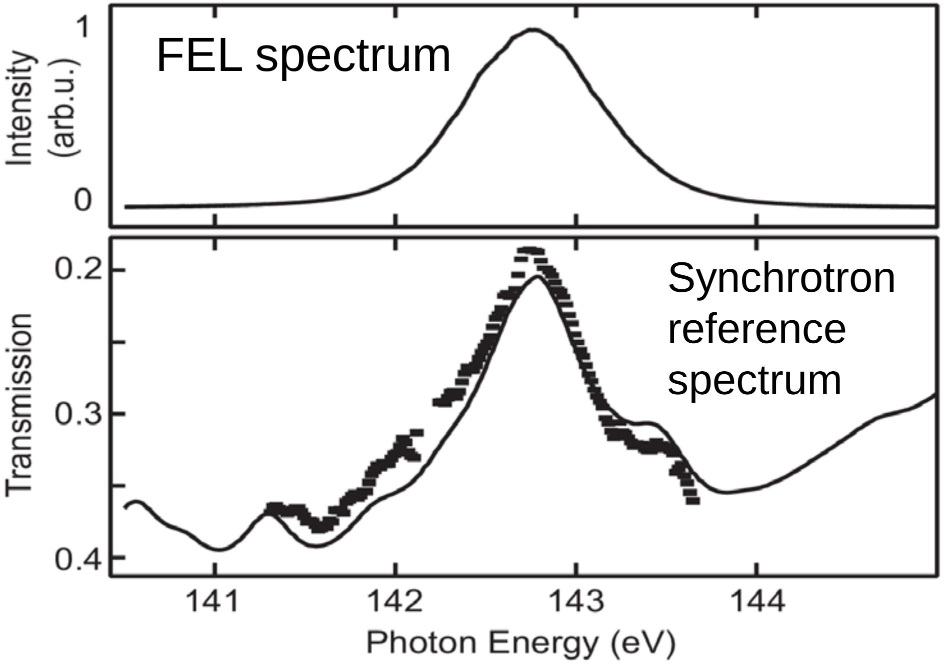
100 meV bandwidth, 100 pulses: below 1% absorption changes can be measured

XAS spectrum measured at PG2



- New normalization scheme used
- Gd sample in signal beam
- Monochromator energy scanned
  (~100 meV energy bandwidth used)

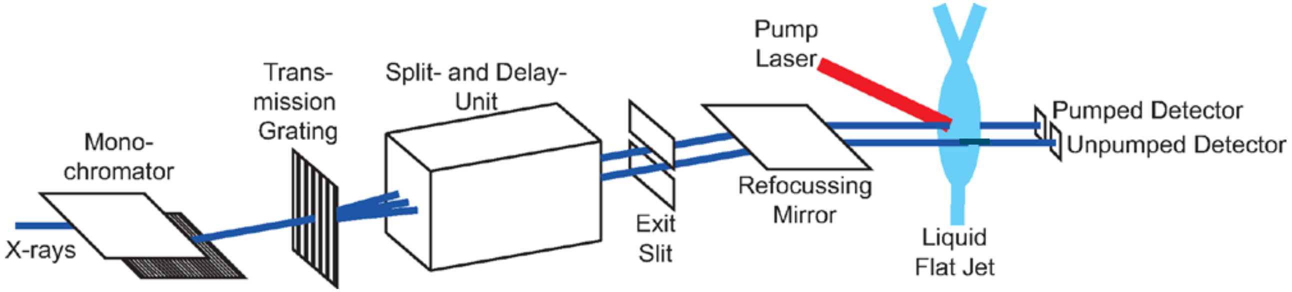
Gd_2O_3 $N_{4,5}$-edge XAS spectrum



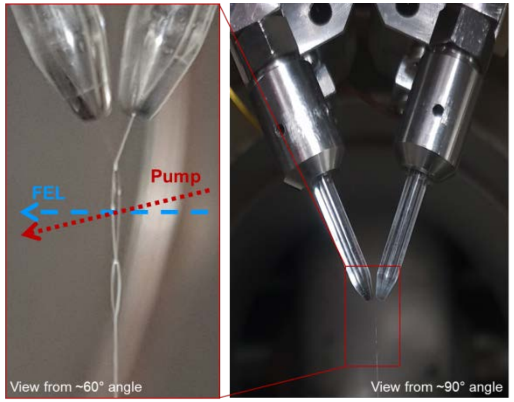
G.Brenner, S. Dziarzhytski, P. Miedema, B. Rösner, C. David and M. Beye

Time-resolved XAS @ Nitrogen K-edge of liquid samples

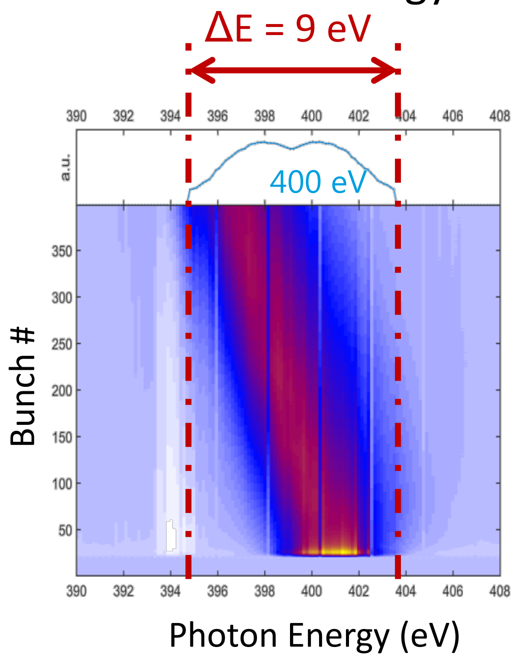
PG2 monochromator beamline



Normalization scheme using diffractive transmission grating



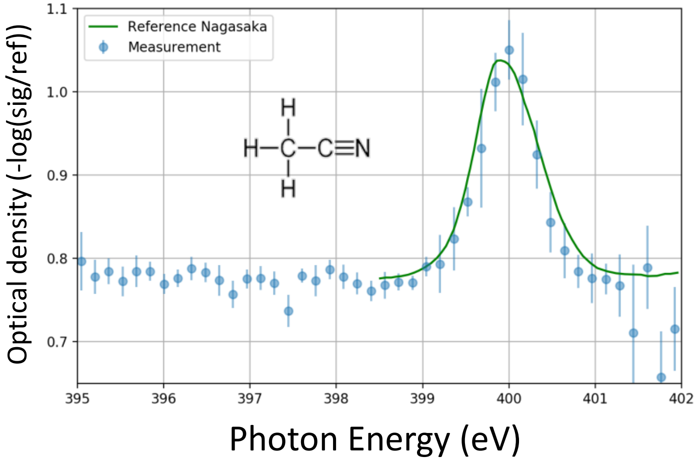
Intra-train FEL energy chirp



Doubling the effective FEL bandwidth

VLS spectrometer & KALYPSO

XAS spectrum Acetonitrile



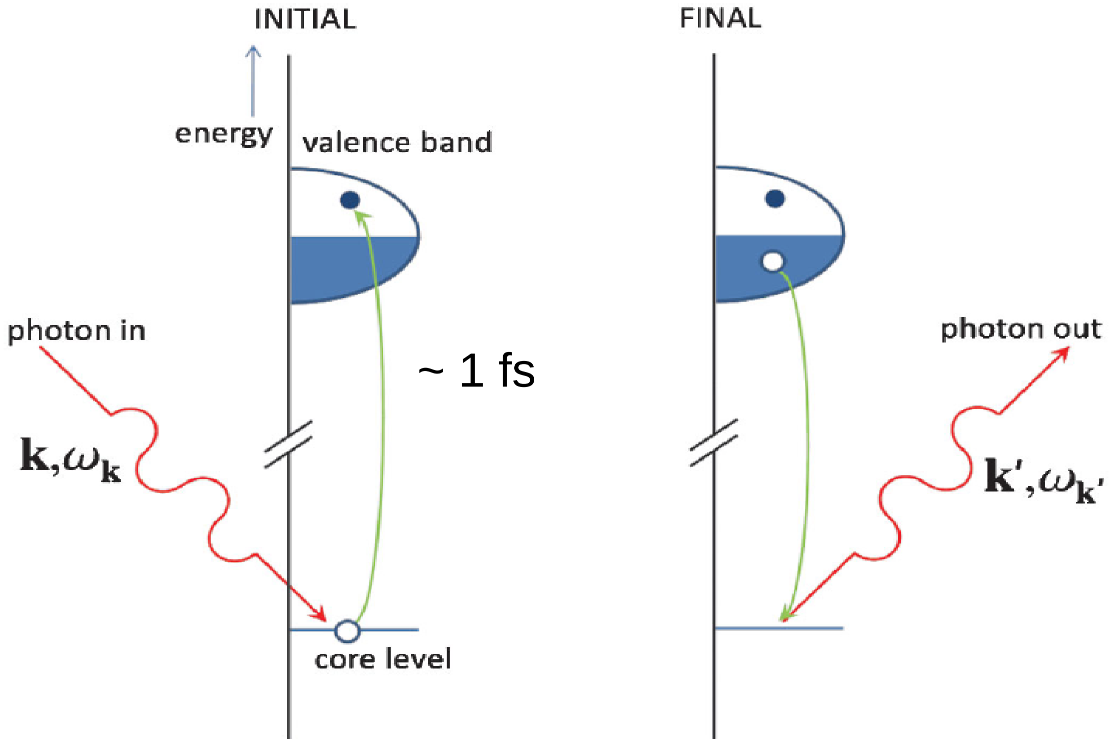
- Acetonitrile solved in Ethanol
- $1s \rightarrow \pi^*$ K-edge transition
- 14min acq time)

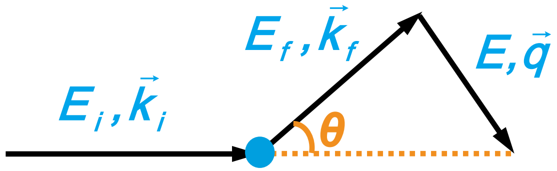
Pump-Probe Data under analysis

N. Huse, M. Beye, G. Brenner, E.Nibbering, C. David

Time-resolved high resolution RIXS at FLASH PG1

RIXS concept



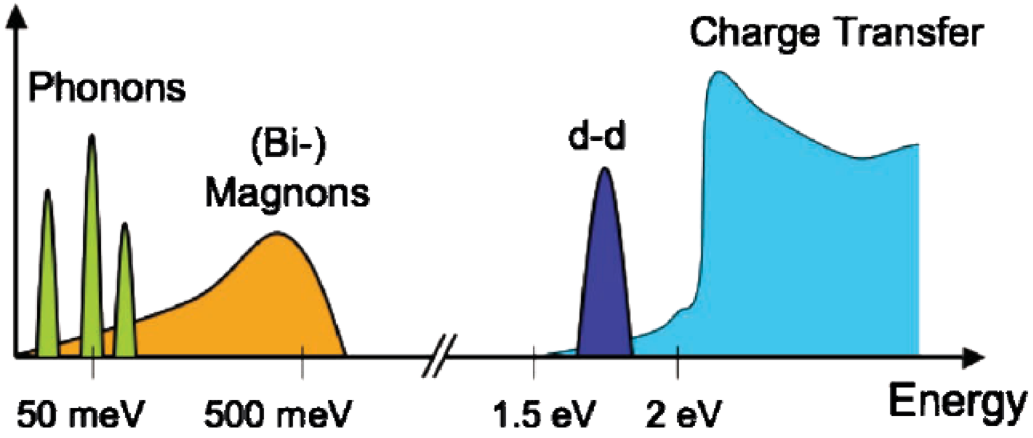


Final state: $\Delta E = E_f - E_i = \hbar\omega_k - \hbar\omega_{k'}$

$\hbar \mathbf{q} = \hbar \mathbf{k} - \hbar \mathbf{k'}$

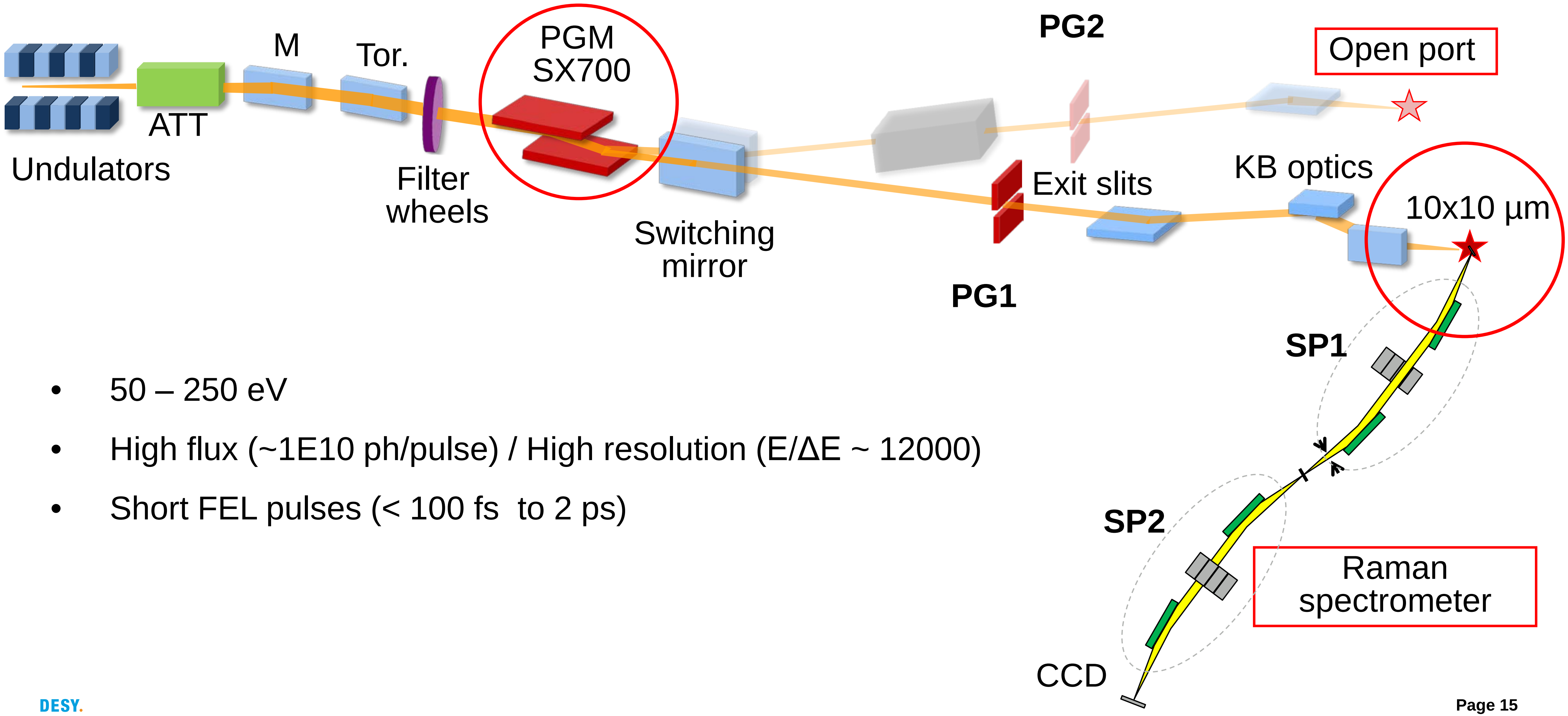
L. J. P. Ament et al. Rev. Mod. Phys., Vol. 83, No. 2, April–June 2011, p.705

RIXS potential



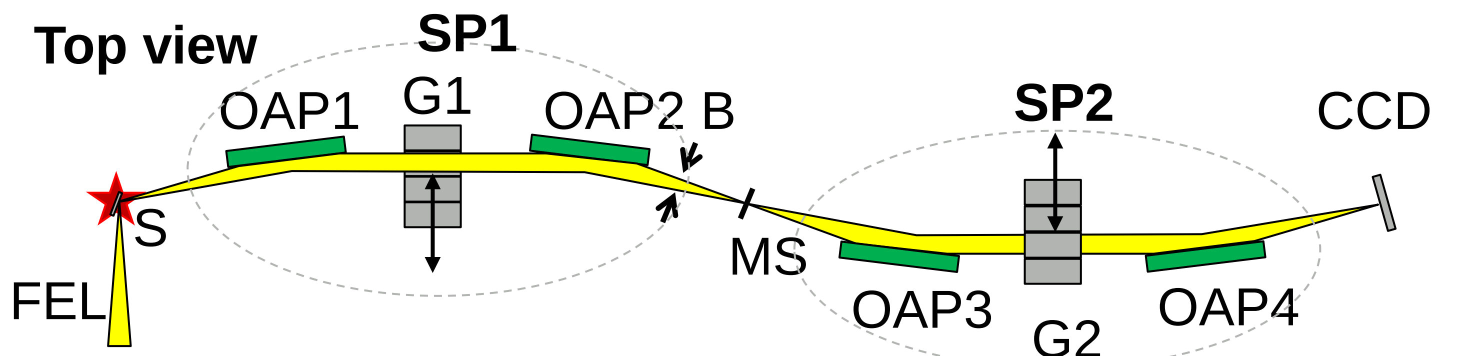
- Functioning of metallo-enzymes
- Charge transfer in bio-relevant molecules
- Vibronic coupling
- Photostability
- Fundamental-to-application questioning of correlated materials

PG1 beamline

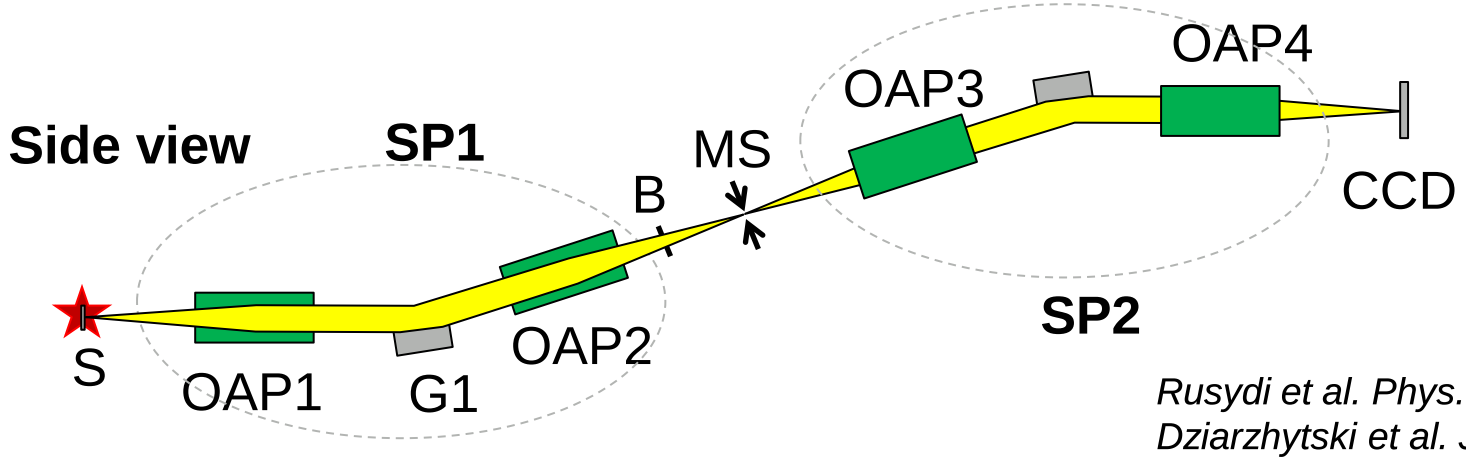


- 50 – 250 eV
- High flux (~1E10 ph/pulse) / High resolution (E/ΔE ~ 12000)
- Short FEL pulses (< 100 fs to 2 ps)

PG1 XUV double stage Raman spectrometer



Slitless
KB vert. focus <10 µm

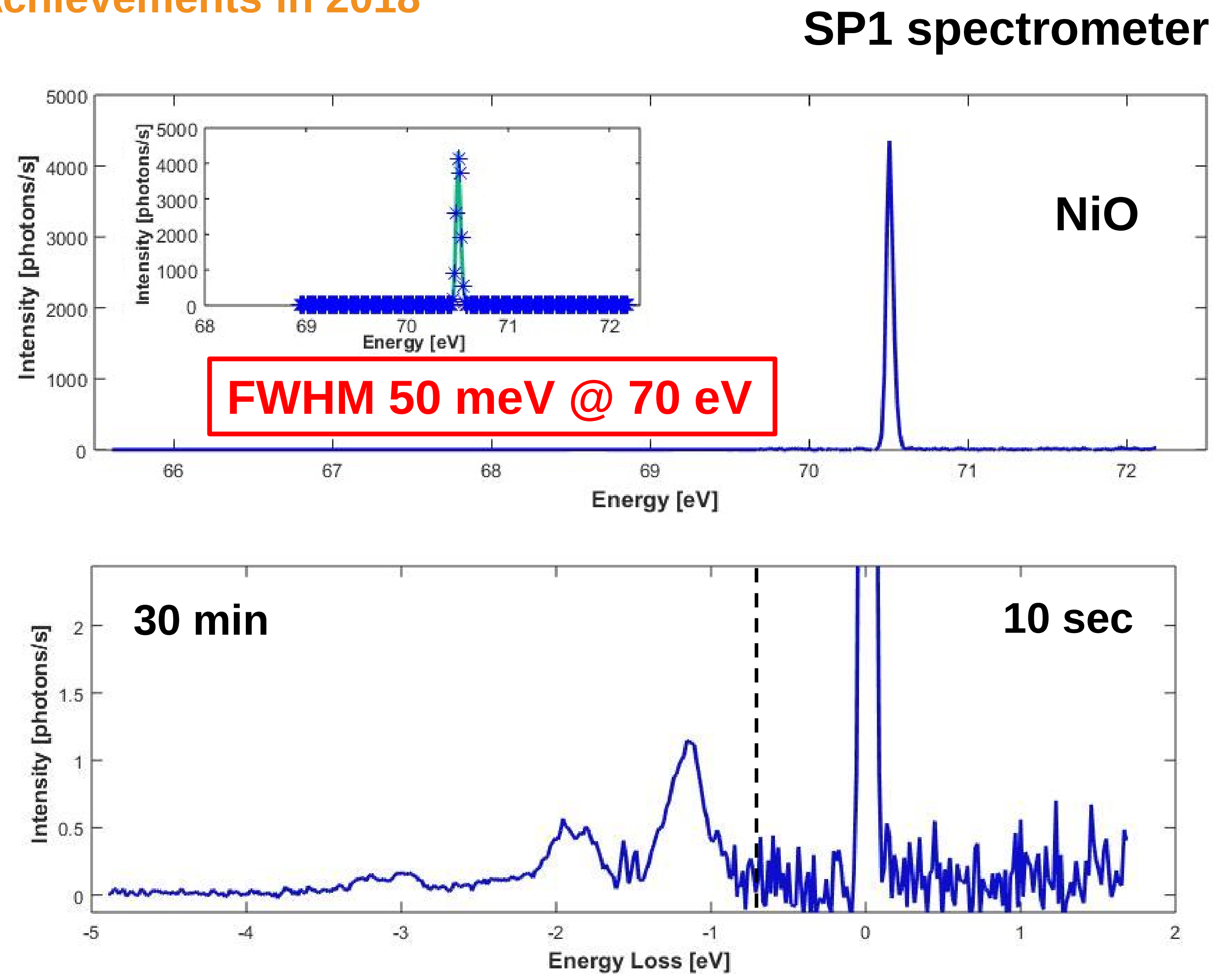


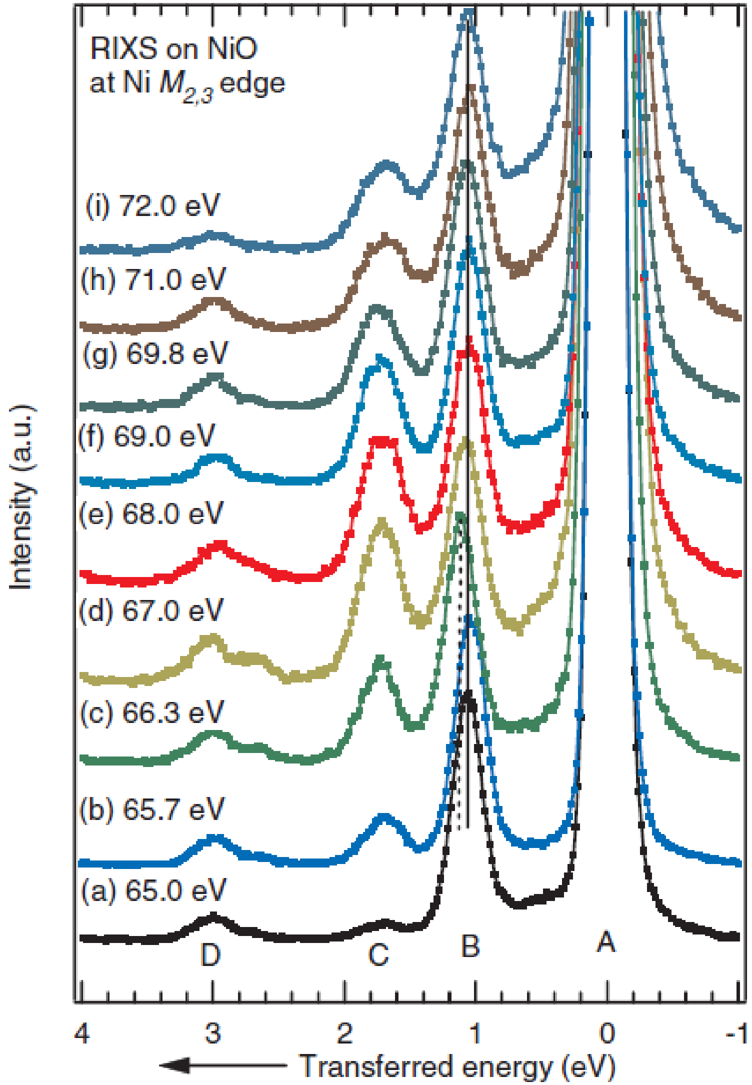
- Double monochromator
- Energy range: 20 – 200 eV
- **Elastic line / stray light suppression**
- **E/ΔE:~ 35000 @ E < 70 eV**
  and ~13000 @ E < 200 eV
- Ang. acceptance V x H = 37x80 mrad
- **Short pulses**

Rusydi et al. Phys. Rev. Lett. 113, 067001 (2014)
Dziarzhytski et al. J. Synchr. Rad. 25, 138-144 (2018)

PG1 XUV double stage Raman spectrometer

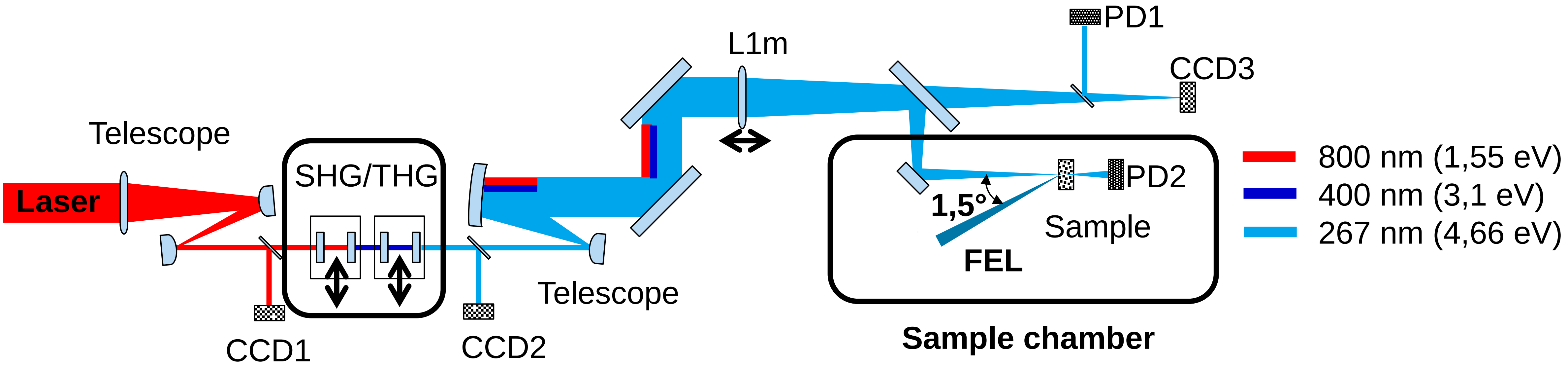
Achievements in 2018

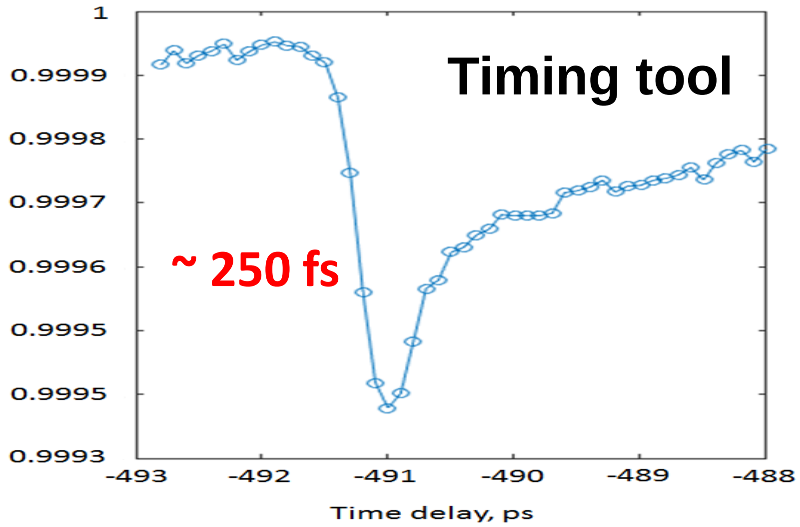




S. Chiuzbaian et al. PRL 95 (2005)

Approaching fs time resolution RIXS at FLASH





Transient optical reflectivity change of Si_3N_4

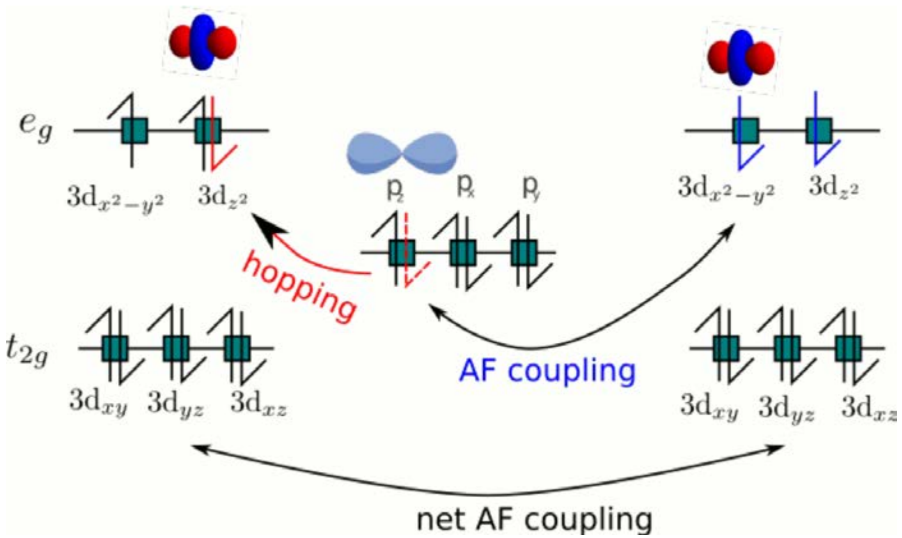
Resolving power ~ 1400 (SP1 only)

Time resolution ~ 250 fs

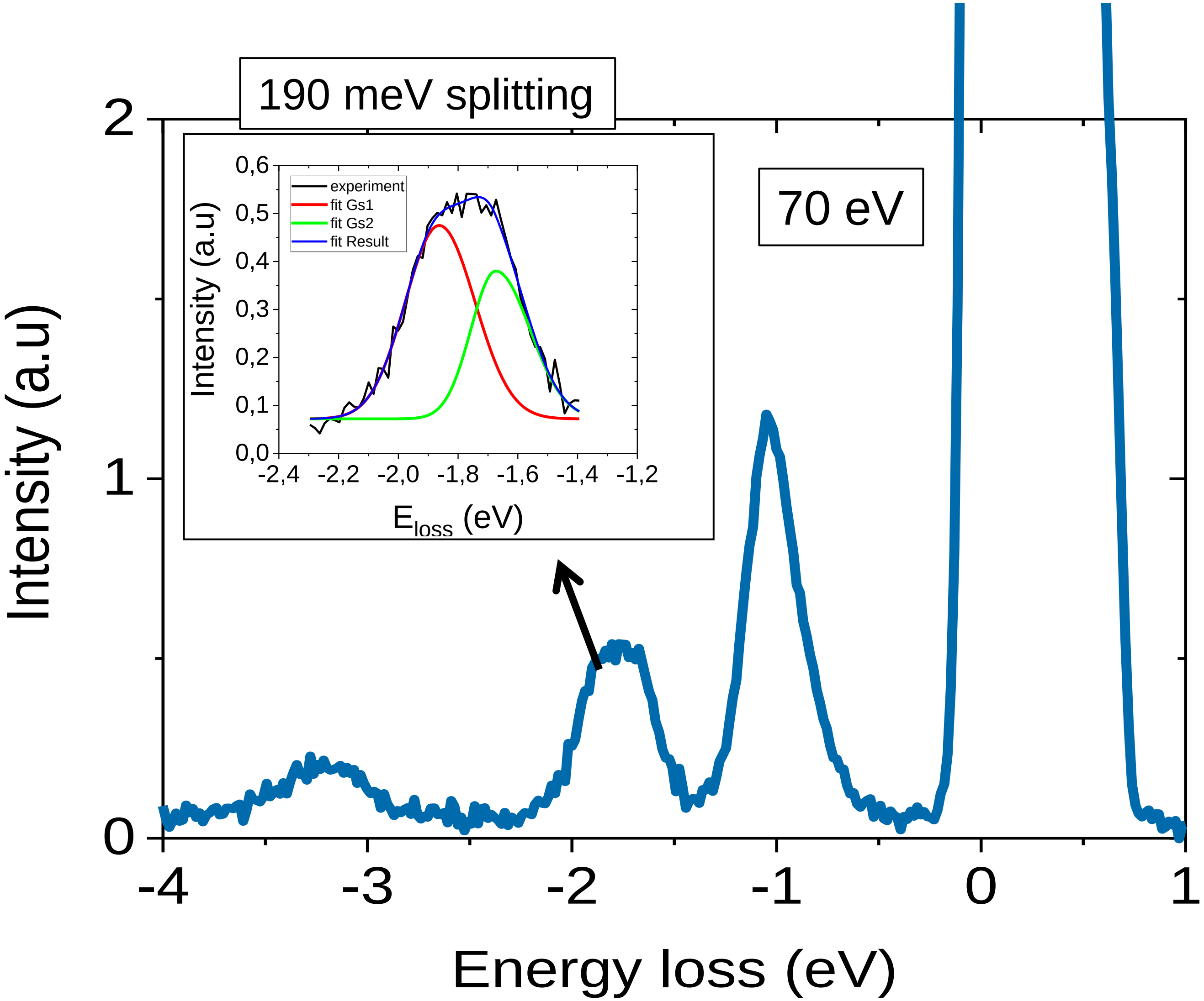
High resolution time resolved RIXS of NiO

First user experiment

NiO at Ni $M_{2,3}$ edges



- **65 meV FWHM** @70eV
- Time resolution ~**250 fs**
- 0.2 eV splitting observed
- Pump-Probe data under analysis



High resolution time resolved RIXS @ FLASH1

Future perspectives

Beamtime in May 2019: P. Miedema

Excited states and decay routes of Cobalt water splitting catalysts followed with XUV-RIXS

Applied for a beamtime in 2nd half 2019: In-house

The speed limit in switching spintronic europium oxide

- **Increase resolution**
- **Broaden spectral range**
- **Variable sample environment**

Increase resolution → **Beating of 20 meV resolution**
Approaching Fourier limit

Broaden spectral range, Variable sample environment → K-edges, L-edges → Life science, Condensed matter

Thanks to

G. Brenner, H. Weigelt, H. Redlin
M. Beye, P. Miedema

AG W. Wurth
AG M. Rübhausen, M. Biednov

A. Schulte (Summer student 2018)

The whole FS-FL FLASH Team and FS-LA

FLASH experts and operators

MEA2 M. Schloesser and colleagues
MEA3 K. Witt and colleagues

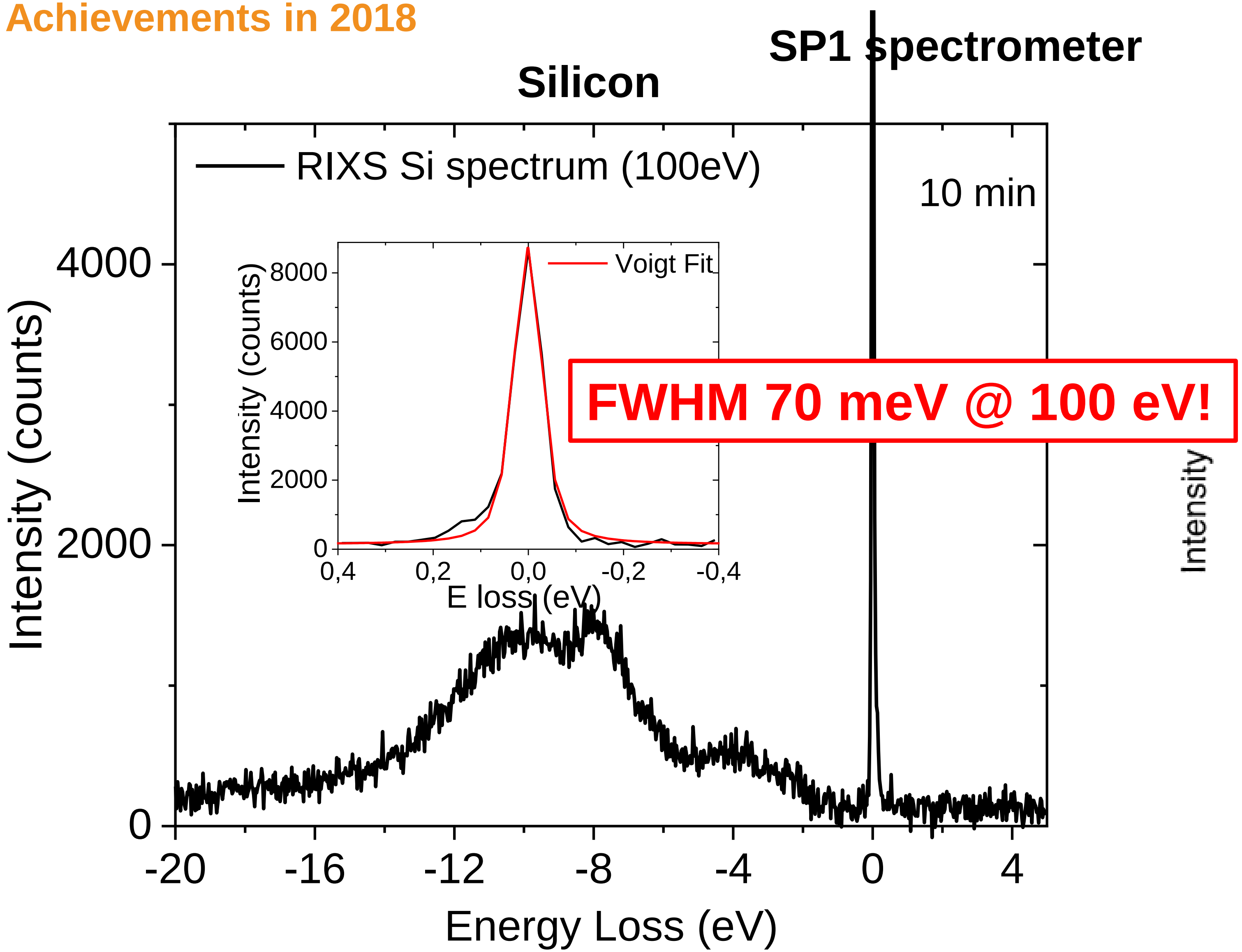
ZM and all workshops…

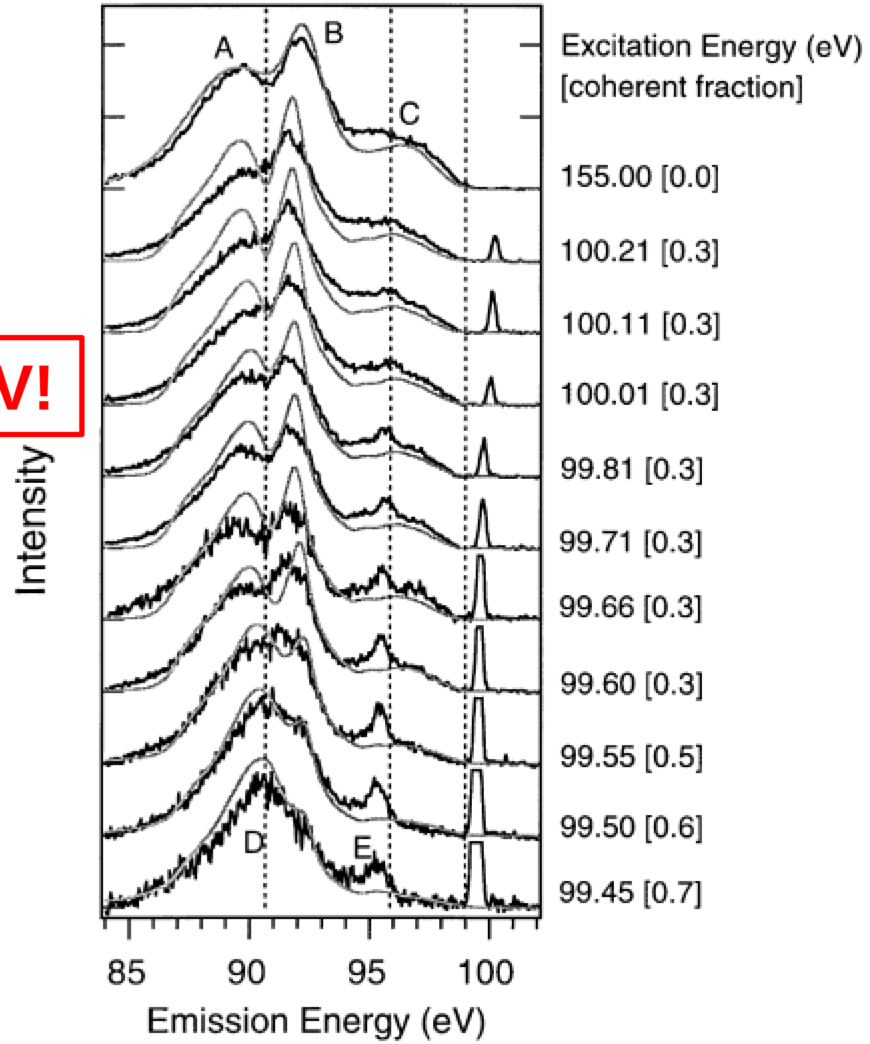
F. Siewert
A. Sokolov

L. Poletto
F. Frassetto

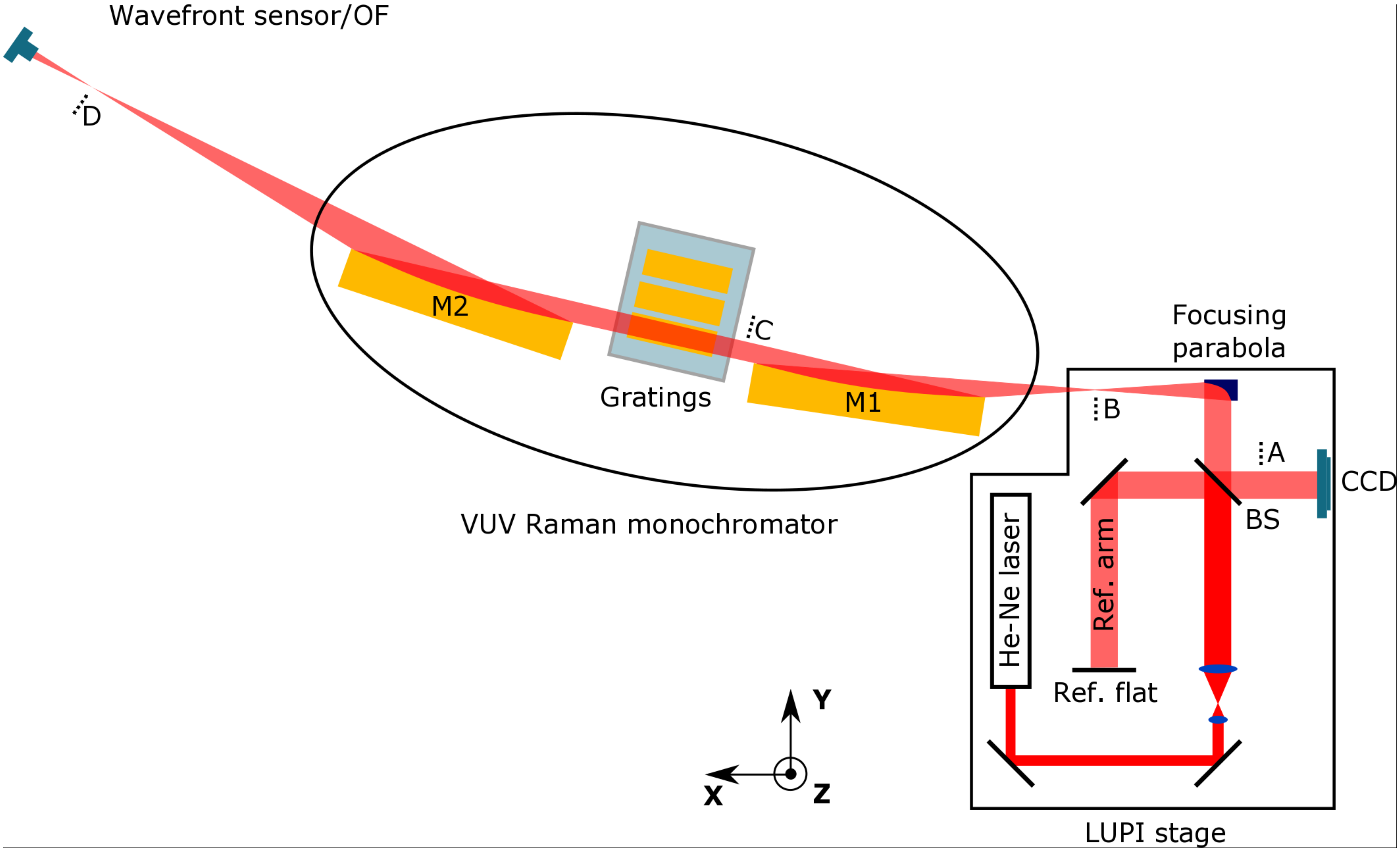
PG1 XUV double stage Raman spectrometer

Achievements in 2018





S. Eisebitt et al. JESRP 93 (1998)


Wavefront sensor/OF
D
M2
Gratings
C
M1
Focusing
parabola
B
A
CCD
BS
VUV Raman monochromator
He-Ne laser
Ref. arm
Ref. flat
Y
X
Z
LUPI stage