

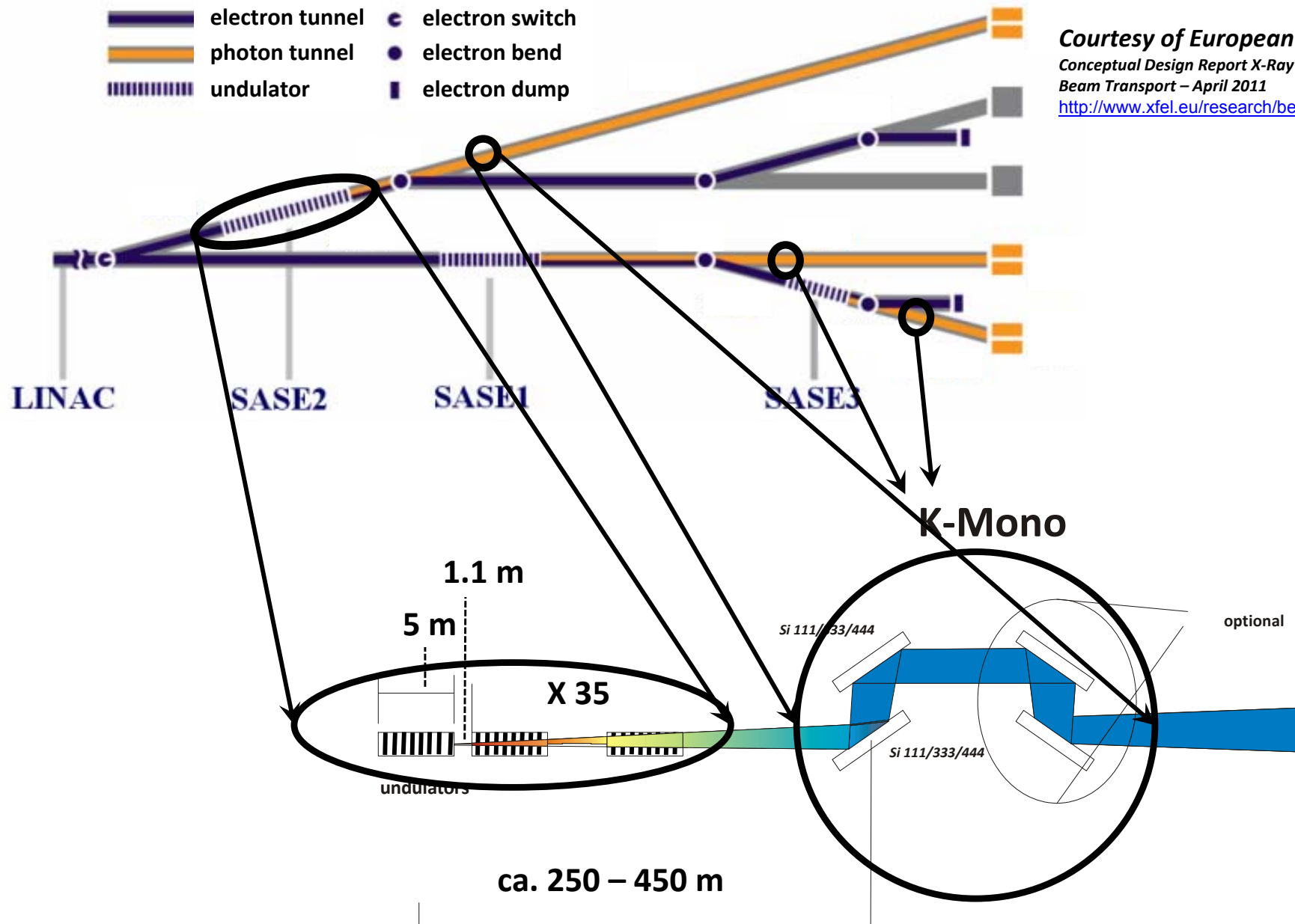


Conceptual raytracing for the X-FEL diagnostic monochromators-spectrometers

J. Rehanek, F. Schäfers, A. Erko

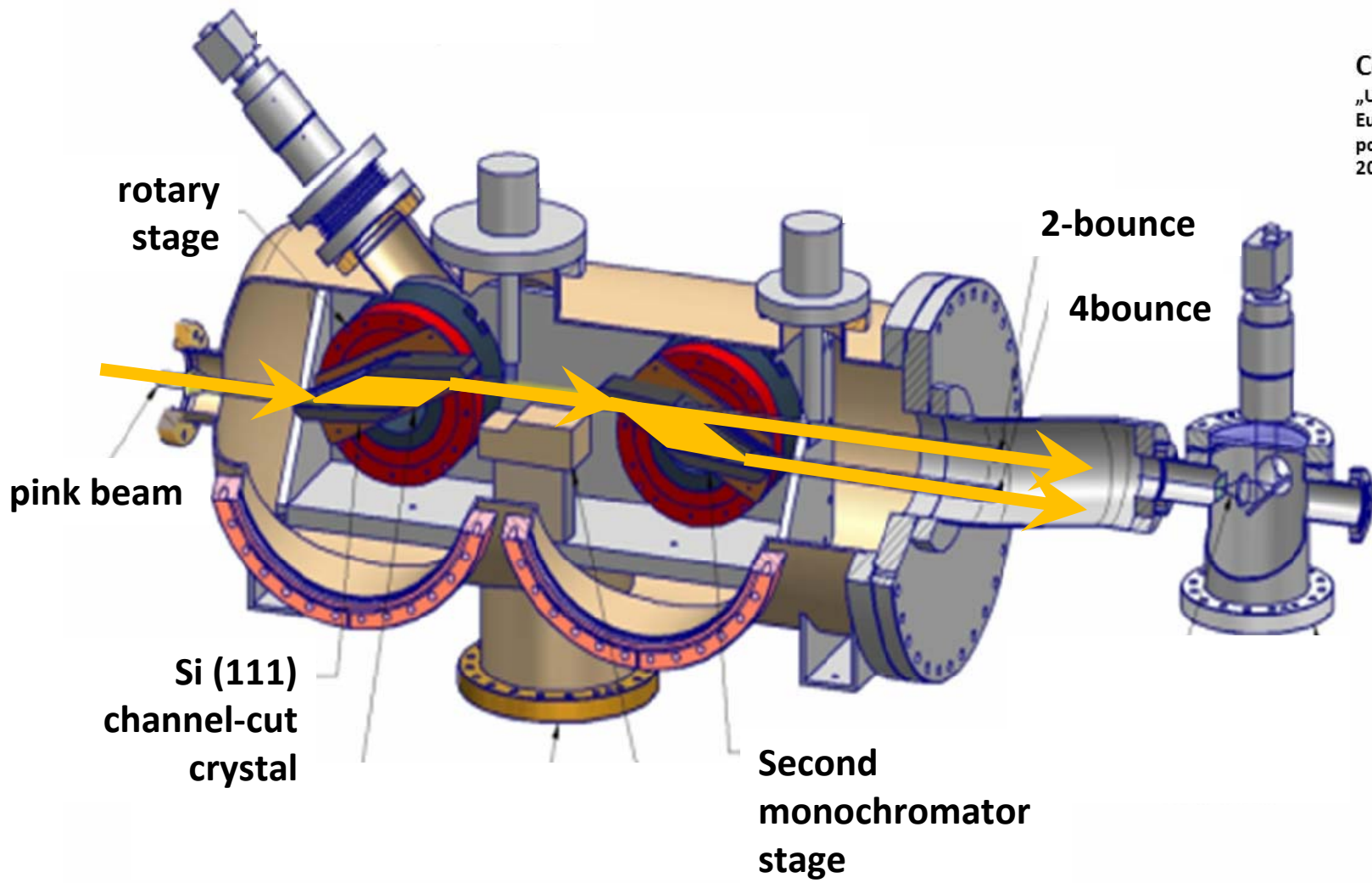
- **Undulator commissioning**
 - **K-Monochromator (Jens Rehanek)**
- **Single-shot spectrometer (Alexei Erko)**
 - **dispersive crystal design**
 - **reflection zone plate (RZP) design**

European XFEL – K-Monochromator



Courtesy of European XFEL
 Conceptual Design Report X-Ray Optics and
 Beam Transport – April 2011
<http://www.xfel.eu/research/beamlines/>

K-Monochromator design concept



Courtesy of European XFEL
„Undulator comissioning spectrometer for the European XFEL“,
poster W. Freund at XFEL-User’s meeting January 2011

Simulate Optical systems up to 10 elements (F. Schäfers)

Beamline design tool

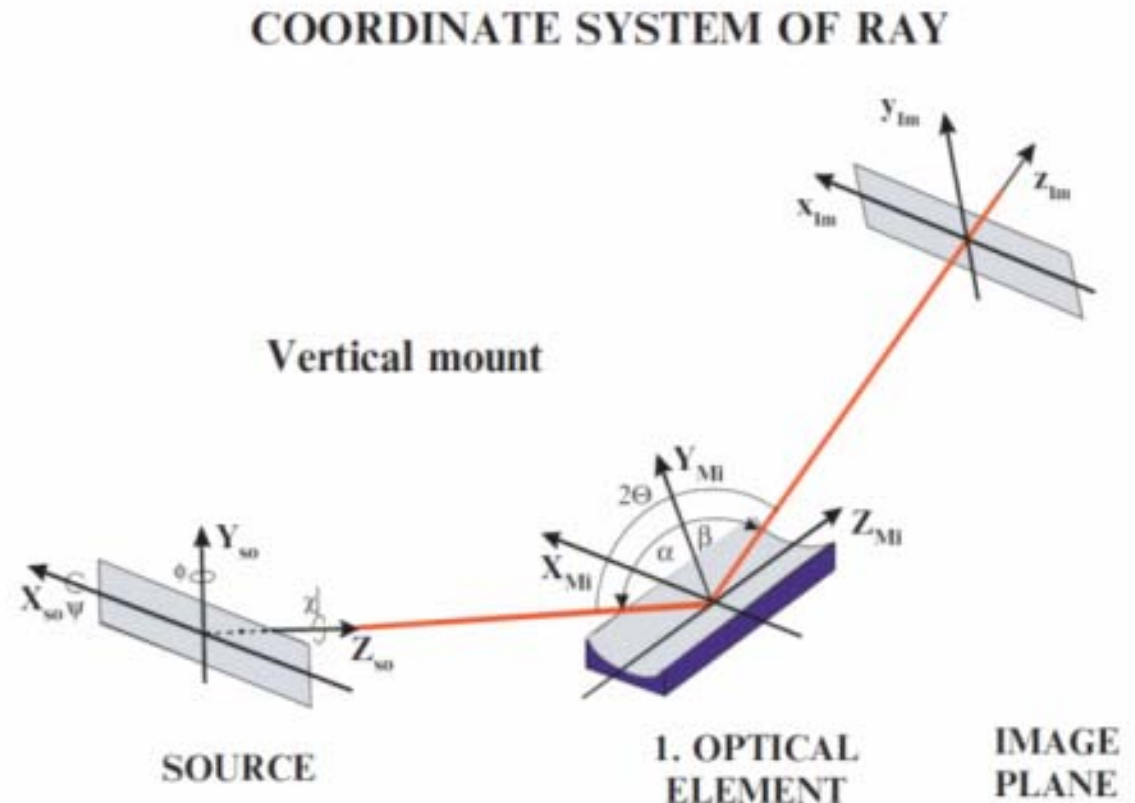
Geometric Optics

Sources

- Point
- Dipole
- Undulator
- External source file

Optical elements

- Reflection Mirrors
- Crystals (graded)
- Gratings (VLS)
- Transmission zone plates
- Reflection zone plates



Electron source parameters

$$\sigma_x = \sigma_z = 34 \mu\text{m}$$

$$\sigma'_x = \sigma'_z = 1 \mu\text{rad}$$

$$\text{Photon Source Size} = \sqrt{\sigma_{x,z}^2 + \sigma_U^2}$$

$$\text{Source divergence} = \sqrt{\sigma_{x,z}'^2 + \sigma_U'^2}$$

Undulator radiation*

$$\sigma_U = \frac{\sqrt{2\lambda L}}{2\pi}, \sigma_U' = \sqrt{\frac{\lambda}{2L}}$$

1 undulator segment L= 5 m

Electron beam parameters:

Electron energy: 14 GeV

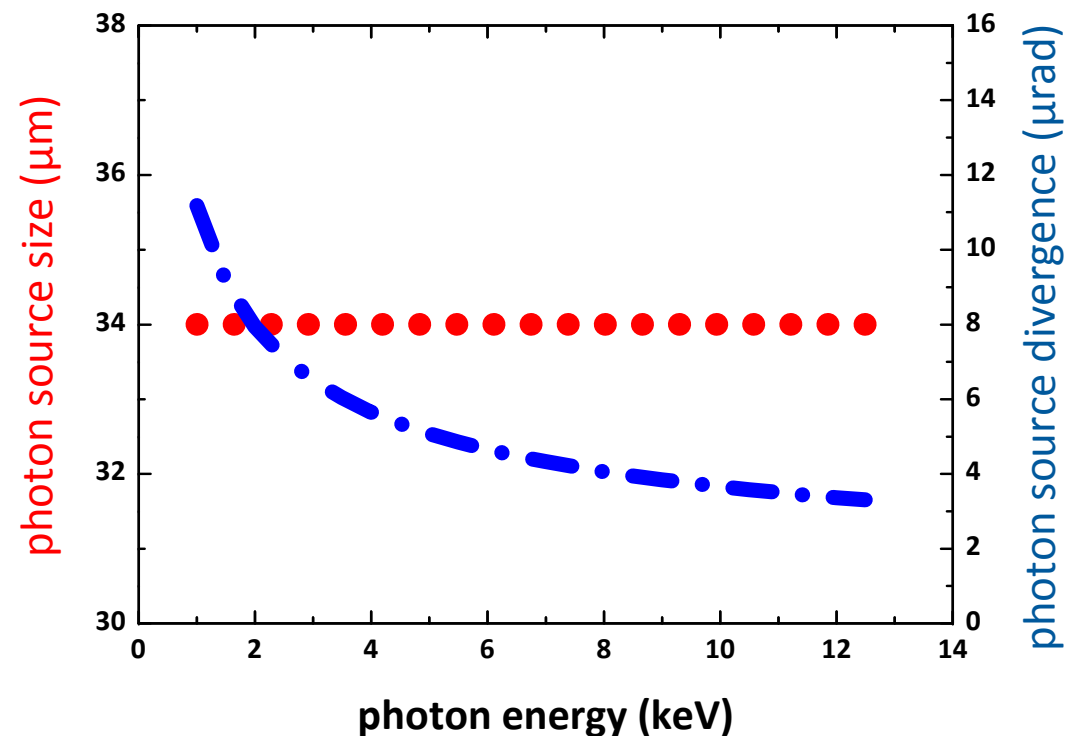
Emittance: 0.97 mm mrad

Beta function: 32 m

Period length: 40 mm

No. periods: 125

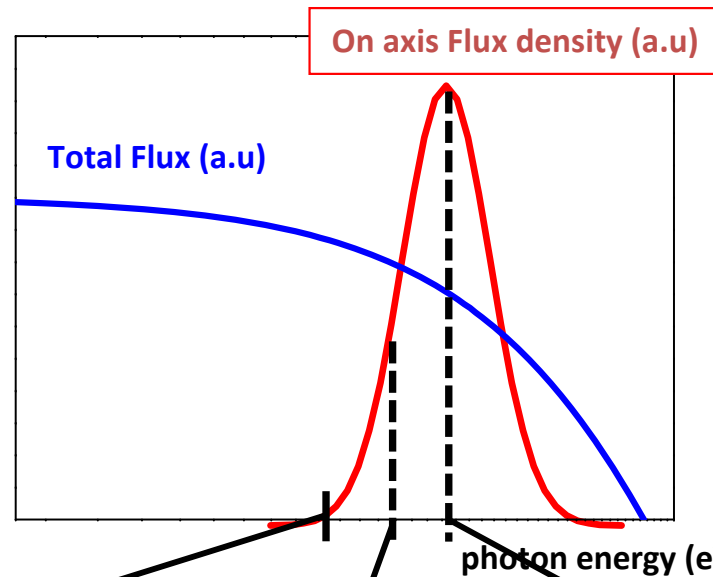
Gap-range: 10-28 mm



* Onuki, Elleaume:Wigglers Undulators and their application, Tylor and Francis 2003, page 79

Radiation field (450 m after source point)

WAVE simulation
as input to RAY



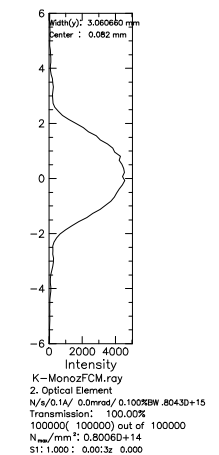
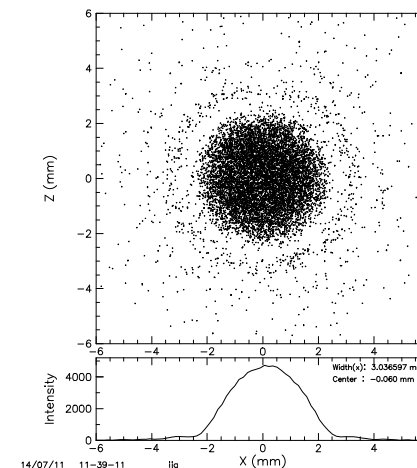
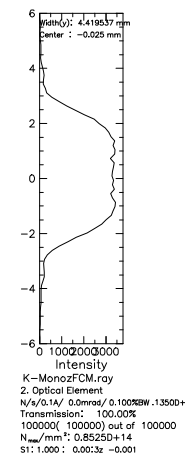
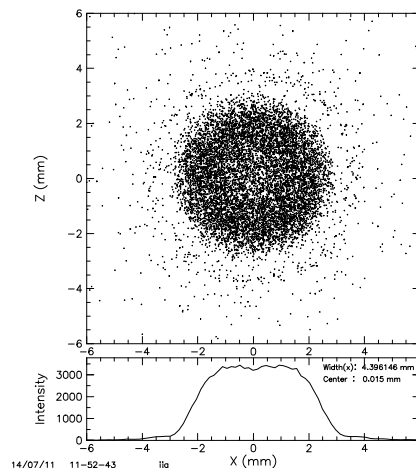
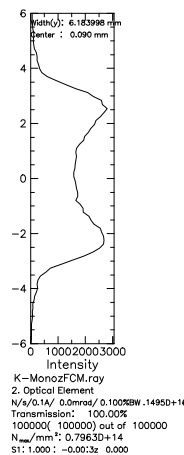
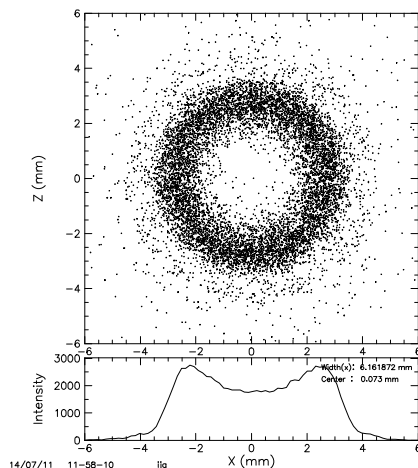
➤ spontaneous radiation

➤ at $K = 2.3$

@12300eV

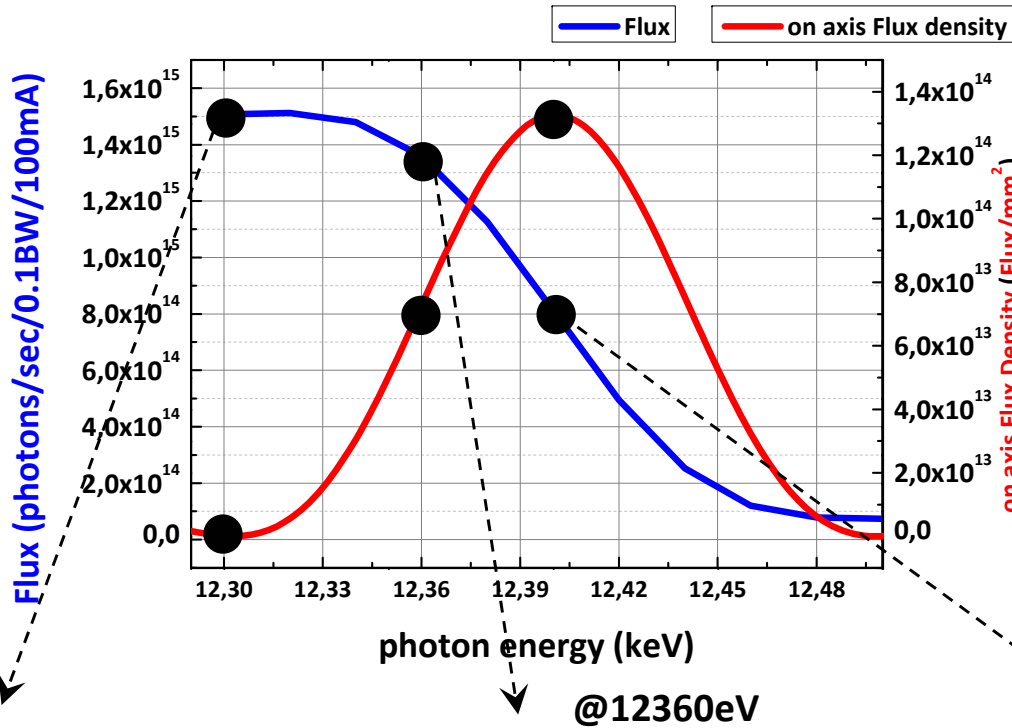
@12360eV

@12400eV

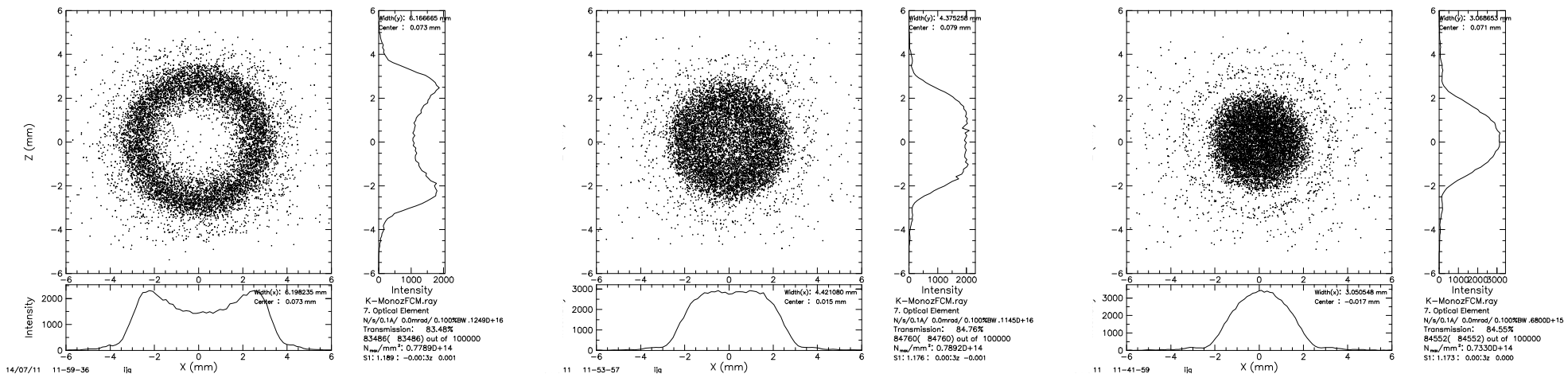


0.5 m after K-Mono

$$\Delta E / E (\text{K-Mono})_{12.4\text{keV}} \approx 1.2 \times 10^{-4}$$



- spontaneous radiation of one undulator segment
- at K = 2.3
- change observation energy

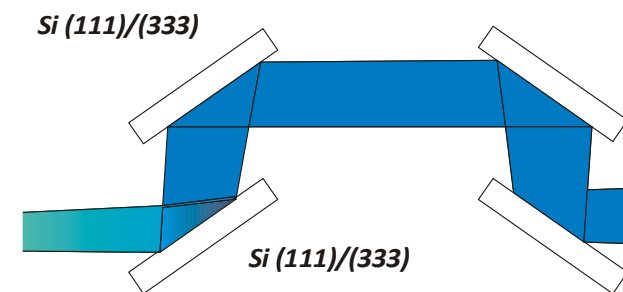


Crystals: 2 x Si 111 (**333**) channel-cut monochromators

Energy range: 2 – 20 keV

Energy resolution:

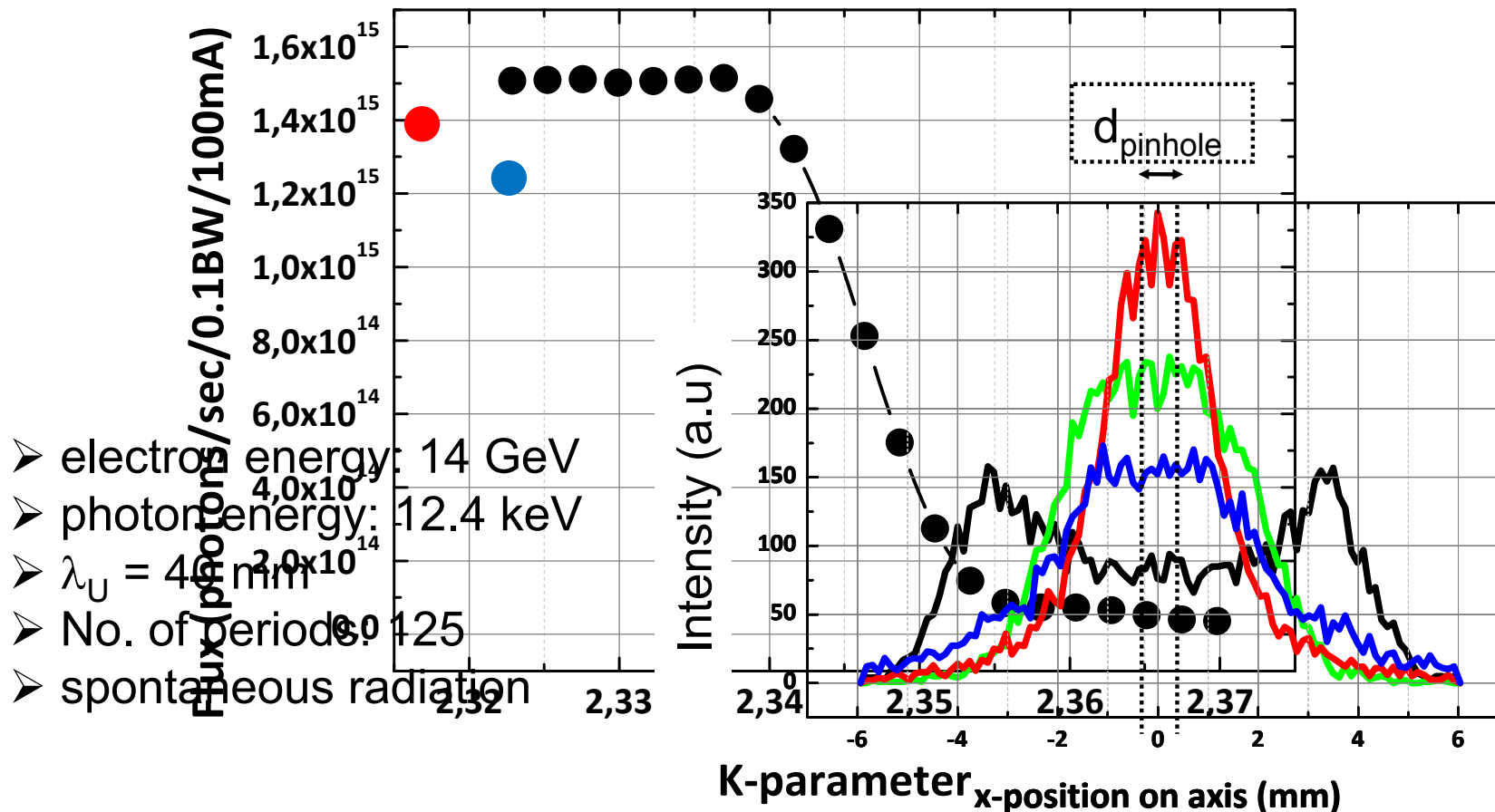
| photon energy (keV) | ΔE (eV) | $\Delta E / E$ |
|---------------------|-----------------|--|
| 5 | 0.49 | 1×10^{-4} |
| 10 | 1.2 | 1×10^{-4} |
| | 0.065 | 6.5×10^{-6} |
| 20 | 2.3 | 1×10^{-4} |
| | 0.104 | 5×10^{-6} |

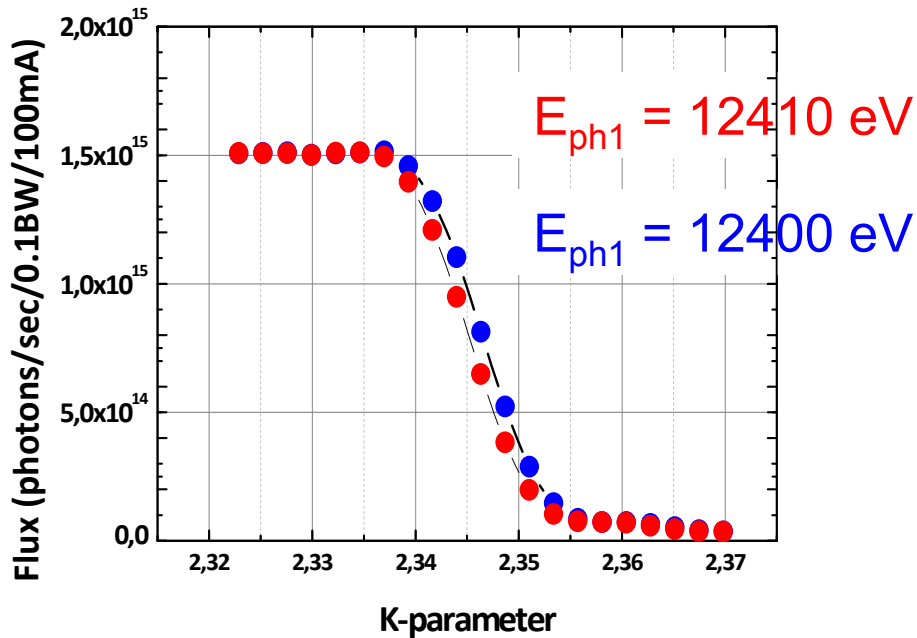


horizontal beam profile

➤ spontaneous
radiation

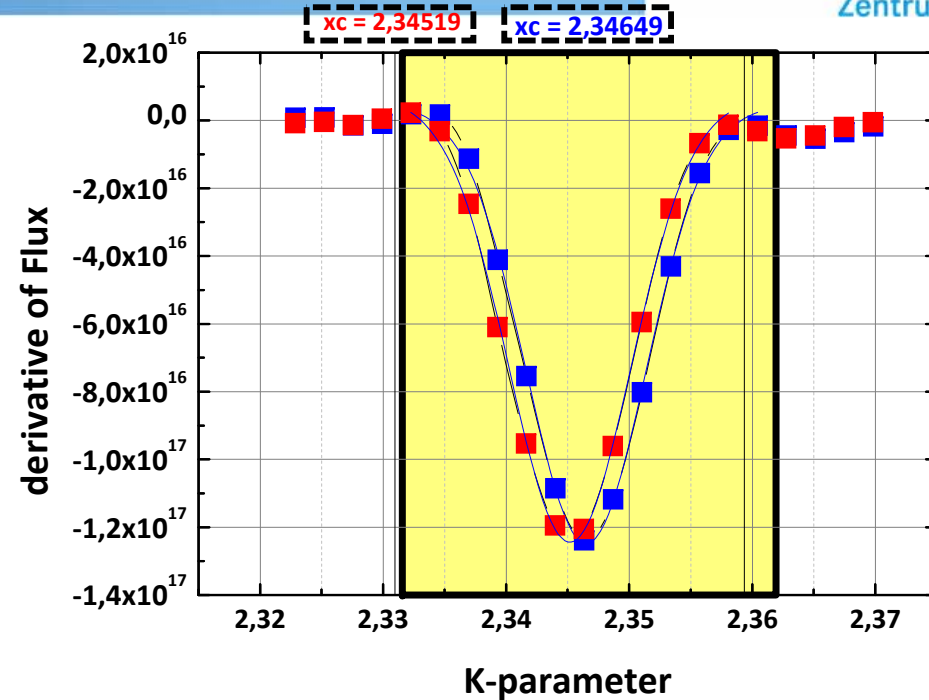
➤ at E = 12.4 keV





Flux at full beam aperture

$$E_{ph} [keV] = 0.950 \frac{E_e^2 [GeV]}{\left(1 + \frac{K^2}{2}\right) \lambda_U [cm]}$$



Flux differential

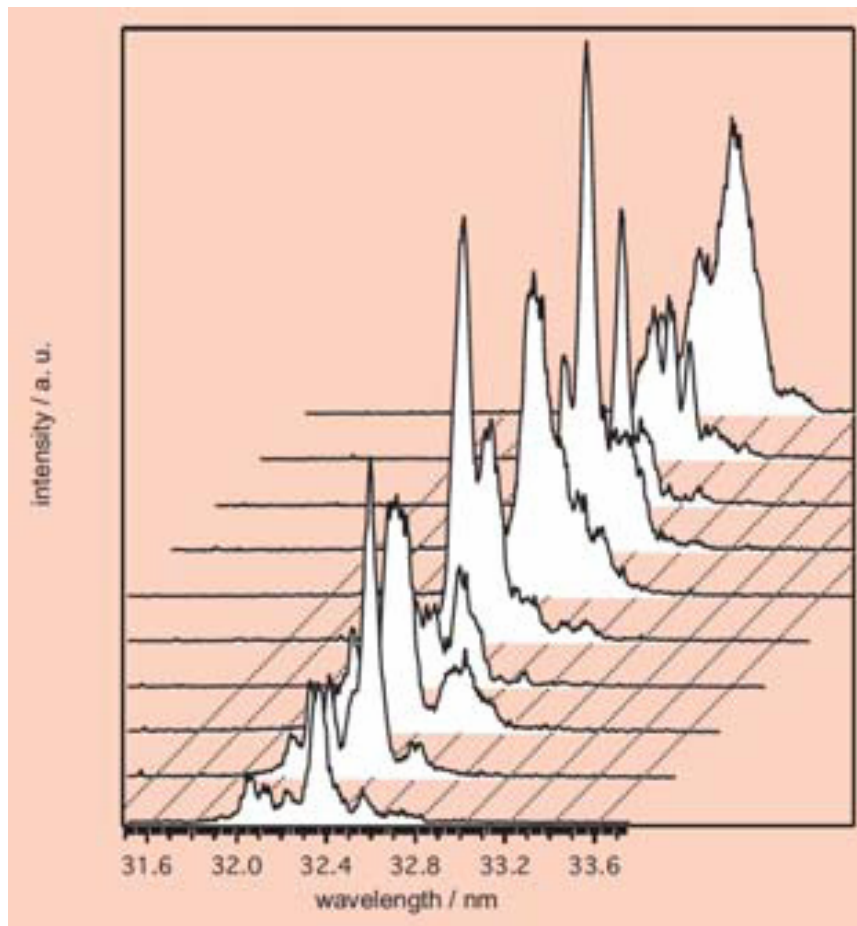
$$\frac{\Delta E}{E} = \frac{K^2}{\left(1 + \frac{K^2}{2}\right)} \frac{\Delta K}{K} \approx 1.46 \frac{\Delta K}{K} \quad / \quad K=2.35$$

„Gaussian fit method“

| | |
|---------------------------------|---------------------------------|
| $E_{ph1} = 12400 \text{ eV}$ | Center @ K = 2.34649 |
| $E_{ph2} = 12410 \text{ eV}$ | Center @ K = 2.34519 |
| $\Delta E/E = 8 \times 10^{-4}$ | $\Delta K/K = 5 \times 10^{-4}$ |

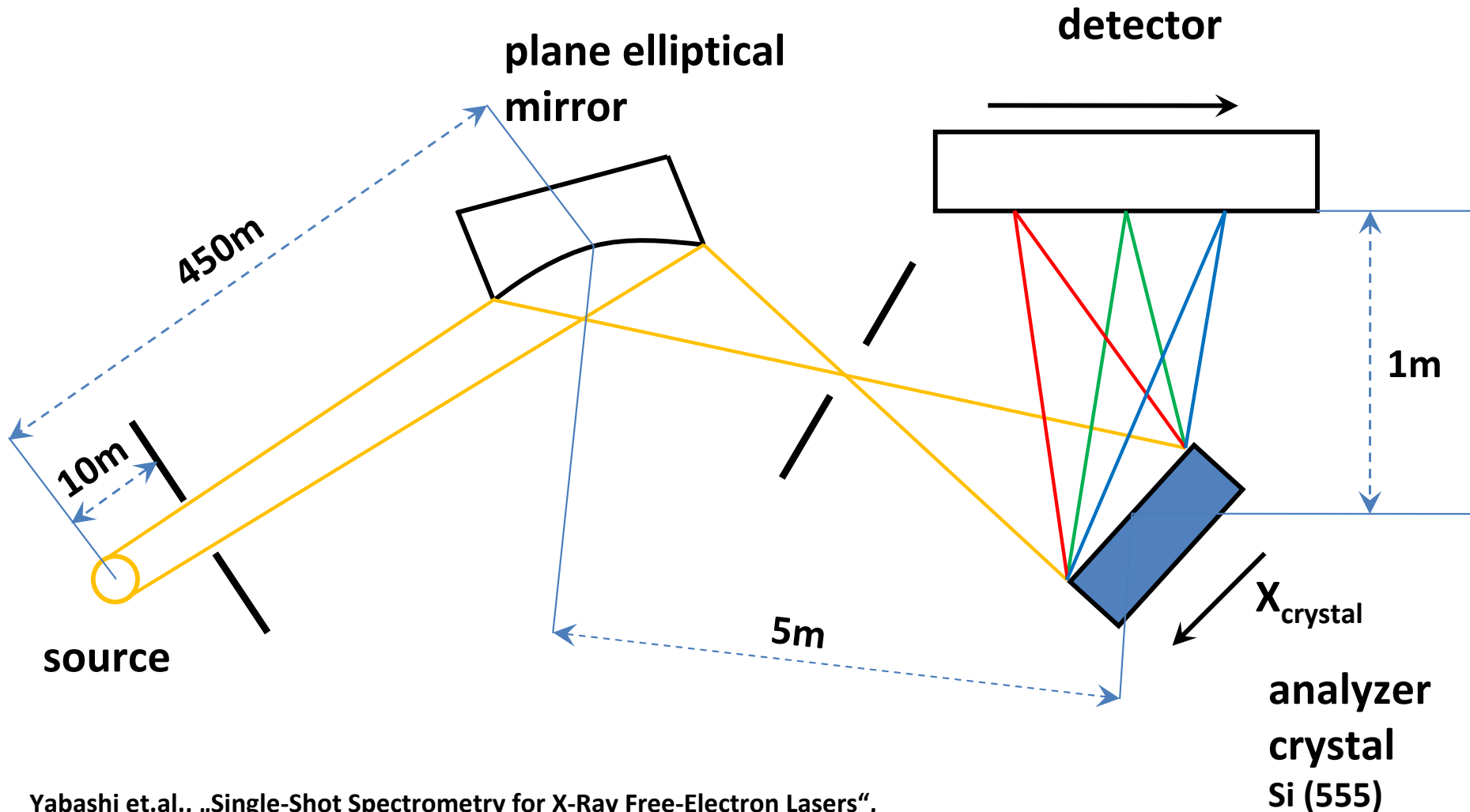
Motivation

- Typical SASE Single Shot Spectrum

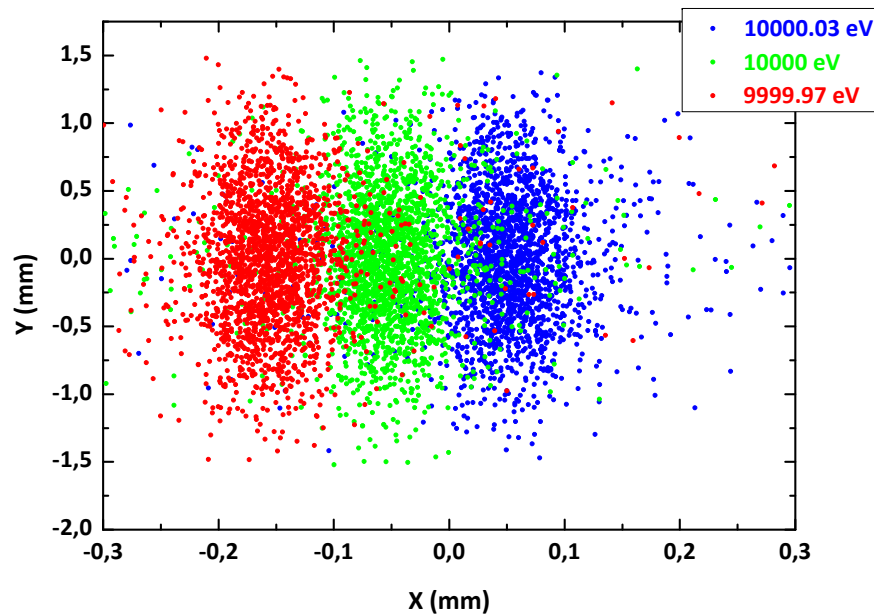


- intensity at one wavelength varies from pulse to pulse significantly
- wavelength spectrum varies considerably

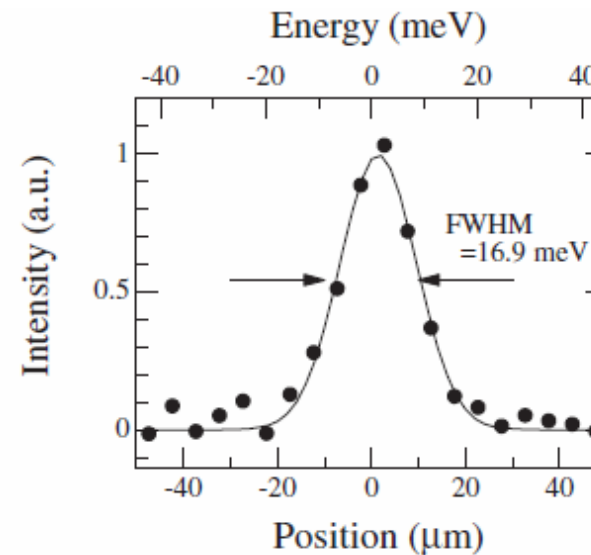
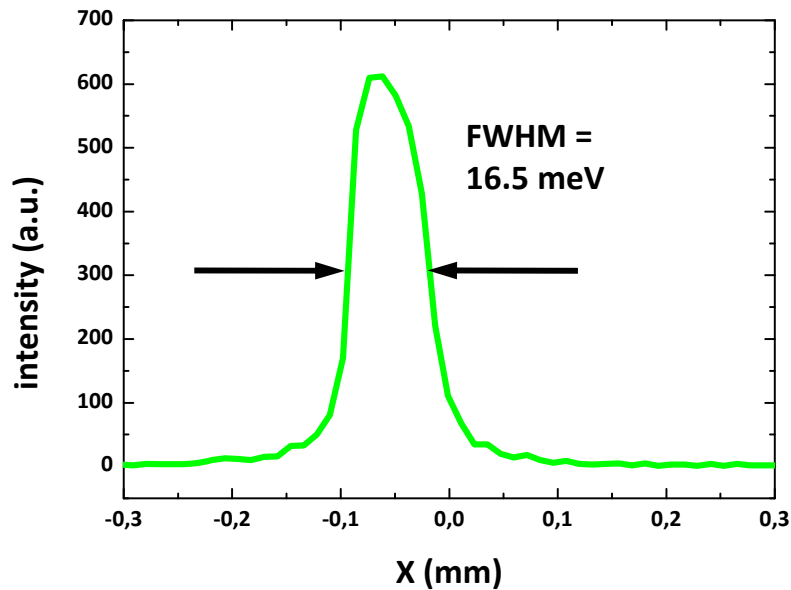
top view



Yabashi et.al., „Single-Shot Spectrometry for X-Ray Free-Electron Lasers“,
Phys.Rev.Lett. 97, 084802 (2006)



- resolution: $\Delta E = 30 \text{ meV} / 0.1 \text{ mm}$
- dispersion: $300 \text{ meV} / \text{mm}$ (0.5 eV/mrad)
- FWHM: 16.5 meV ($55\mu\text{m}$)
- slope errors: $< 1.0 \text{ arcsec}$
(state of the art: 0.3 arcsec)

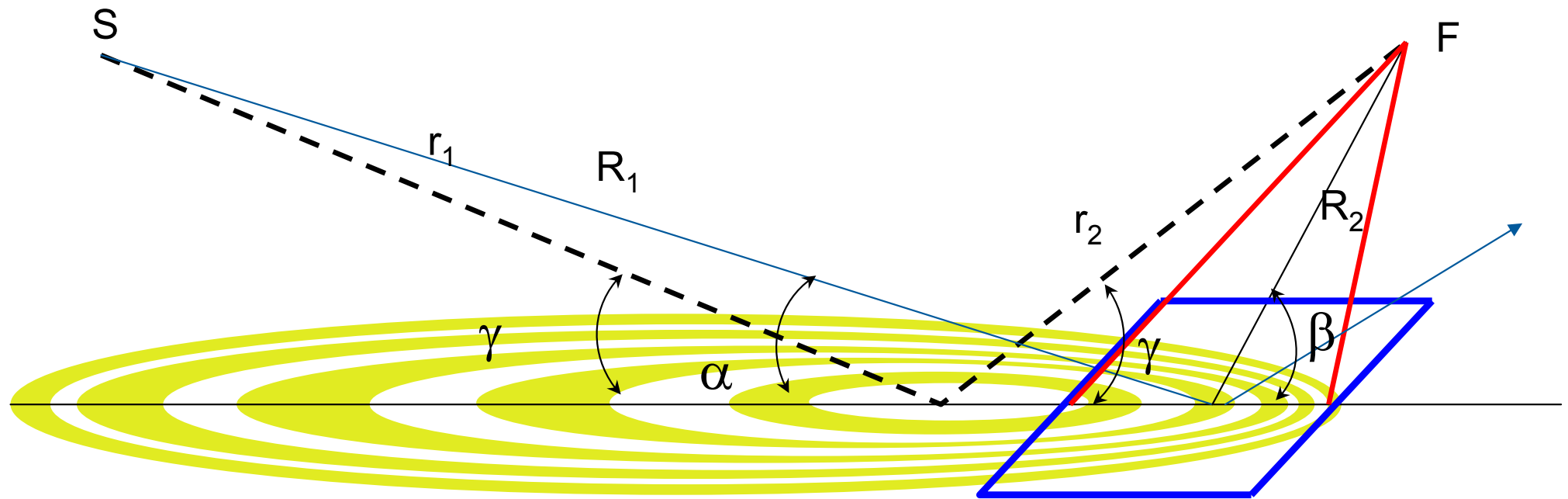


picture: Yabashi et.al.,
„Single-Shot
Spectrometry for X-Ray
Free-Electron Lasers“,
Phys.Rev.Lett. 97,
084802 (2006)

FIG. 3. Spatial profile of dispersed beam (lower axis). The corresponding energy scale is shown on the upper axis.

Reflection Zone Plate Single - Shot Monochromator

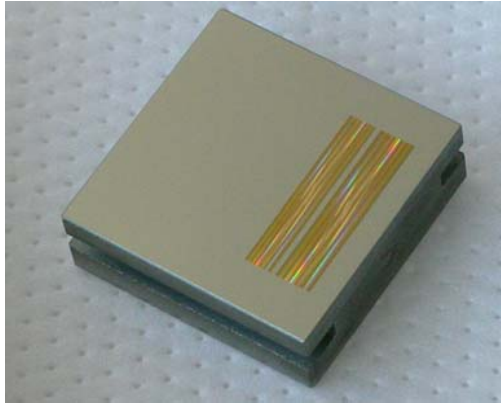
- **X-ray laser** is a source of coherent short-pulse radiation. Each optical element in the beam transport line will induce absorption, scattering, distortion etc. Normally, after interaction with 5 – 7 mirrors, the absorption reduces the flux by several orders of magnitude. Scattering and speckle formation processes will destroy all unique properties of the laser beam. Coherent experiments are very problematic.
- If a radiation of 1000 eV is reflected by 7 mirrors with Au coating, **only 1.7 %** of the radiation will go through the optics.
- **X-ray lasers** require new non-traditional solutions and non-conventional designs to ensure that their unique properties can be fully exploited.



Wavelength range: 0.025 nm (50 keV) – 200 μm (0.062 eV)

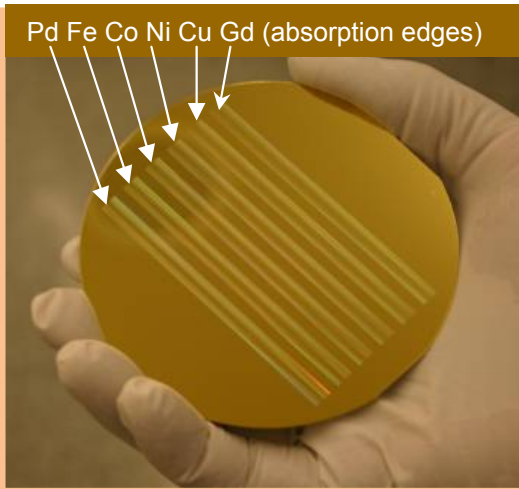
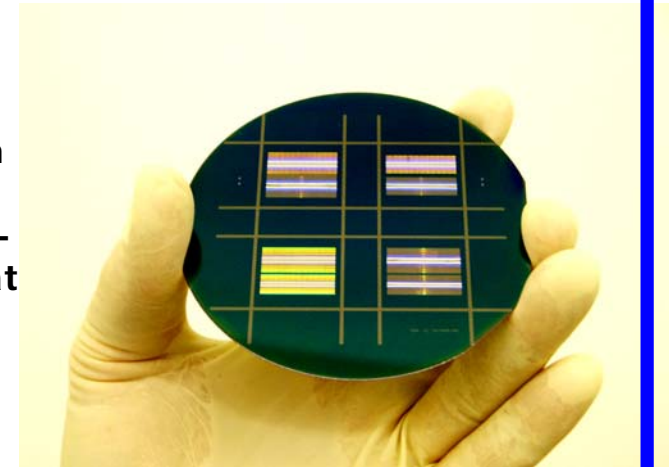
Efficiency: 5% - 30 %

Energy resolution $\lambda / \Delta\lambda$: 100 – 50 000



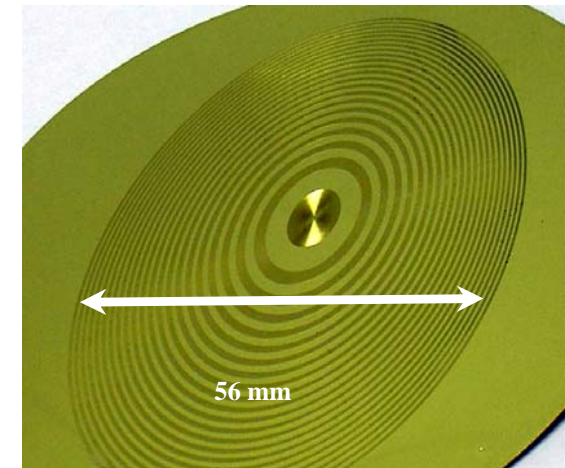
5 keV - 16 keV
Bragg-Fresnel Lens
on the second
monochromator
crystal at MySpot
beamline

10 eV – 60 eV
Total reflection
zone plate as
monocromator-
spectrometer at
HHG harmonic
selector



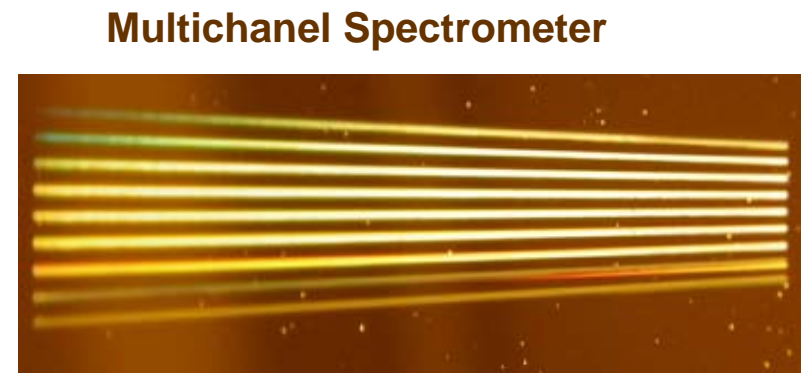
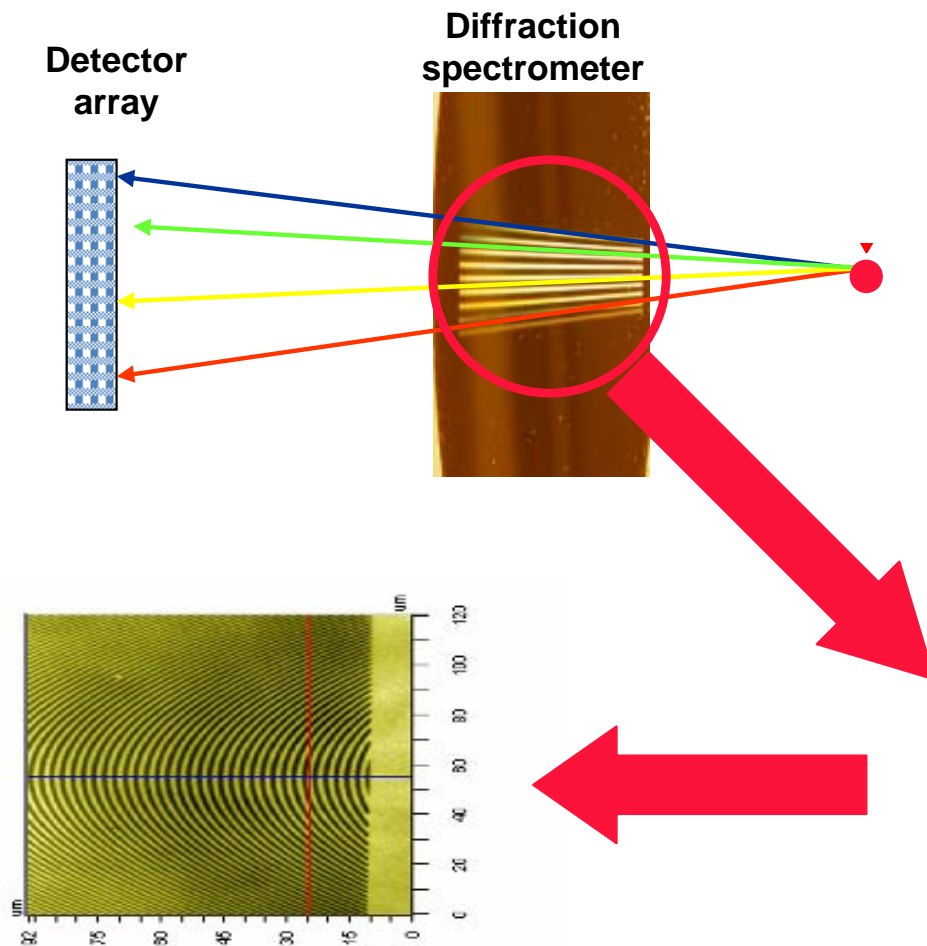
0.5 keV – 1.2 keV
Total reflection
zone plate as
monocromator-
spectrometer at
Slicing beamline

$6.2 \cdot 10^{-3}$ eV
Total reflection
zone plate as
monocromator-
spectrometer at
THz beamline

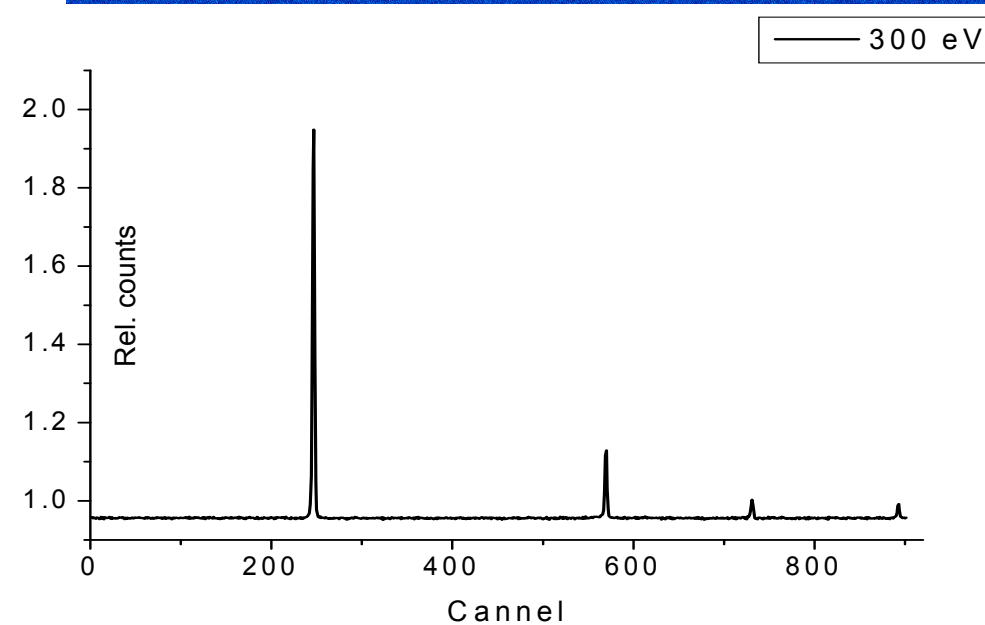
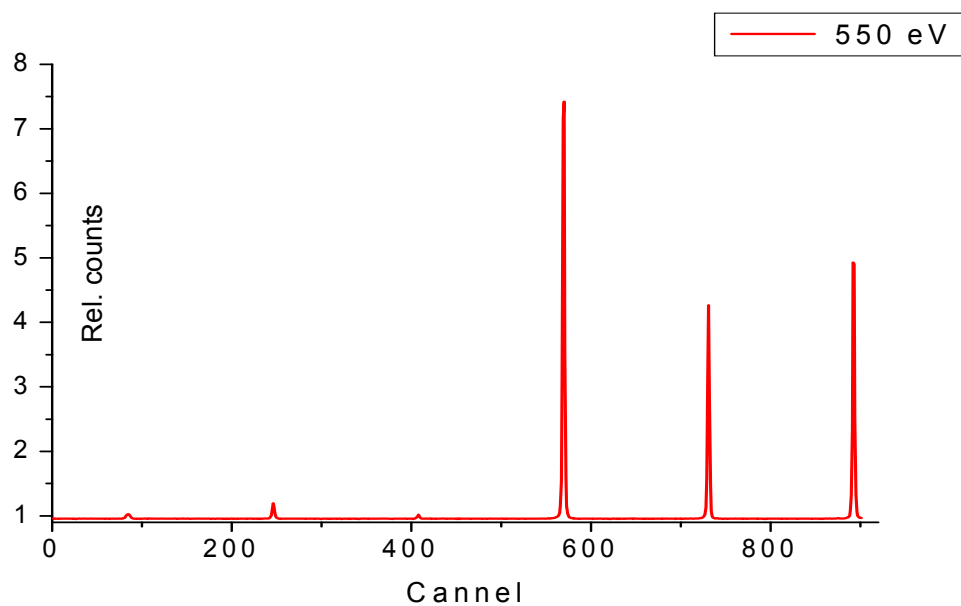
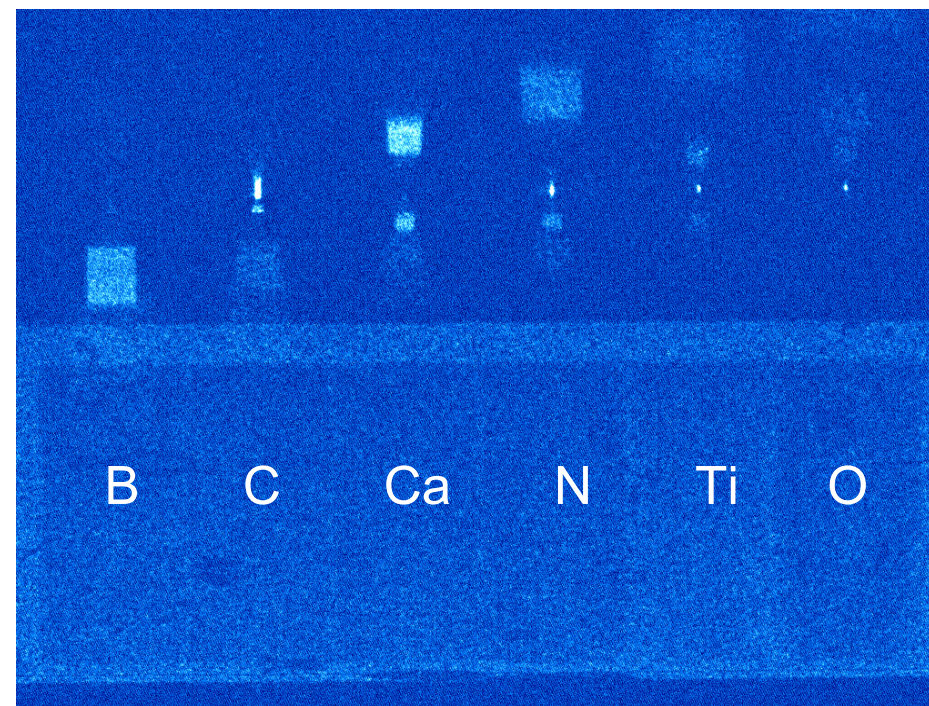
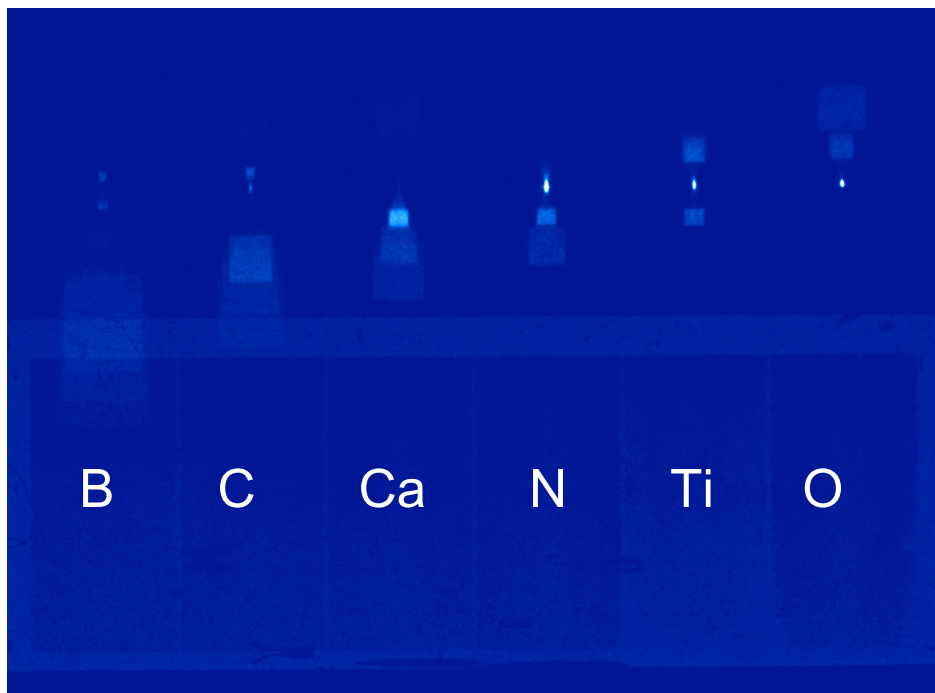


One pulse, one spectrum: Ultra-fast X-ray spectroscopy spectroscopy

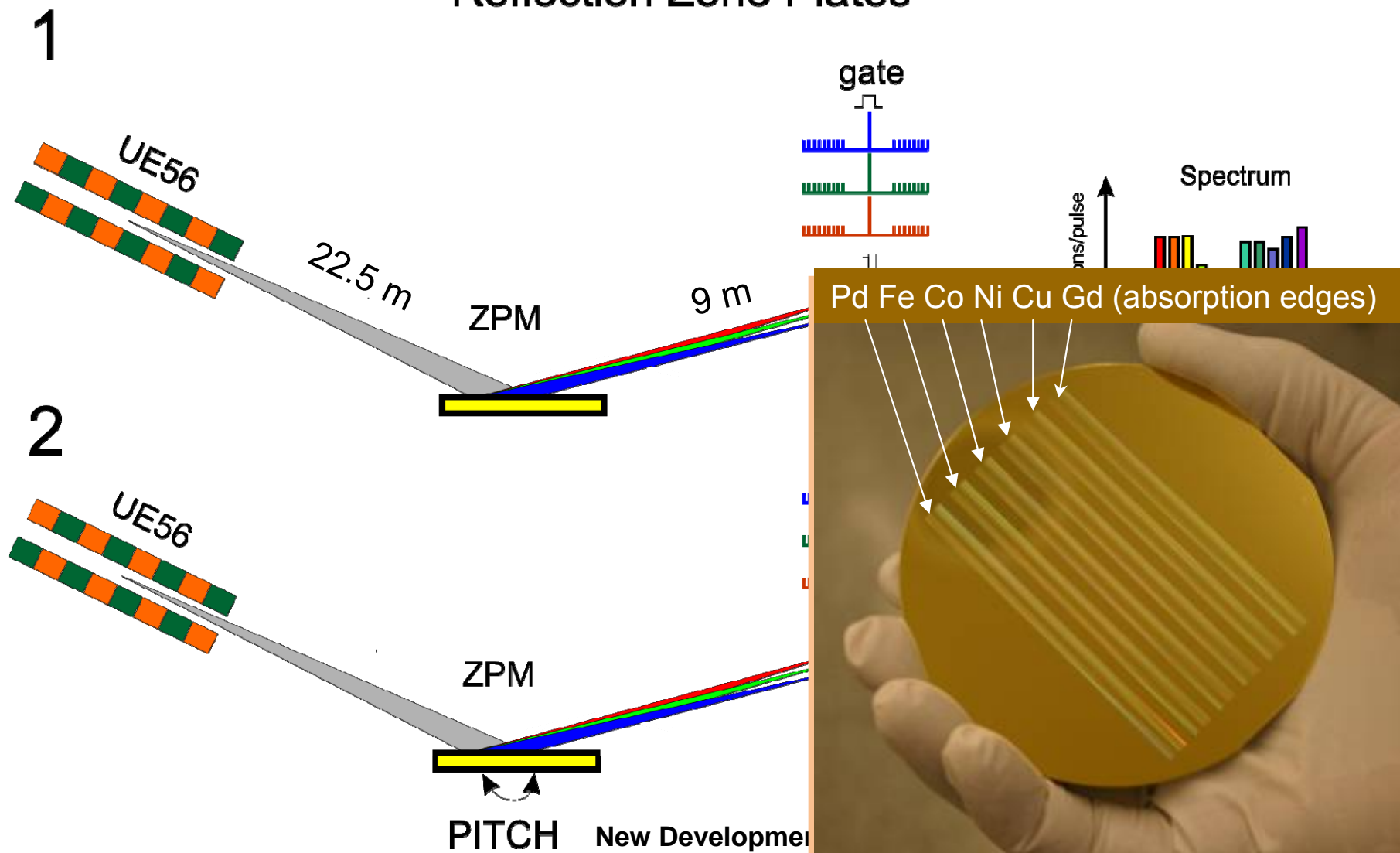
A. Erko, et al., Novel parallel vacuum ultra-violet/X-ray fluorescence spectrometer, Spectrochim. Acta Part B (2012), doi:10.1016/j.sab.2012.01.001



New generation: tests at RIXS beamline



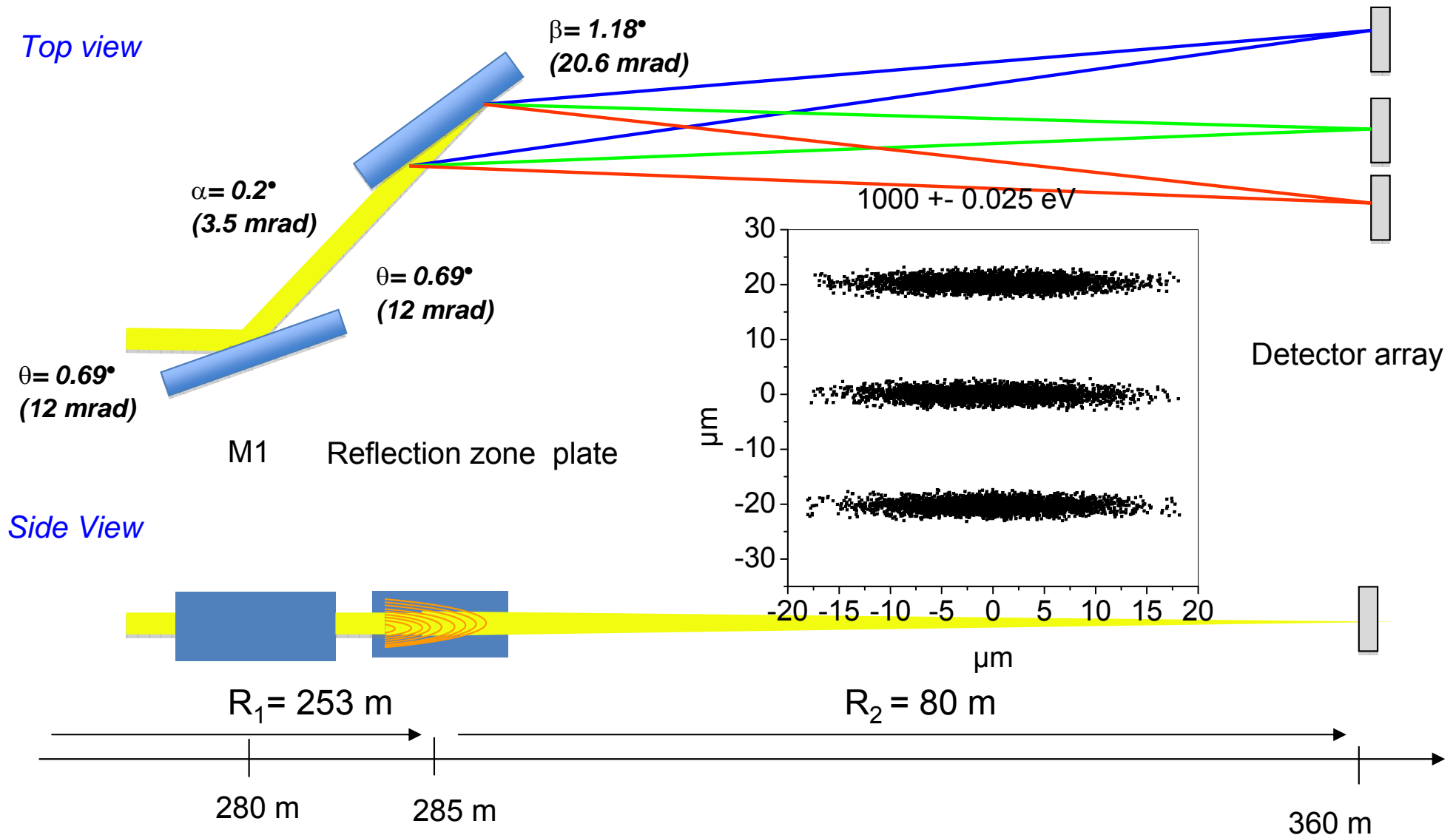
Time-Correlated Parallel detection with Reflection Zone Plates



A. Erko, A. Firsov, K. Hollack, AIP CONF. PROC. 2010 1234, 177-180)

Concept Single-Shot monochromator

$E = 1 \text{ keV}$, $E/\Delta E = 40\,000$ (25 meV at 1 keV), Detector pixel size = 20 μm



Beam parameters at 253 m

| λ/E | Beam size D | Δt |
|------------------|-------------|------------|
| 1.24nm (1keV) | ~7 mm | < 100 fs |

$$\Delta t = \frac{\lambda}{c} N$$

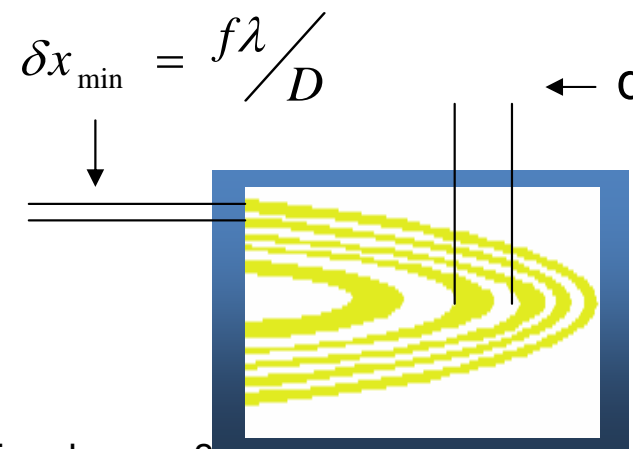
$$\Delta t \sim 4.1 \cdot 10^{-18} \text{ s}, N = 25000$$

Diffraction structure parameters

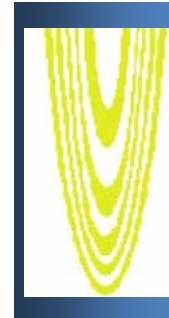
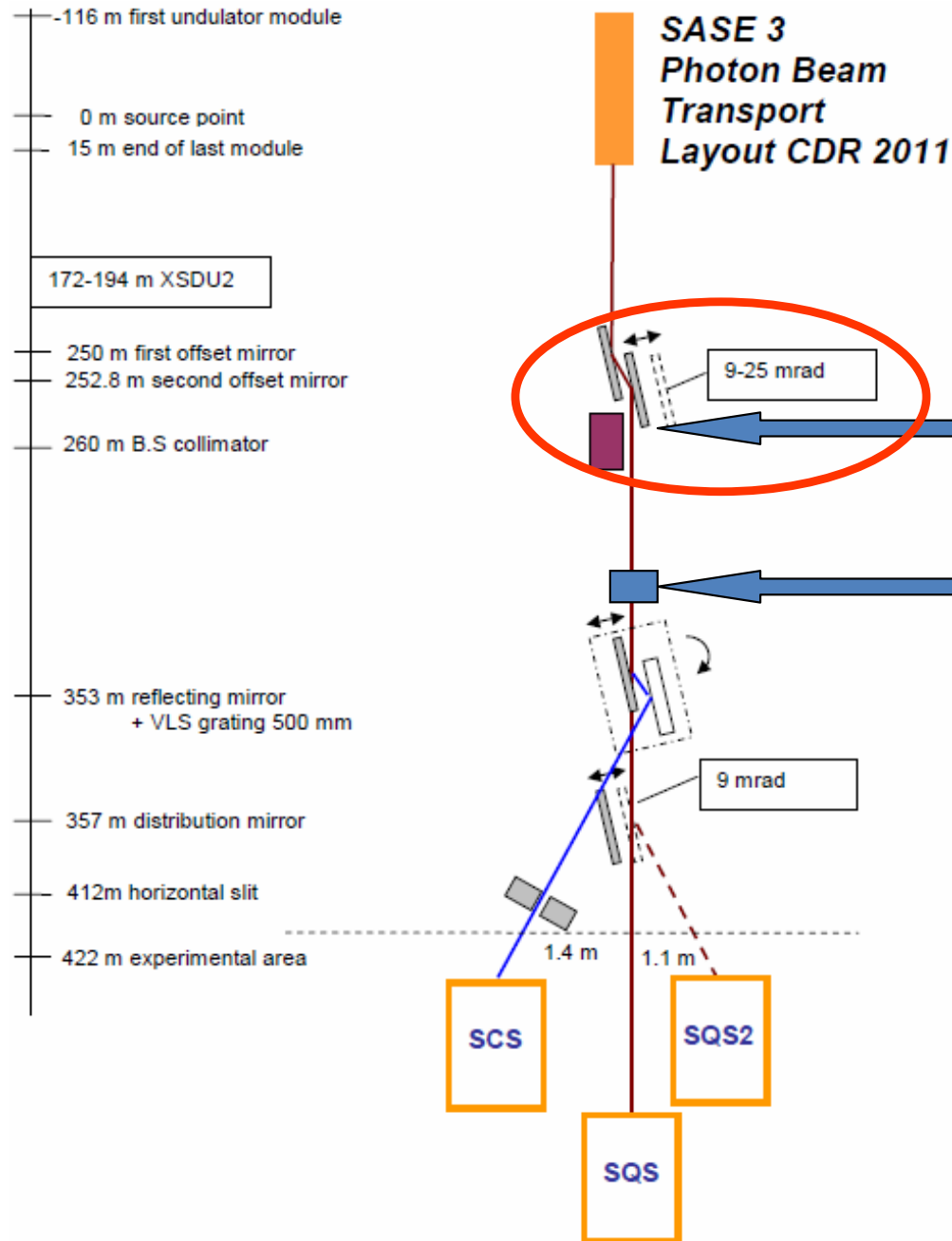
| L | α | β | d | Δx | $\lambda/\Delta\lambda$ | 2θ | R_1 | R_2 |
|-------|--------------------|---------|---------------------------------|------------------|-------------------------|-----------|-------|-------|
| 155mm | 0.2° (3.5 mrad) | 1.18° | 6.2 μm (160 l/mm) | 20 μm | 25000 | 1.38° | 253m | 80m |

Reflection zone plate parameters

| γ | r_1 | r_2 | δx_{\min} |
|----------|---------|---------|--------------------|
| 0.44° | 116.2 m | 216.8 m | 10.8 μm |



Single-Shot monochromator position SASE3



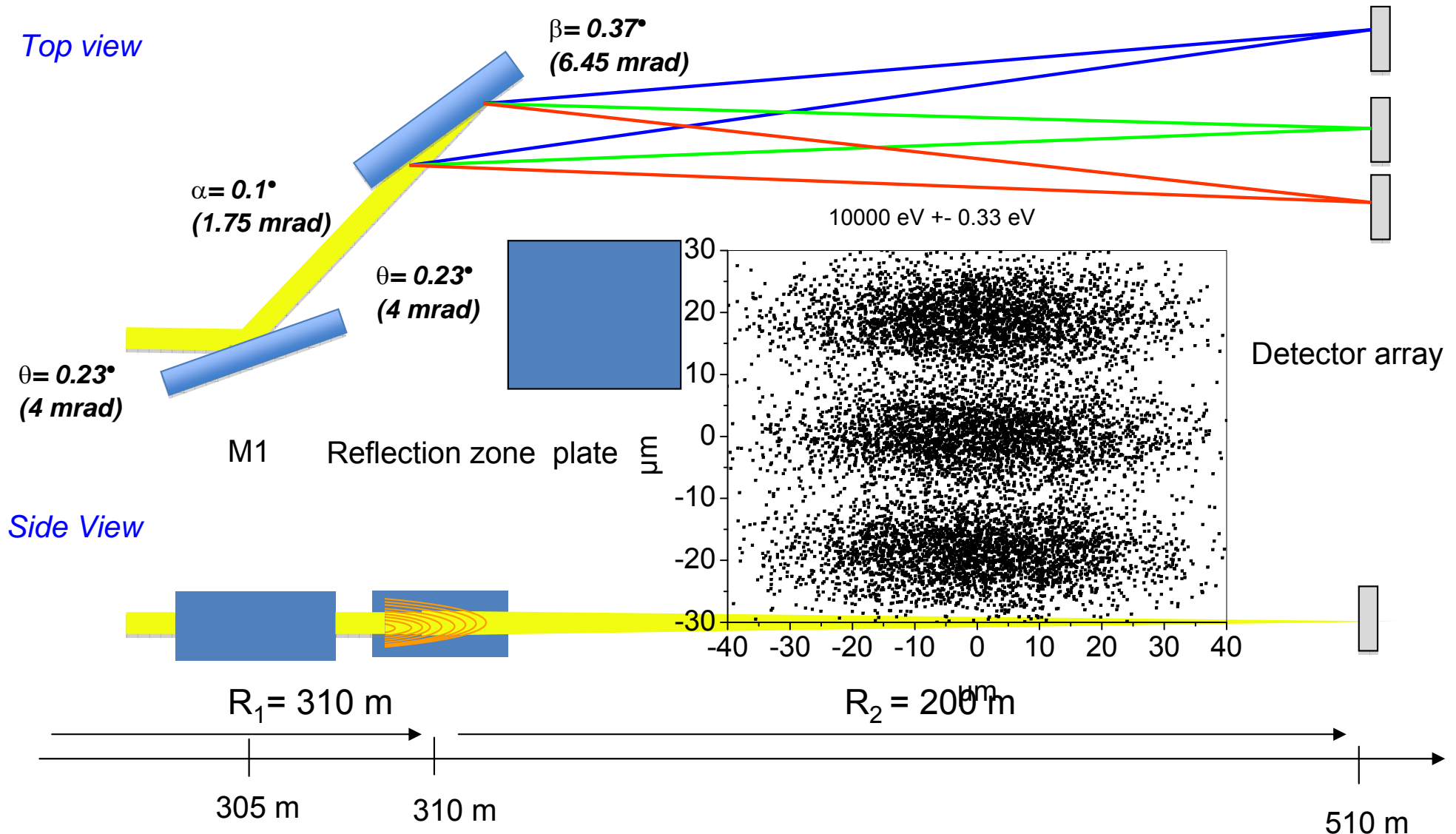
Reflection zone plate

Parallel detector array



Concept Single-Shot monochromator

$E = 10 \text{ keV}$, $E/\Delta E = 30\,000$ (0.33 eV at 10 keV), Detector pixel size = 20 μm



Beam parameters at 310 m

| λ/E | Beam size |
|---------------------|-----------|
| 0.124nm (10 keV) | ~ 1 mm |

$$\Delta t_N \sim 4.1 \cdot 10^{-19} \text{ s, at } 0.124 \text{ nm}$$

$$N \sim 30000$$

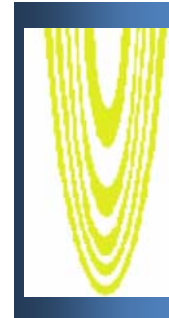
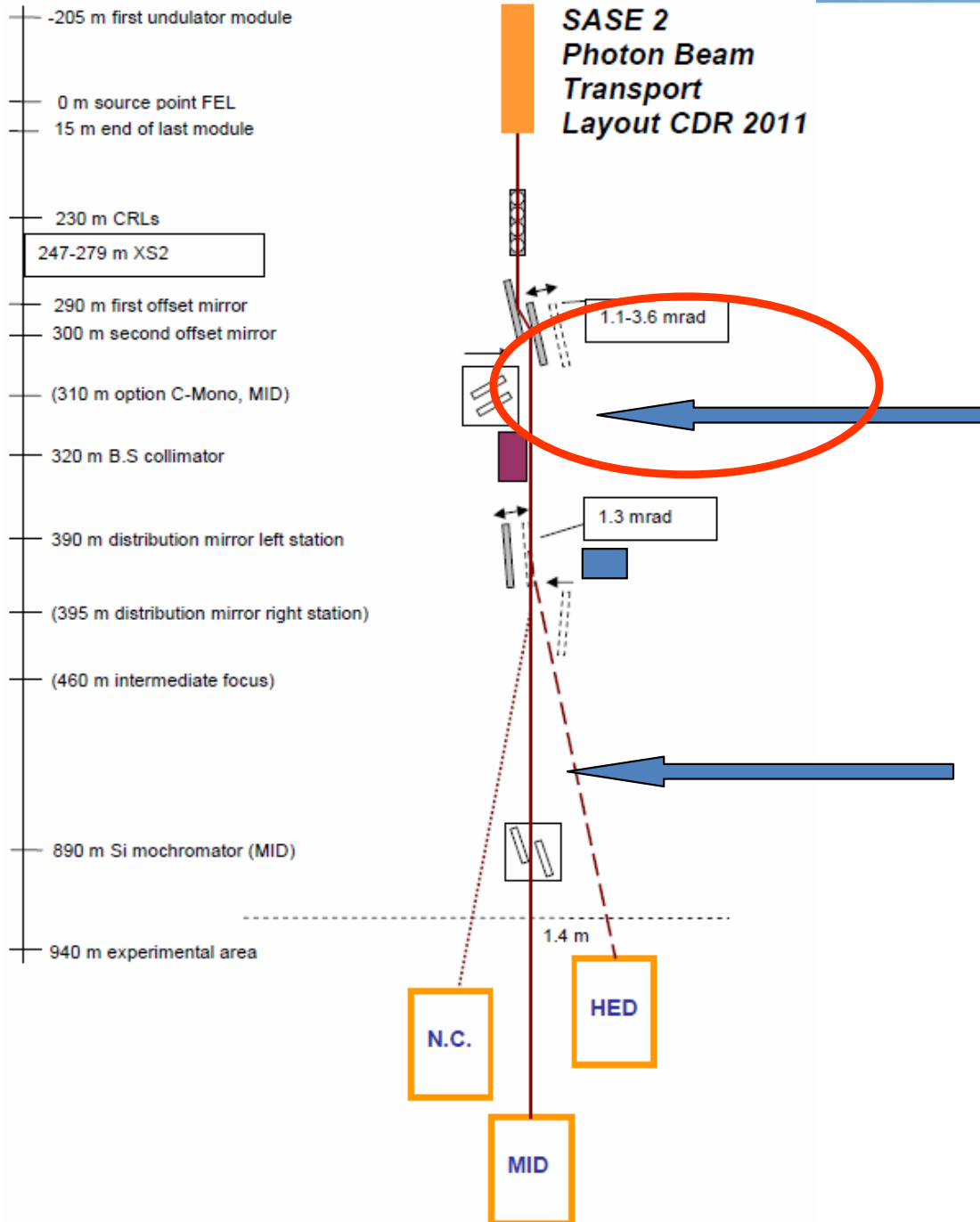
Diffraction structure parameters

| α | β | d | $\lambda/\Delta\lambda$ | 2θ | R_1 | R_2 |
|---------------------|---------|---------------------------------|-------------------------|-----------|-------|-------|
| 0.1° (1.75 mrad) | 0.37° | 6.4 μm (156 l/mm) | 30000 0.33 eV | 0.47° | 310 m | 200 m |

Reflection zone plate parameters

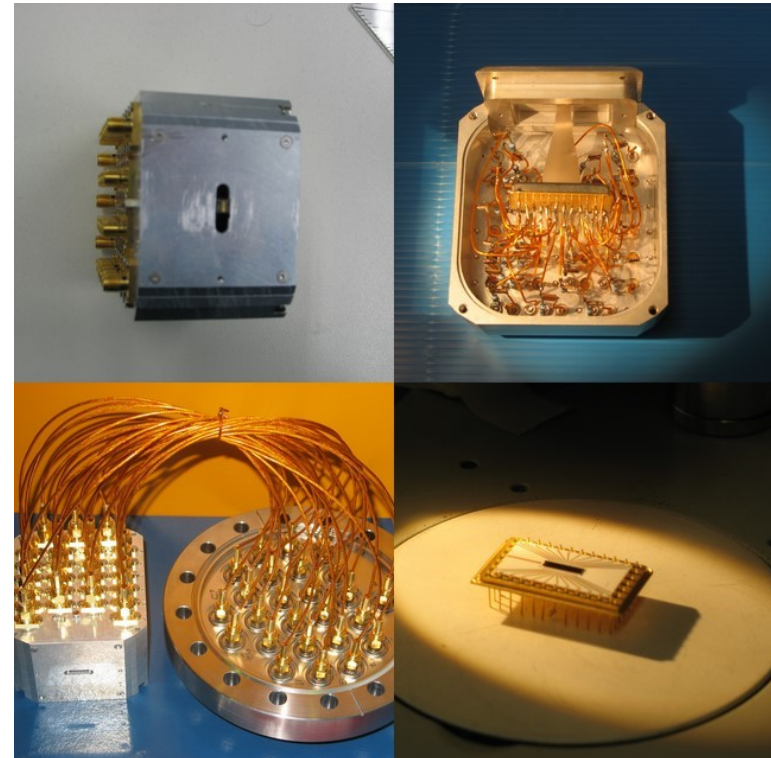
| L | γ | r_1 | r_2 | δx_{min} | Δt | Δx detector resolution |
|--------------------|----------|-------|-------|-------------------------|--------------------|--------------------------------|
| 200 mm (400 mm) | 0.2° | 144 m | 356 m | 10.8 μm | ~ 12 fs (25 fs) | 20 μm |

Single-Shot monochromator position SASE 2



Reflection zone plate

Parallel detector array



We propose minimizing the number of optical elements in the beamline by combining reflection, focusing and dispersion in one single element. We considerably increase efficiency (20 times in the example of the BESSY II Slicing beamline), reduce scattering and slope errors using flat substrates and PRESERVE COHERENCE.

Reflection zone plates have been experimentally tested in the energy range 0.062 eV to 20 keV at several BESSY II beamlines and show high stability, efficiency and energy resolution.

The radiation stability tests are necessary to confirm advantages of reflection zone plates in XFEL applications.

Franz Schäfers

Alexei Erko

Michael Scheer

Frank Siewert

Alexander Firsov

Heike Löchel



Wolfgang Freund

Jan Grünert

Cigdem Özkan

Serguei Molodtsov

Thank you!