



Rolf Follath:: SwissFEL Photonics :: Paul Scherrer Institut

Beamlines Design for Synchrotron Radiation

HESEB Soft X-ray Lecture & Training Course

4.12.2024

Properties of synchrotron radiation

2

SESAME, 2.5 GeV

133 m circumference

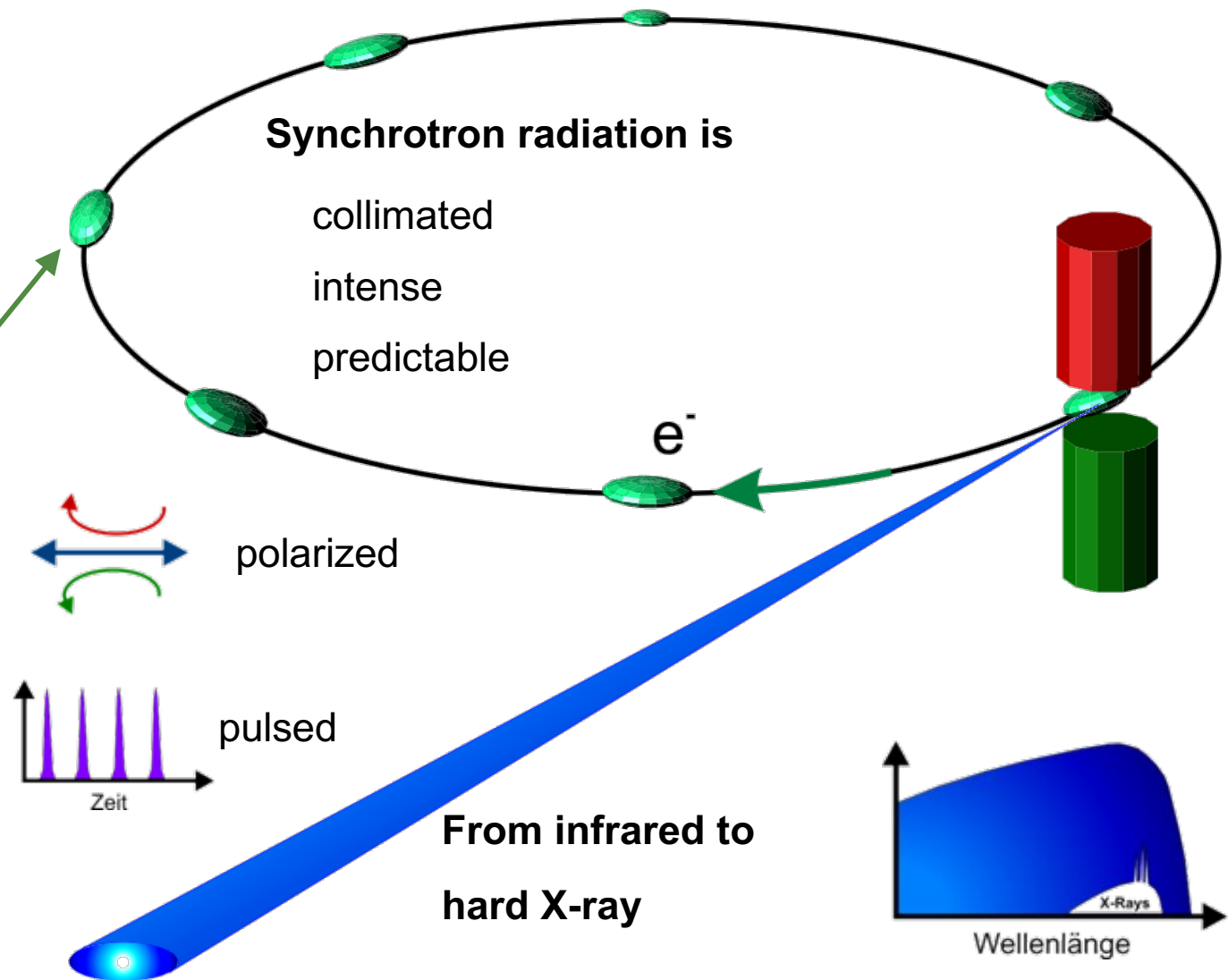
222 buckets

200 electron bunches

Stroboscopic flashes of light

50 ps flashes

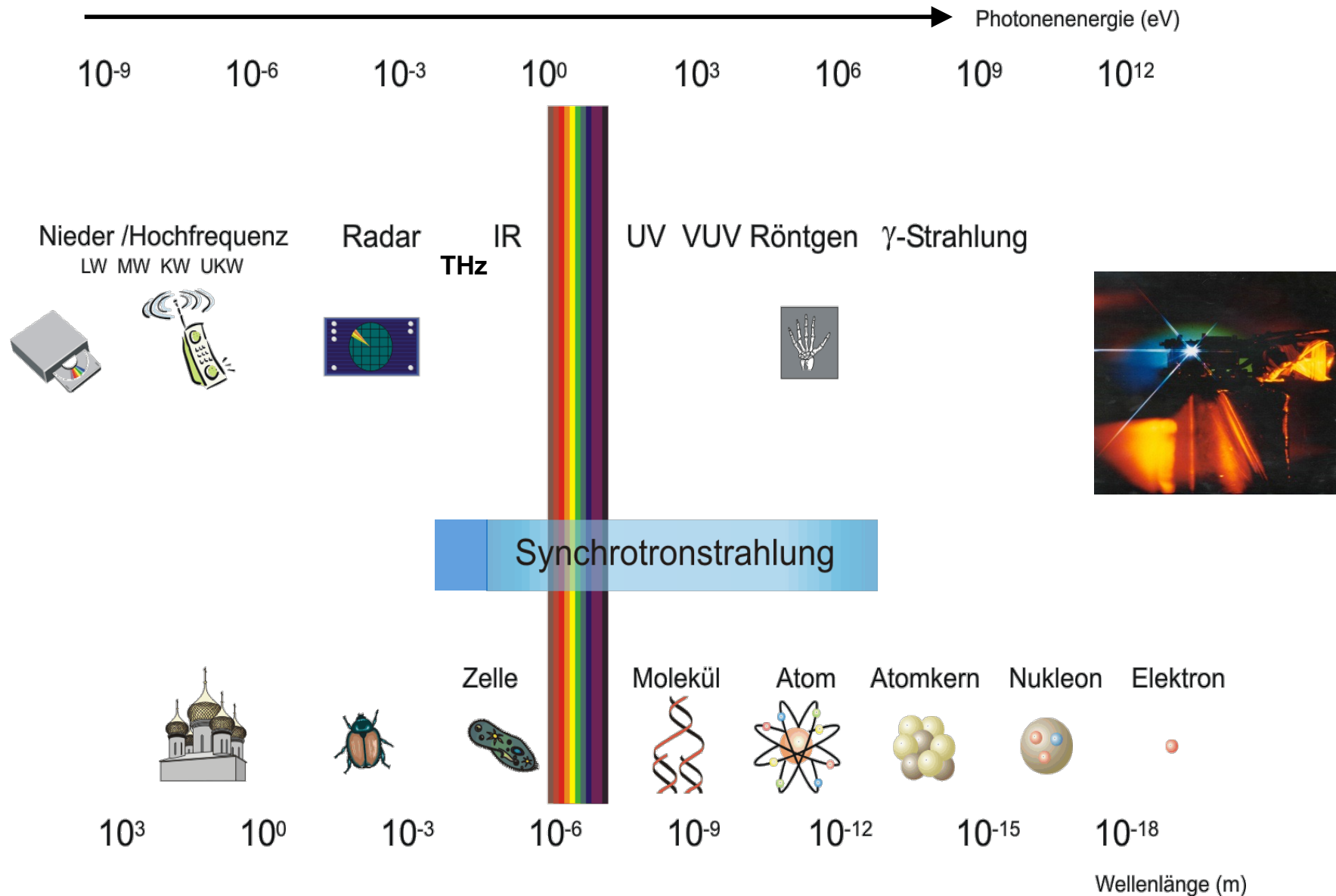
500 000 000 per second.



Courtesy BESSY II

Wavelength of synchrotron radiation

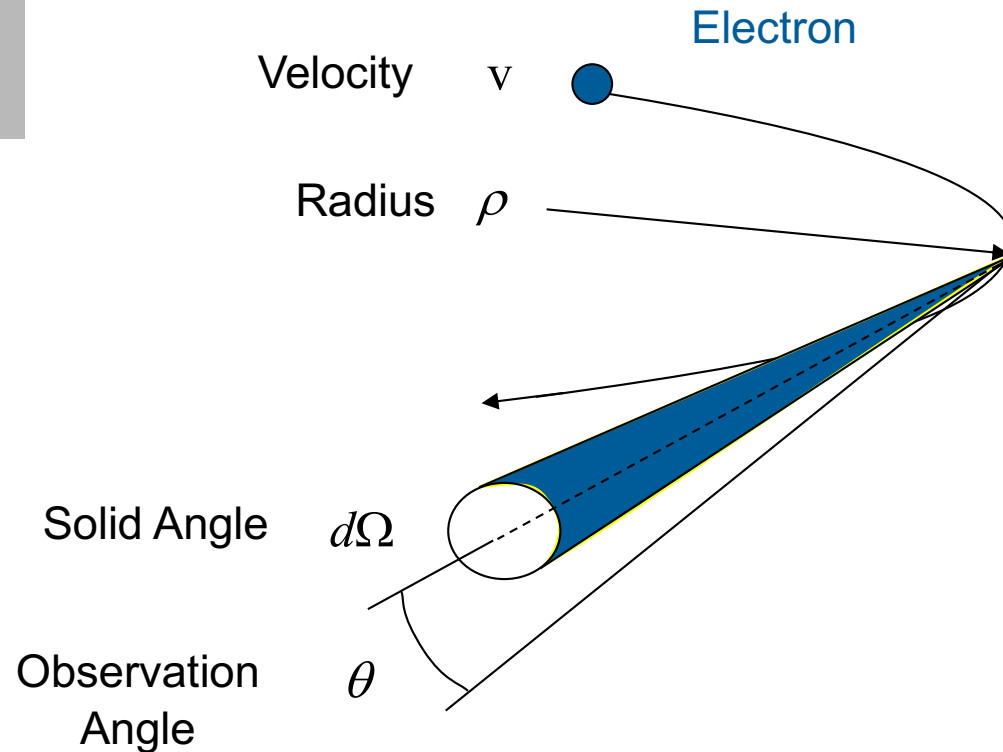
3



Courtesy BESSY II

Predictability of synchrotron radiation

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$$\beta = \frac{v}{c} \quad \gamma = \frac{1}{\sqrt{1-\beta^2}}$$

ω : frequency

$$\xi = \frac{\omega \rho}{3c} \left(\frac{1}{\gamma^2} + \theta^2 \right)$$

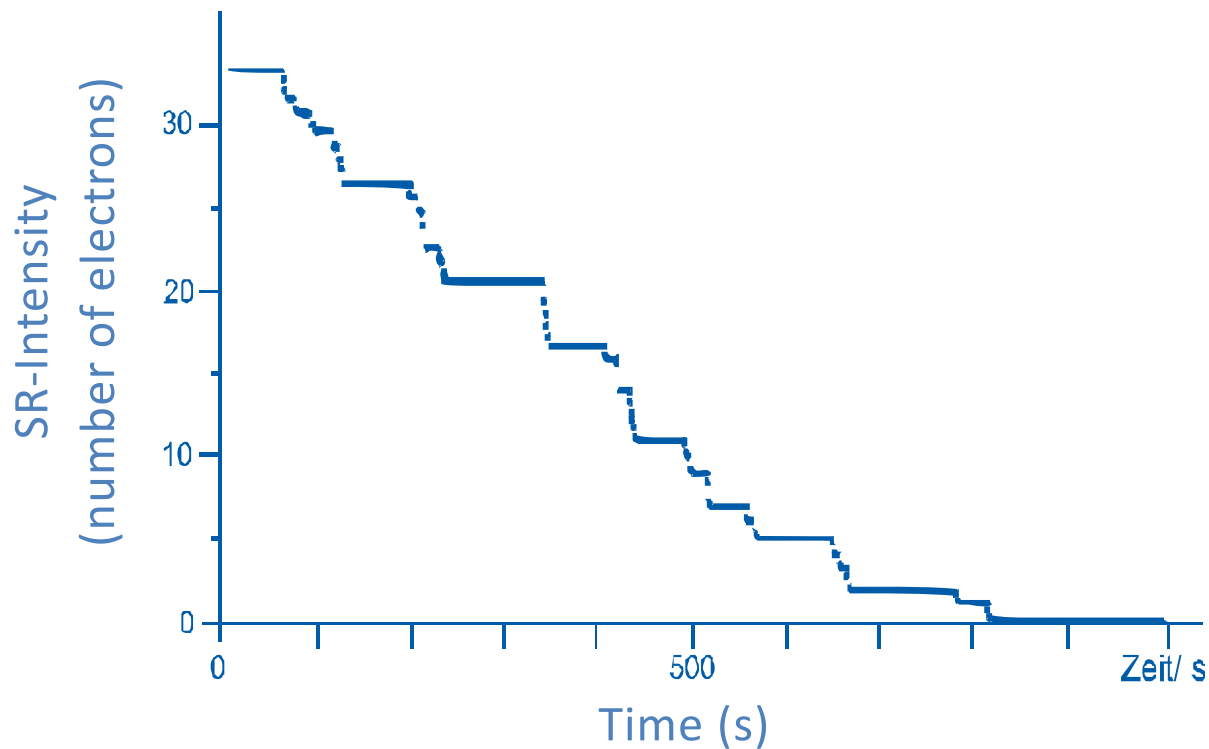
K : mod. Bessel functions

$$\frac{d^2 I}{d\omega d\Omega} = \frac{e^2}{3\pi^2 c} \left(\frac{\omega \rho}{c} \right)^2 \left(\frac{1}{\gamma^2} + \theta^2 \right) \left[K_{2/3}^2(\xi) + \frac{\theta^2}{(1/\gamma^2) + \theta^2} K_{1/3}^2(\xi) \right]$$

Exactly predictable -> Used as radiation standard in national metrology labs
need to know the electron beam energy.

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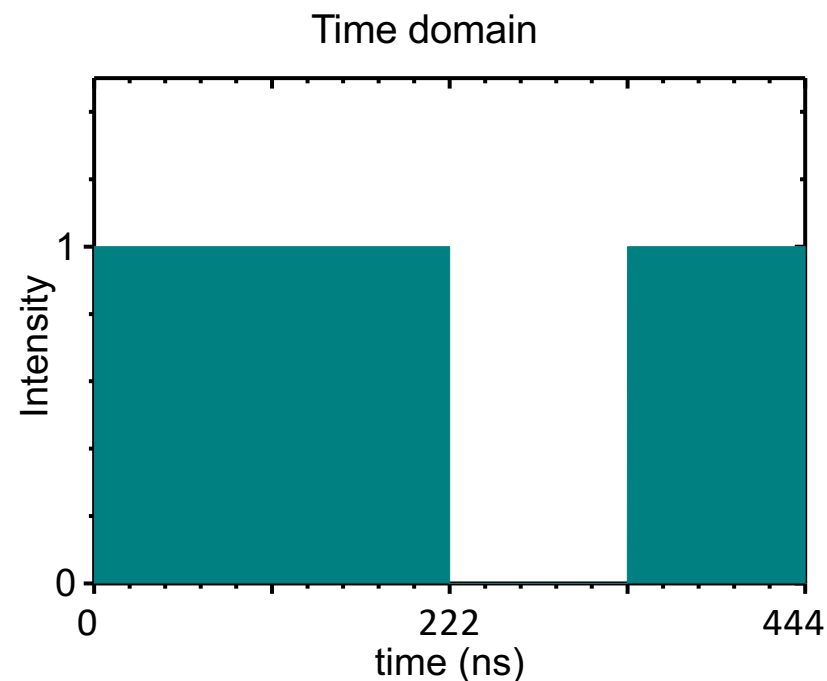
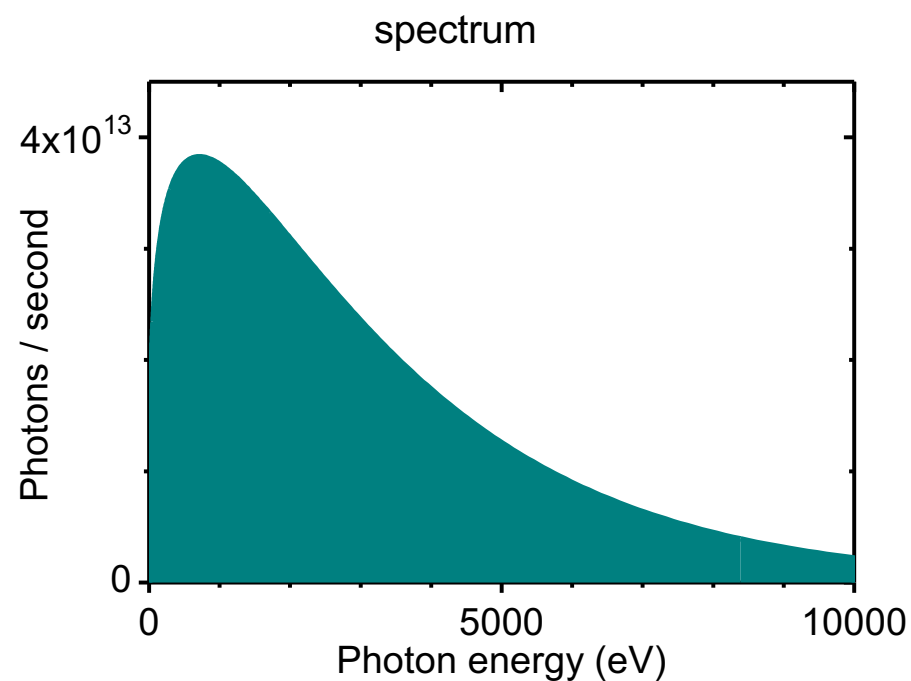
Detector of ESA satellite
Solar and heliosphere observer (SOHO)



Variation of beam intensity by nine order of magnitude

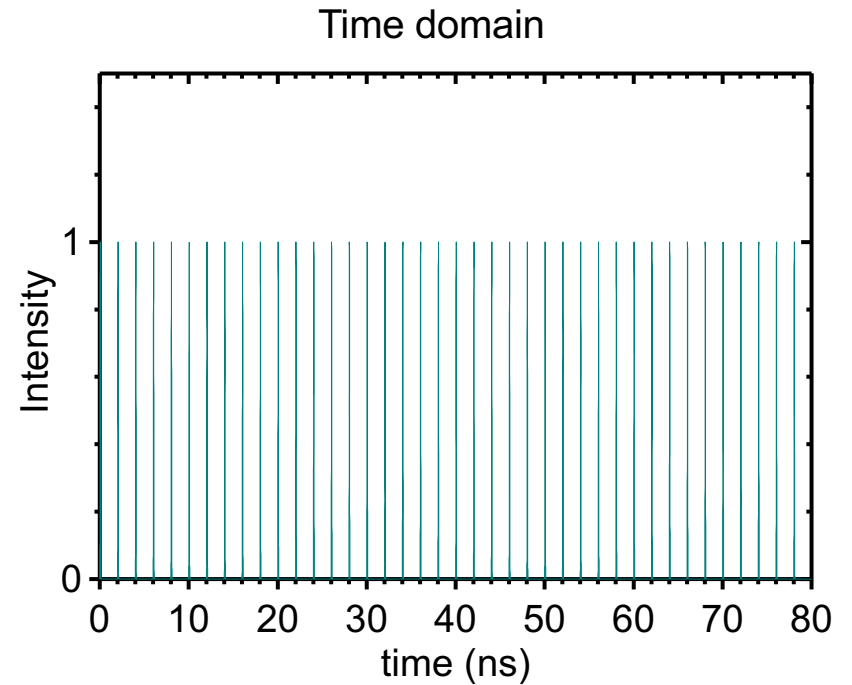
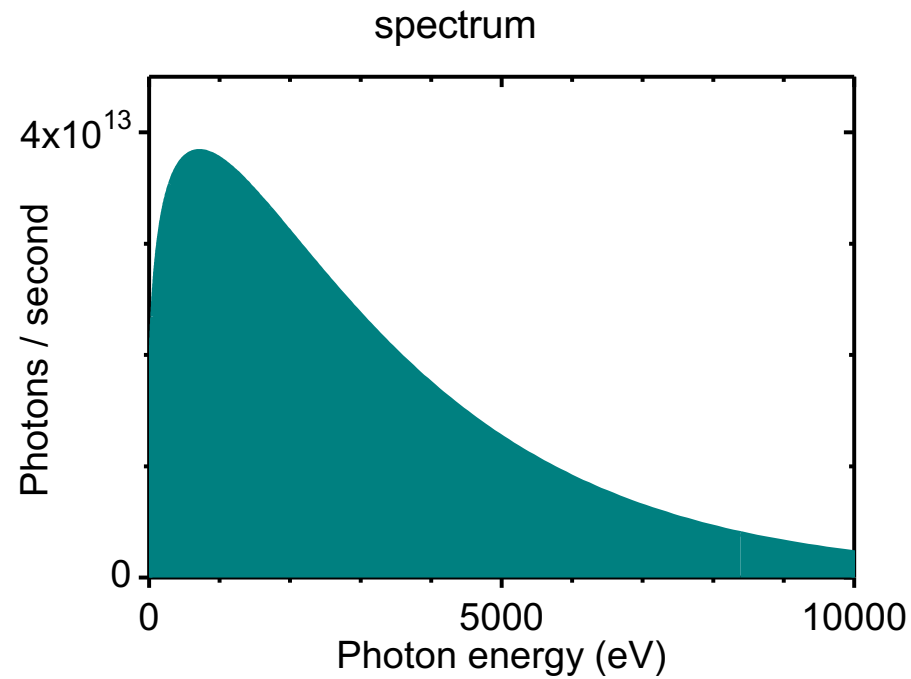
6

Dipol radiation



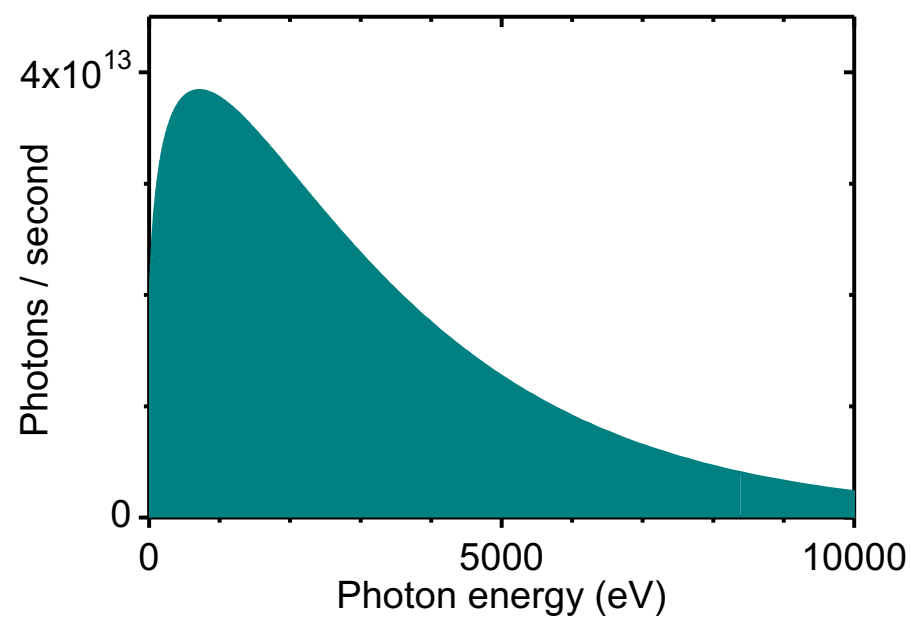
1 revolution
(gap to increase live time)

Dipol radiation

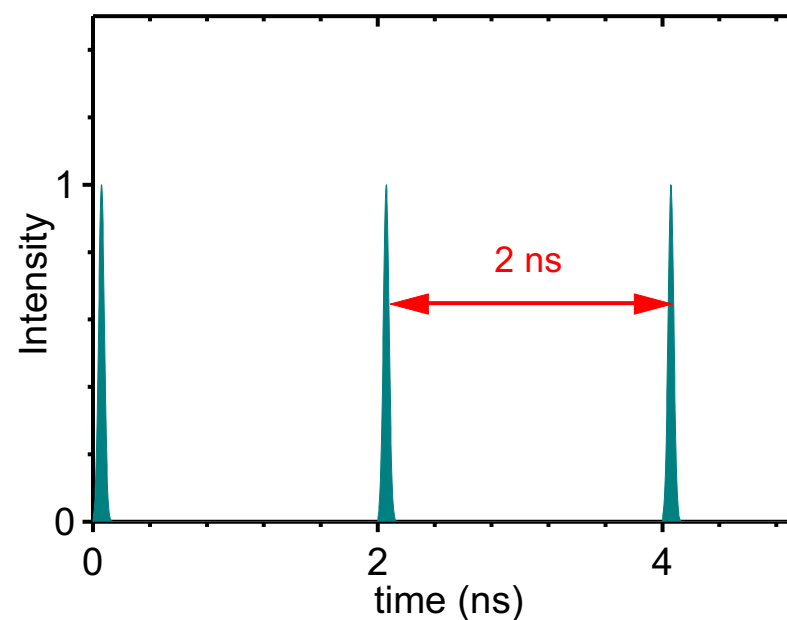


Dipol radiation

spectrum

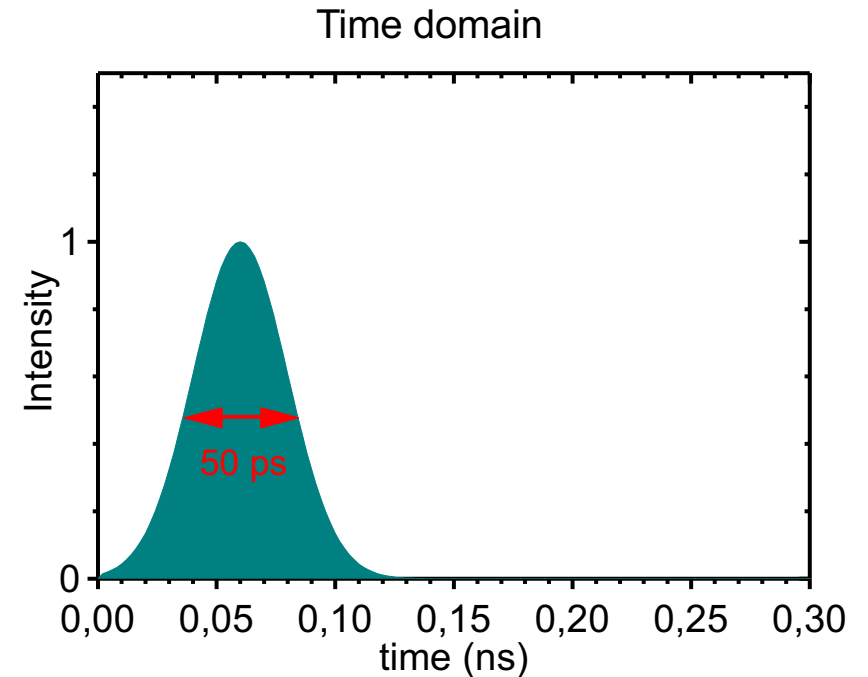
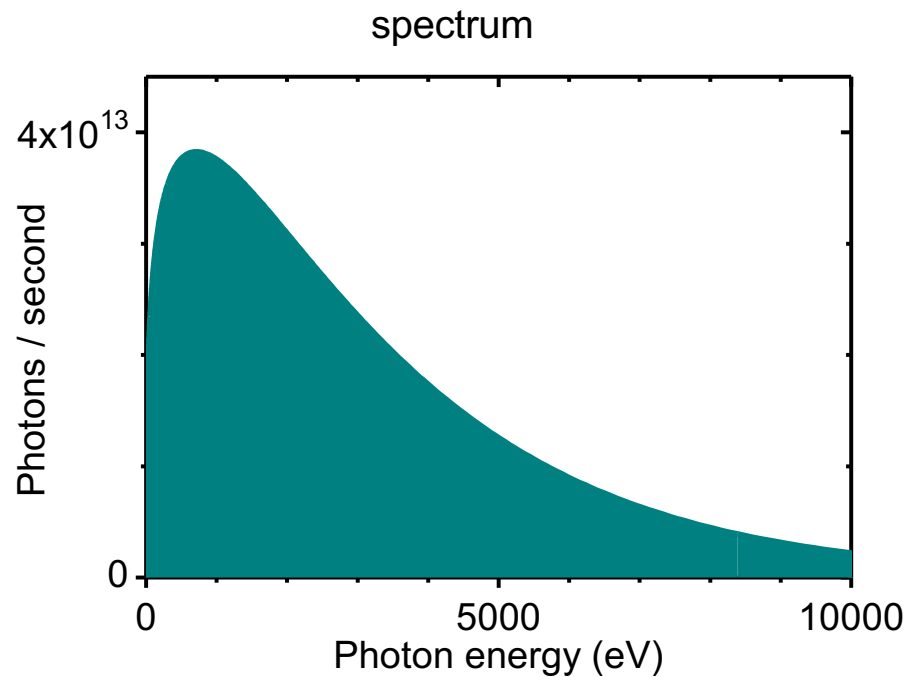


Time domain



2 ns : period of accelerator RF

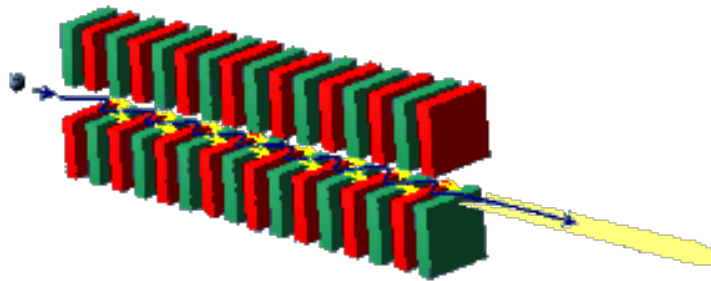
Dipol radiation



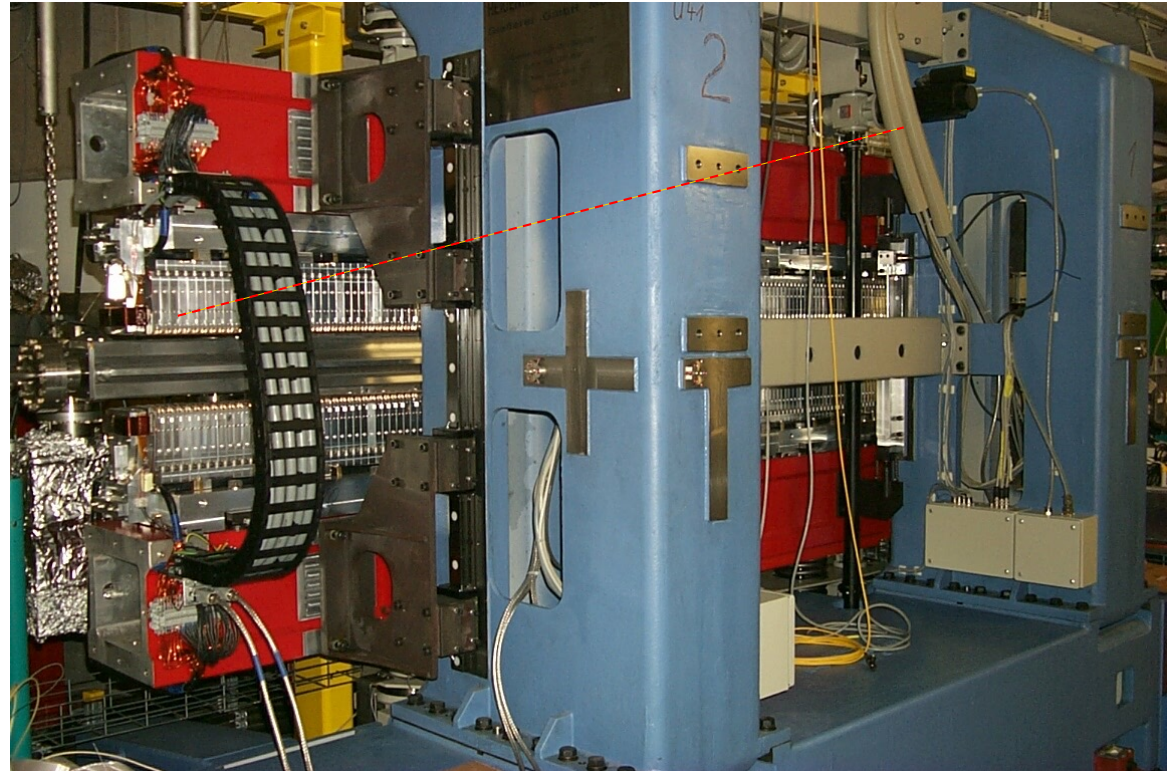
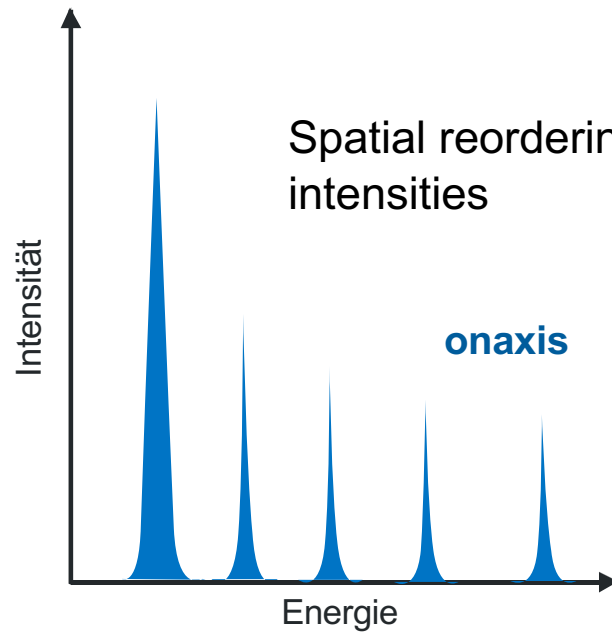
Bunchlength down to 1 ps in low- α mode of a storage ring

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Magnetic array



Spatial reordering of intensities

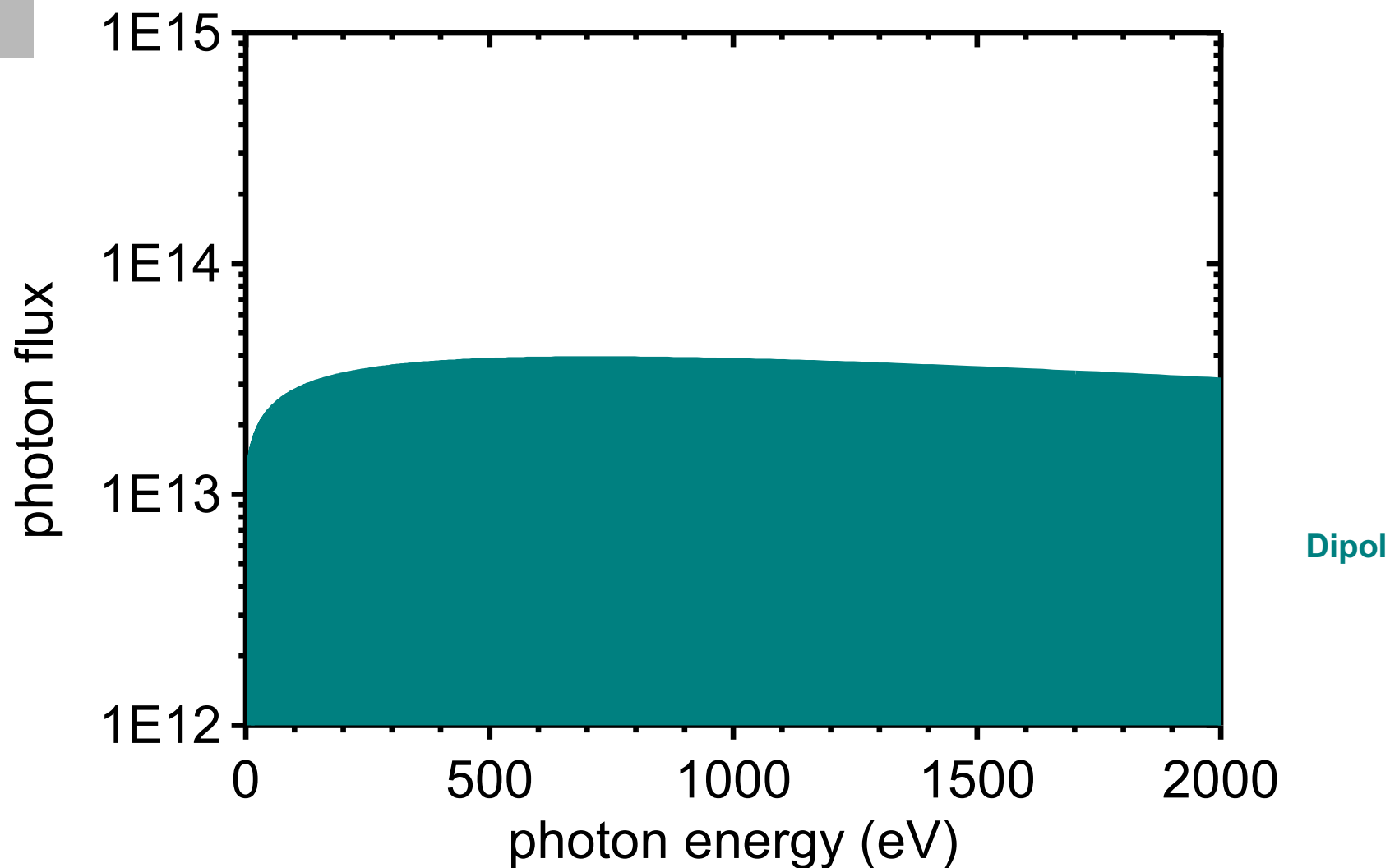


Typical values

Undulatorlength	2 - 4 m
Period length	15 - 150 mm
Number of periods	20 - 100

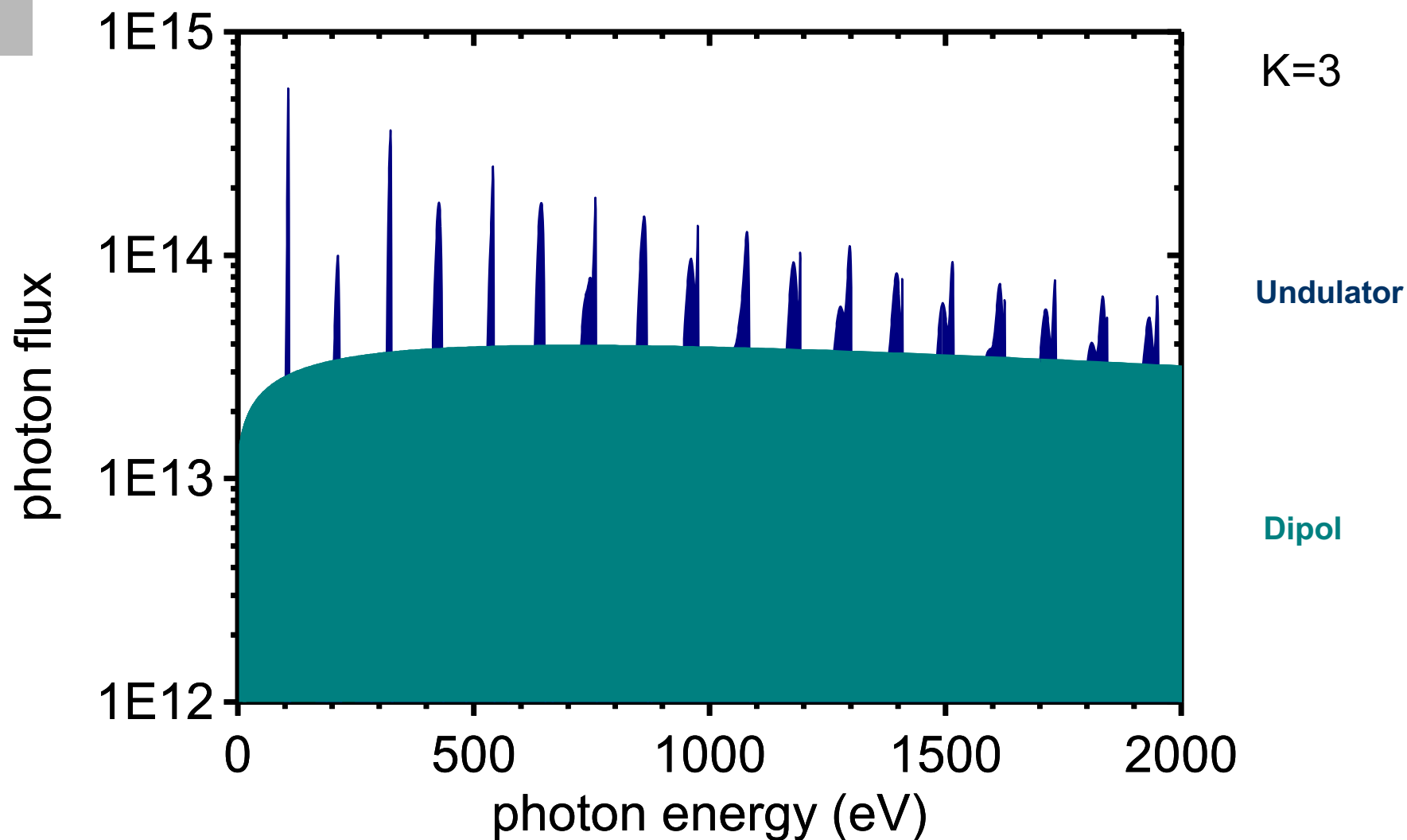
Courtesy BESSY II

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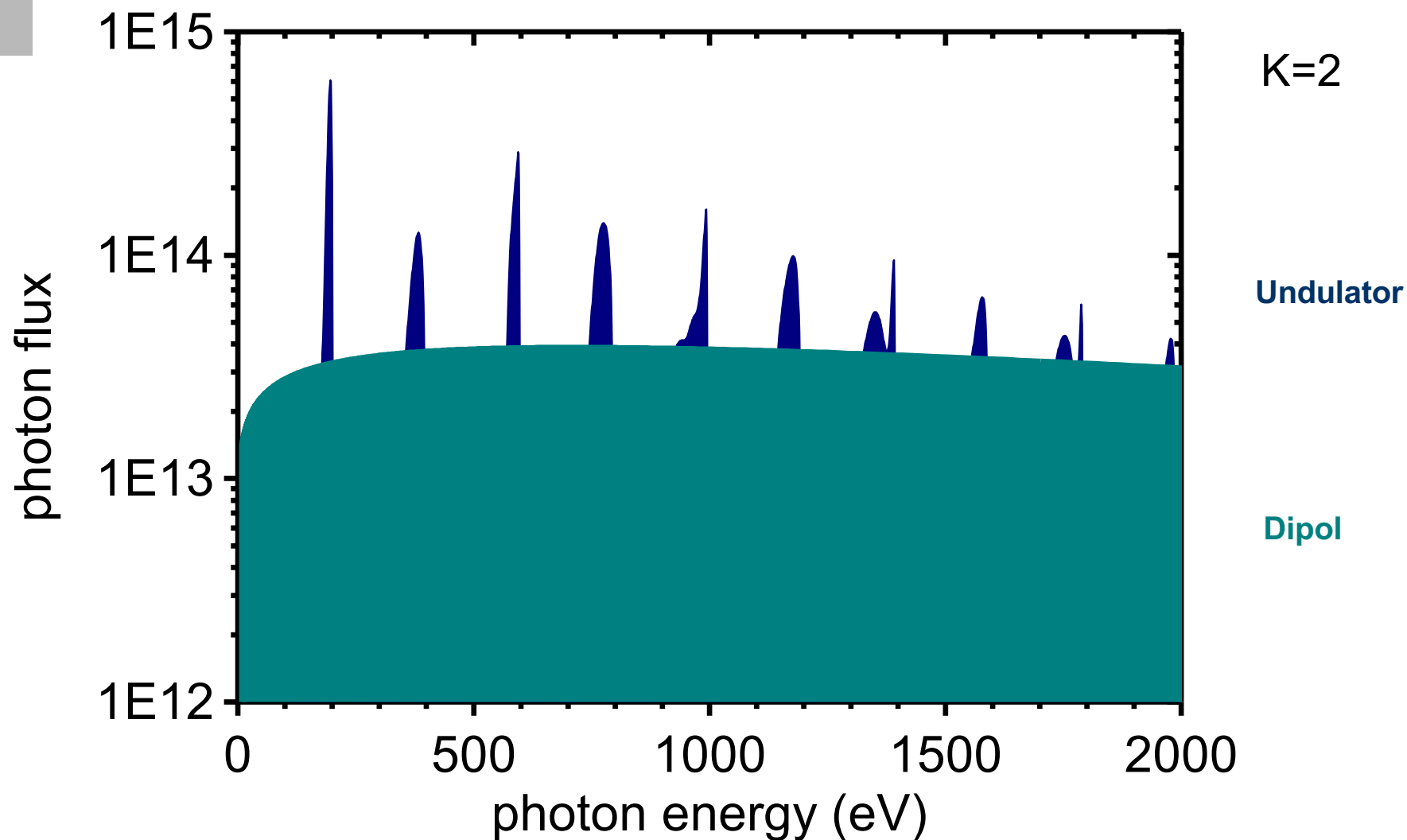
Scan k-value to extend the photon energy range.

12



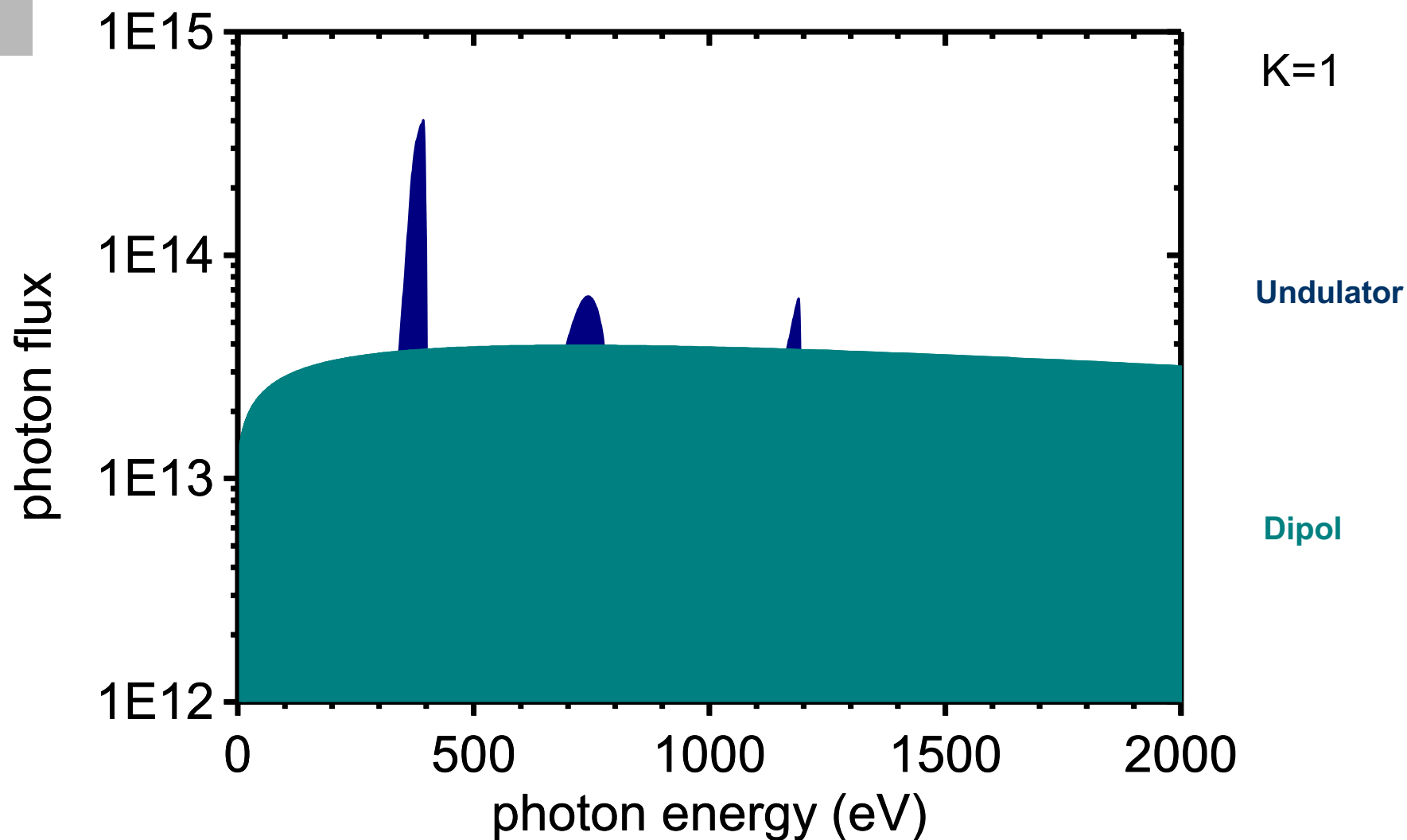
Scan k-value to extend the photon energy range.

13



Scan k-value to extend the photon energy range.

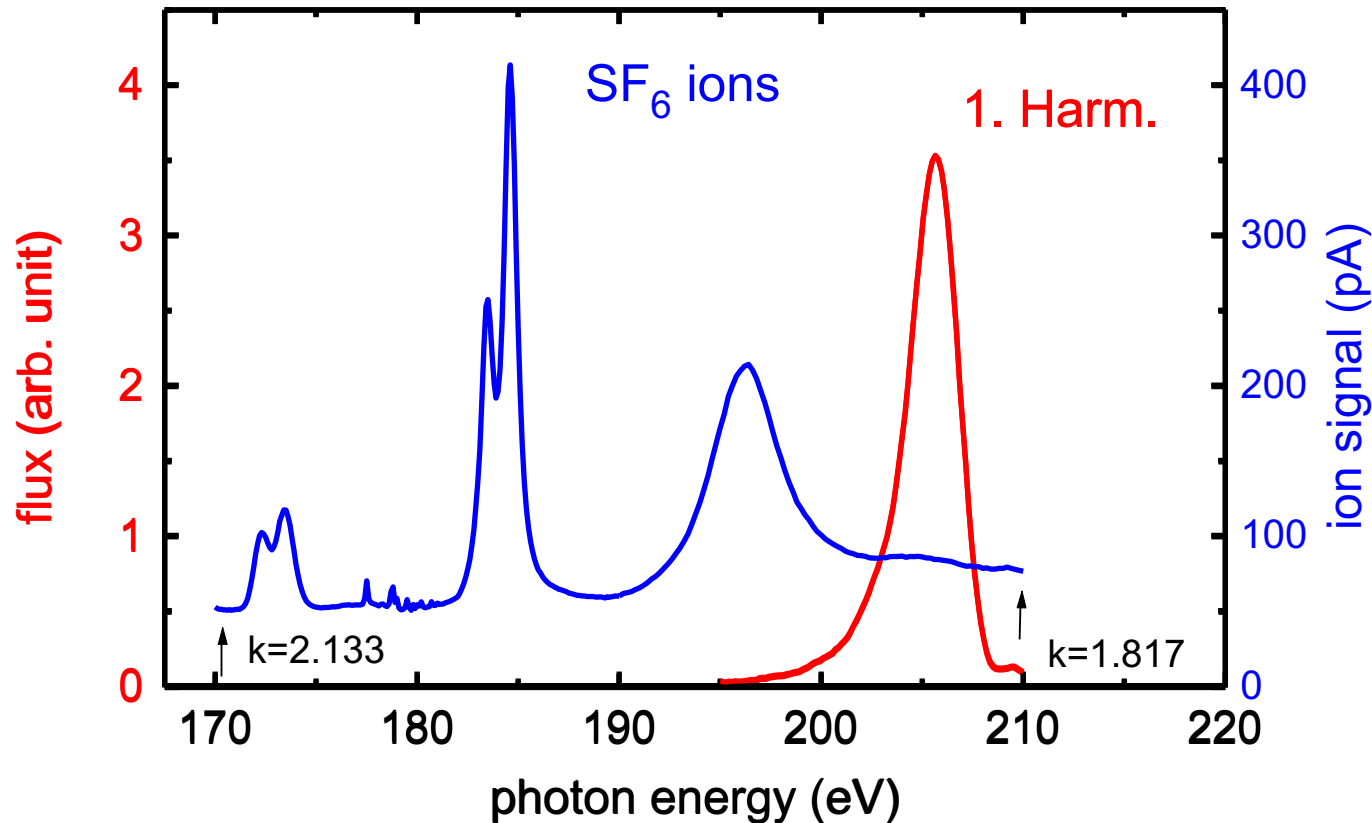
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Scan k-value to extend the photon energy range.

Photoabsorption of SF₆ gas

U49/1-SGM

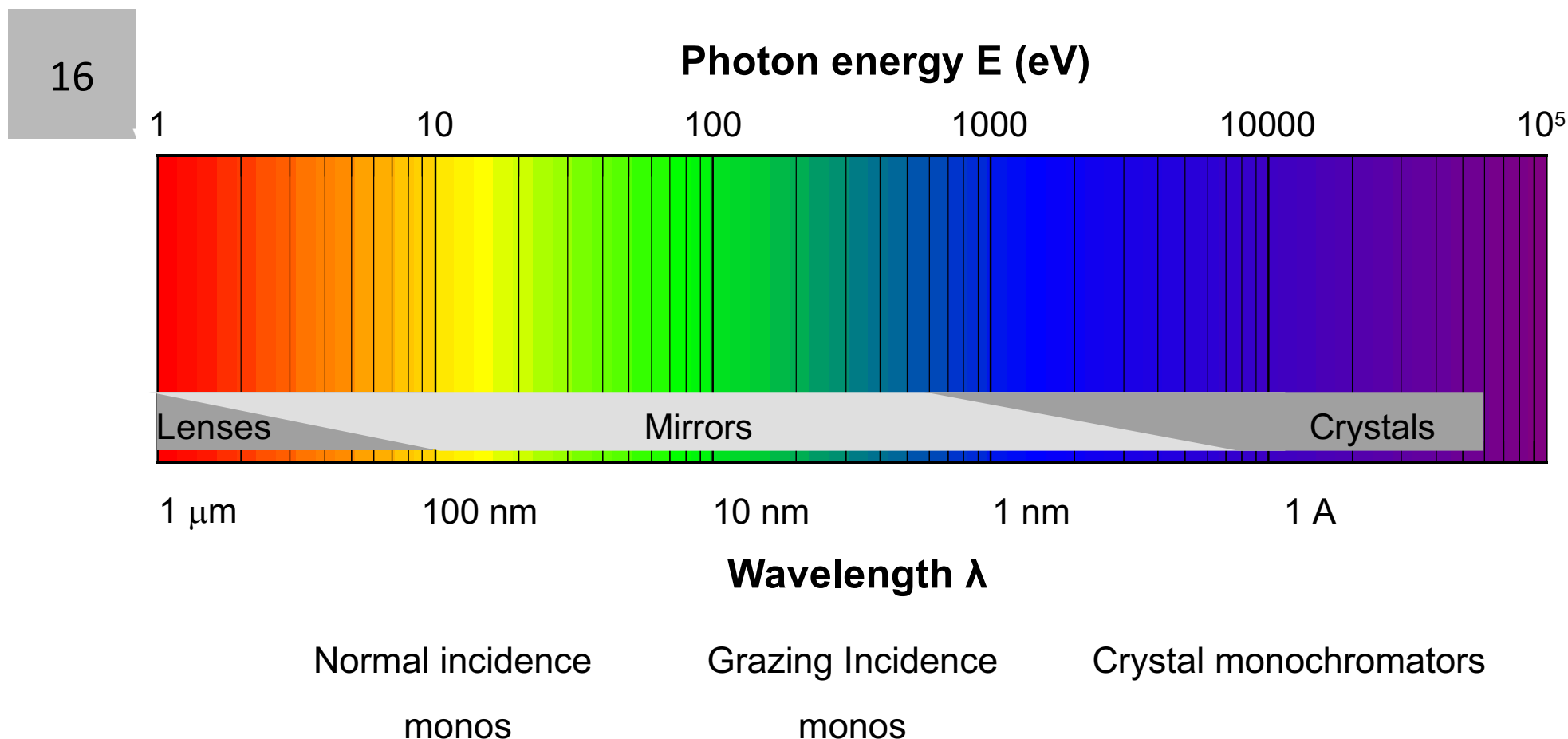


- Undulatorharmonic too broad for spectral features,
- But too small to cover complete spectrum

need for monochromator.

simultaneous scanning of ID and mono

Spectral range at Synchrotrons



$$E = \frac{12.4 \text{ keV} \cdot \text{nm}}{\lambda}$$

Reflectance

Matter is almost opaque for soft X-ray radiation

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Photon energy

- **Visible light**

- Lenses in axial-symmetric configurations
(Microscopes, Cameras, Binoculars)
- mirrors in axial symmetric configuration (achromatic)
(Astronomical telescopes)

- **VUV**

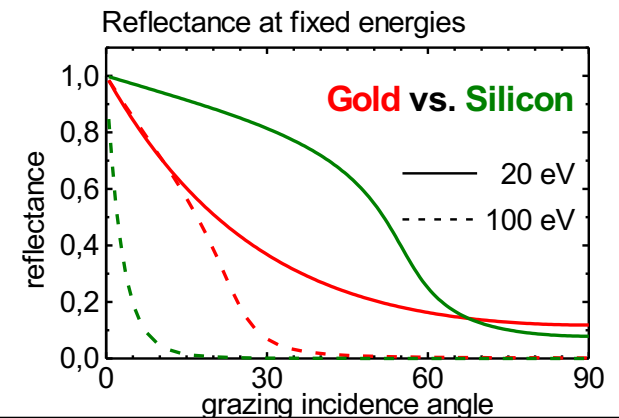
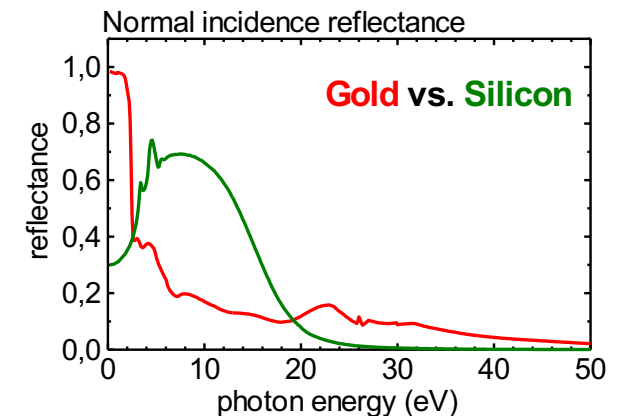
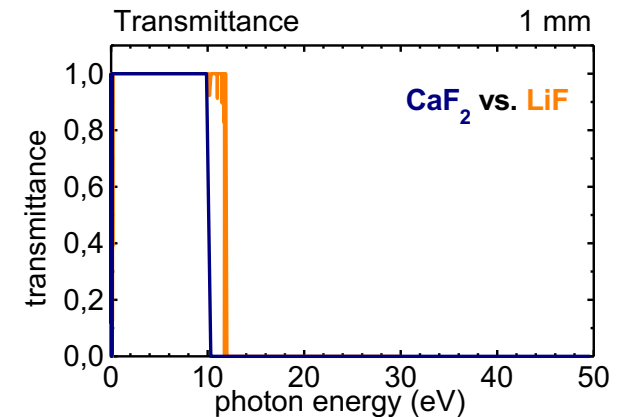
- mirrors and gratings in axial-symmetric configurations
(Normal Incidence Mono, EUV lithography)

- **Soft X-rays**

- mirrors and gratings in grazing incidence configurations
(Grazing Incidence Mono)
- Zone plates, multilayers
- Microscopes

- **Hard X-rays**

- crystals



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Fresnel formulas

- incident intensity I_0 , reflected I_r and transmitted intensity I_t
- boundary conditions of amplitudes (E,H)
- conservation of energy
- angle of reflection = incident angle
- separately for s- and p-polarised light

$$I_r = R_{s,p} \cdot I_0 \quad I_t = T_{s,p} \cdot I_0$$

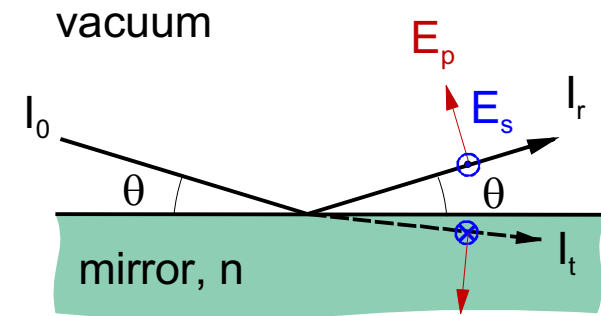
We are only interested in the reflected intensity

s- polarised

$$R_s = \frac{\sin \Theta - \sqrt{n^2 - \cos^2 \Theta}}{\sin \Theta + \sqrt{n^2 - \cos^2 \Theta}}$$

p- polarised

$$R_p = \frac{n^2 \sin \Theta - \sqrt{n^2 - \cos^2 \Theta}}{n^2 \sin \Theta + \sqrt{n^2 - \cos^2 \Theta}}$$



e.g. for solids with only one type of atoms:

index of refraction $n = n + ik$

$$n = 1 - \delta + i\beta$$

$$n = 1 - \frac{r_e}{2\pi V_A} \cdot \lambda^2 \cdot (f_1 + i f_2)$$

V_A : Atomic volume = $1 / n_A$

r_e : classical electron radius ($2.82 \times 10^{-15} \text{ m}$)

f_1, f_2 : atomic scattering factors

(f_1, f_2) in the Henke tables (n, k) in the book of Palik

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Brewster angle

At the Brewster angle the reflected light is s-polarised ($R_p=0$). The reflected beam is **perpendicular** to the transmitted one.

The electrons oscillate always along an axis parallel to the electric field of the transmitted light.

If the reflected light should propagate parallel to this axes, no power is emitted in this direction.

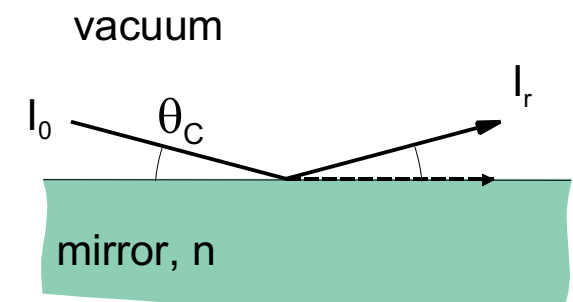
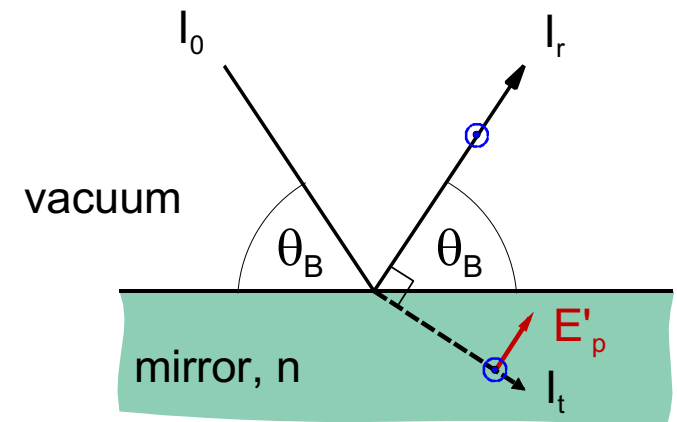
$$\Theta_B = \arctan\left(\frac{1}{n}\right)$$

Total external reflection

If the light comes from the optical denser side of the boundary surface, total reflection can occur (e.g. from under water to air).

In the soft x-ray regime **vacuum is optical denser** than matter. Total reflection occurs when the angle of the transmitted light equals zero.

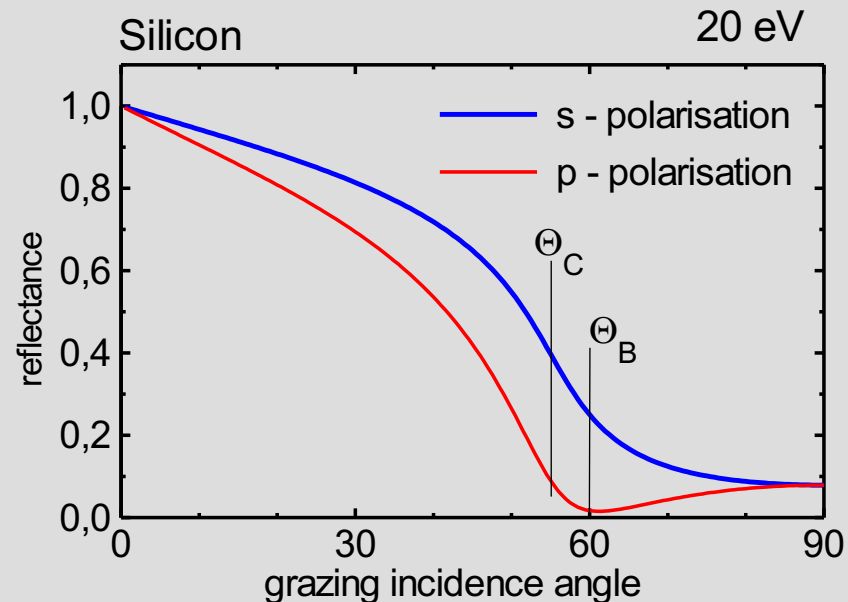
$$\Theta_C = \arccos n$$



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Example 1

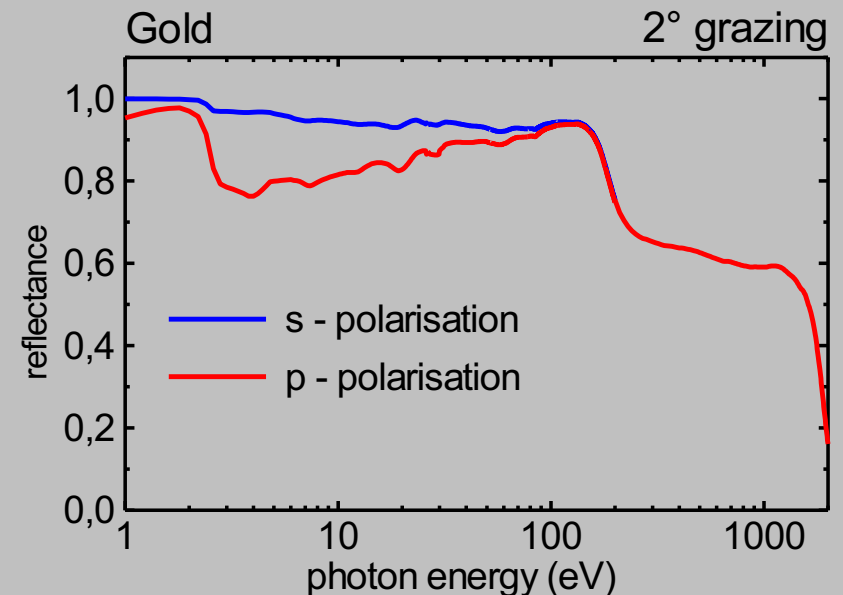
- silicon at 20 eV
- $n = 0.567$, $k = 0.0835$
- critical angle $\theta_C = 55^\circ$
- Brewster angle $\theta_B = 60^\circ$



Always $R_s \geq R_p$

Example 2

- gold at 2° grazing incidence angle



Good reflectance up to 2000 eV

Difference between s- and p- polarisation up to 100 eV

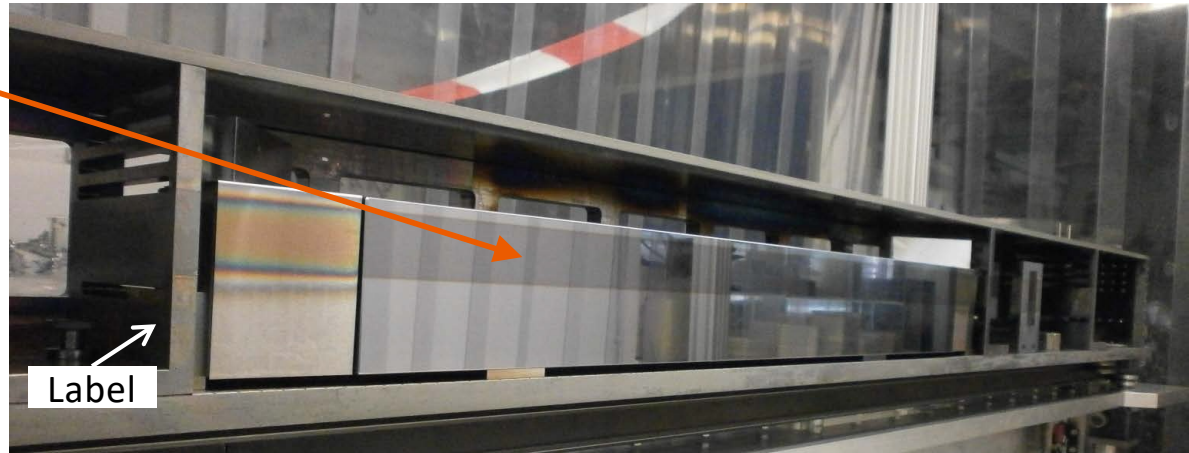
Mirrors

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First stripe: SiC + top B₄C

End of June 2016
Run ID T664

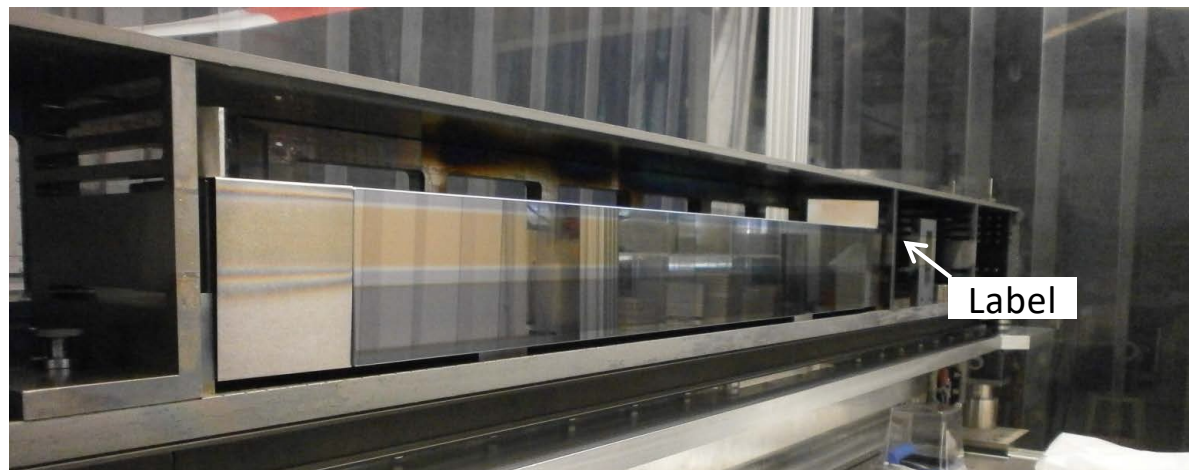
coating area above
width: 44-75 mm (or 44-72 mm)
(uncoated silicon below)



Second stripe: Mo + top B₄C

Beginning of July 2016
Run ID T668

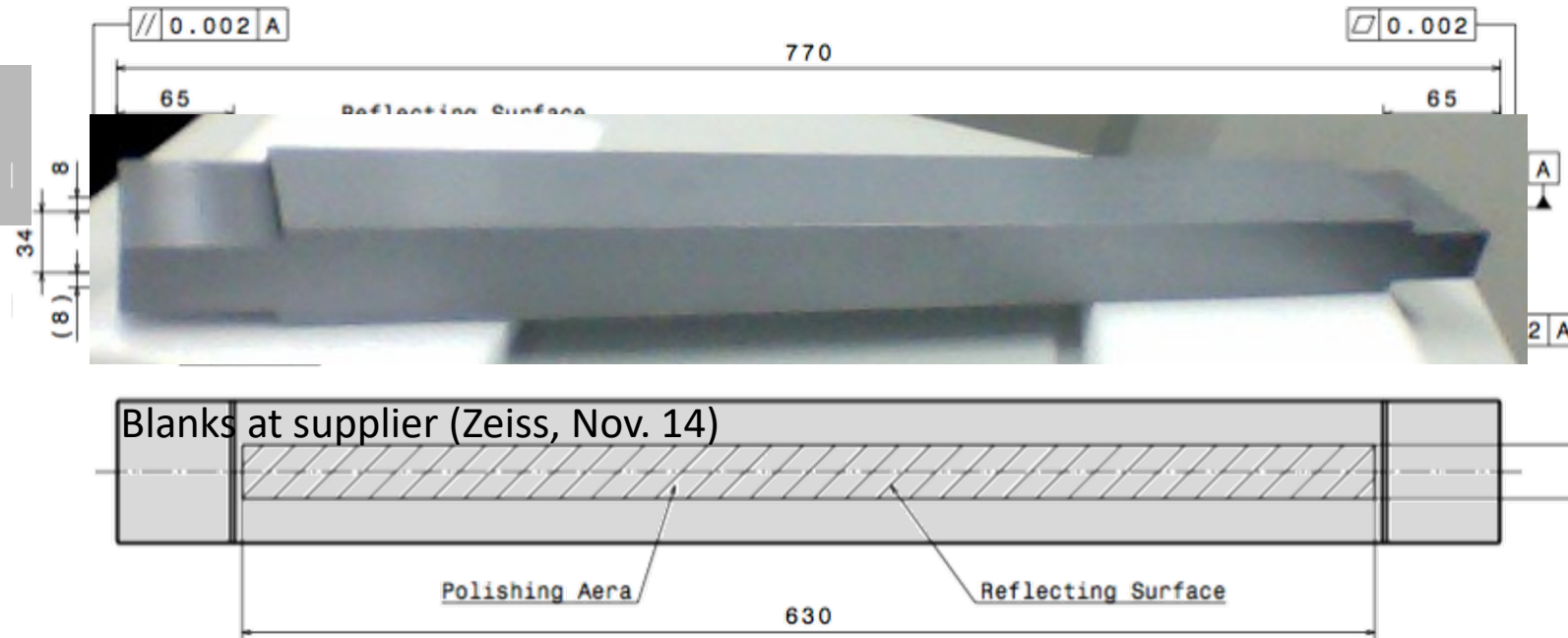
coating area above
width: 44-75 mm (or 44-72 mm)
(first stripe below)



Courtesy, M. Stoermer, HzG Geesthacht

Offset Mirror specification

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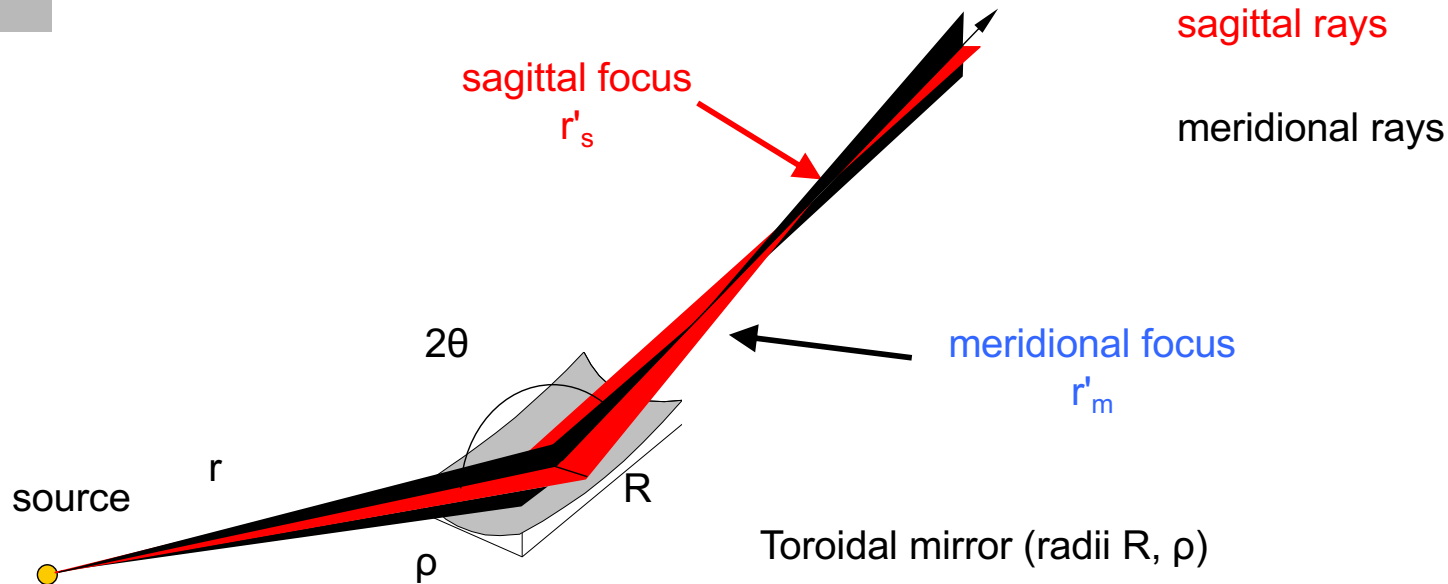


- Bulk : Si (100)
- Height error : < 0.6 nm rms
- Microroughness : < 0.2 nm rms
- Dimensions : 770 x 80 x 50 (80) mm³
- Optical surface : 630 x 30 mm²
- Coatings : SiC/B₄C, Si, Mo/B₄C
- Ordered : Jul. 2014, Zeiss and JTEC
- Delivery : Jul. 2015
- Coating : Start Aug. 2016 (HZ Geesthacht)

Focusing with mirrors

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Because of the small index of refraction we must use grazing incidence to get reflection.



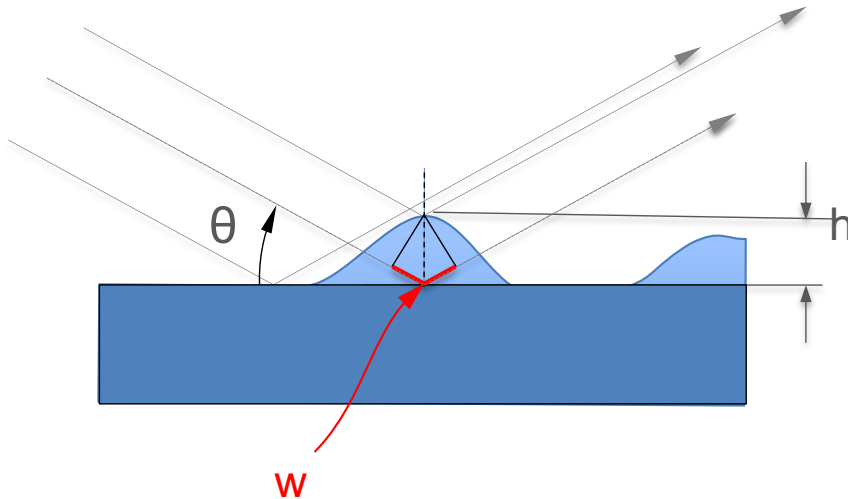
$$\frac{1}{r} + \frac{1}{r'_s} = \frac{2 \cos \theta}{\rho}$$

sagittal focus

„Astigmatic image“ because foci do not coincide
 „Stigmatic image“ match parameters R, ρ

What means ideal optics (1)

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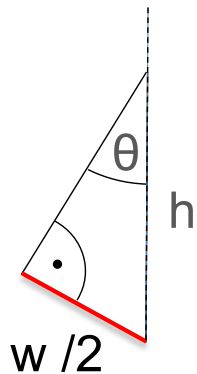


Path difference **w**

$$w = 2h \sin \theta$$

Phase error φ

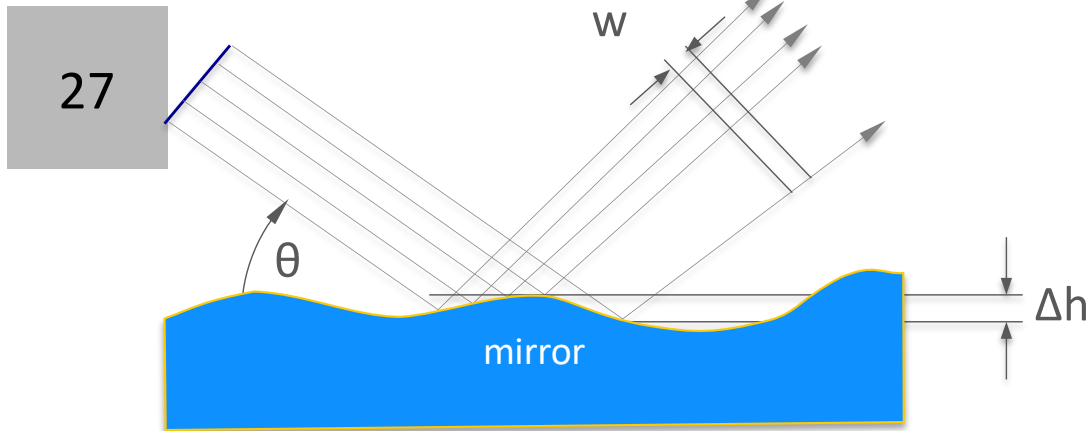
$$\varphi = 2\pi \cdot \frac{2h \sin \theta}{\lambda}$$



$$\frac{w}{2} = h \sin \theta$$

- Abberations reduce with smaller incidence angle
- Abberations stay constant when $\sin \theta / \lambda = \text{constant}$

What means ideal optics (2)



Height error $\Delta h \rightarrow$ wave front distortion w

$$w = 2\Delta h \sin \theta$$

$$w_{rms} = 2\sigma_{rms} \sin \theta$$

Wave front distortion w_{rms}

Surface profile errors σ_{rms}

Diffraction limited optics:

Maréchal criterion

$$w_{rms} \leq \frac{\lambda}{14}$$

Beamline with N surfaces:

$$\sigma_{rms} \leq \frac{\lambda}{14\sqrt{N}2\theta}$$

$$N=4, \theta = 0.75^\circ \quad (13 \text{ mrad})$$

$$1800 \text{ eV } (0.7 \text{ nm}) \rightarrow \sigma_{rms} = 1 \text{ nm}$$

$$600 \text{ eV } (2 \text{ nm}) \rightarrow \sigma_{rms} = 2.7 \text{ nm}$$

$$250 \text{ eV } (5 \text{ nm}) \rightarrow \sigma_{rms} = 6.8 \text{ nm}$$

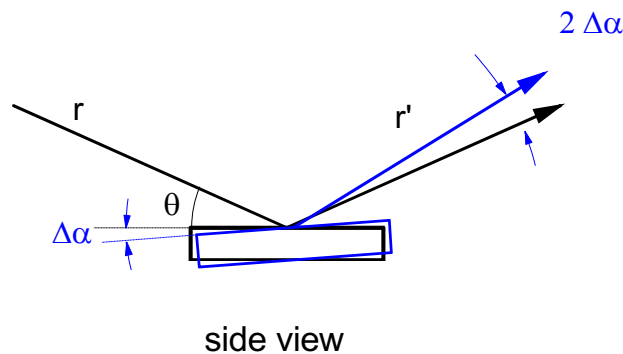
Strongly curved ($\rho = 1.0.. 1.4 \text{ m}$) mirrors

Zeiss $\sigma_{rms} = 10 \text{ nm}$

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Meridional focusing

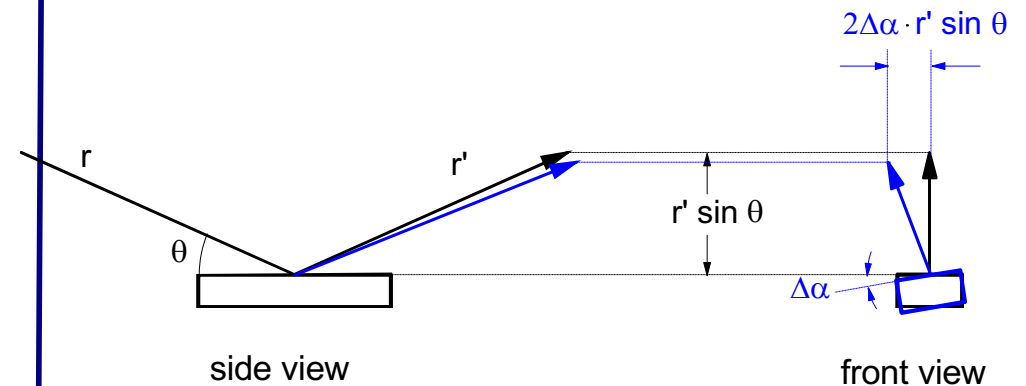
- Focusing in the plane of deflection
- How do surface errors influence the image size?



- Suppose the surface is tilted in the plane of deflection (which is the focusing plane) by $\Delta\alpha$
- the incident beam is then deflected by $2 \cdot \Delta\alpha$
- and the Image size in the focusing plane is increased by $\Delta S = 2 r' \Delta\alpha$

Sagittal focusing

Focusing in the plane perpendicular to deflection

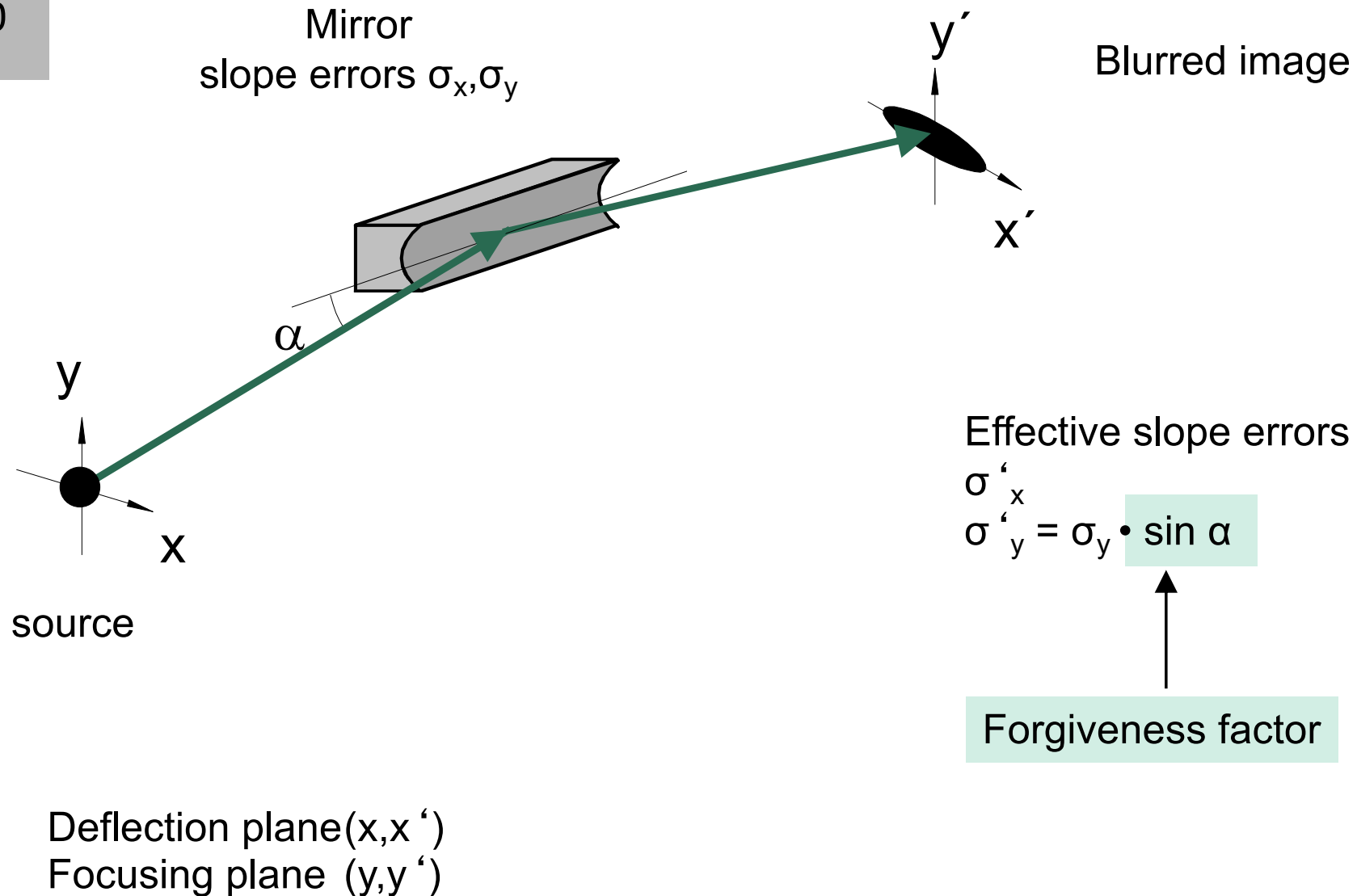


- Surface tilts in the plane of deflection do not affect the image size in the focusing plane.
- A surface tilt in the focusing plane causes the incident beam to be deflected by $2 \cdot \Delta\alpha$,
- and the image size in the focusing plane is increased by $\Delta S = 2 r' \Delta\alpha \sin \theta$

Sagittal focusing reduces the effective slope errors by $\sin \theta$ (reduction by a factor 10-30).

W. Cash, Applied Optics **26** (1987) 2915.

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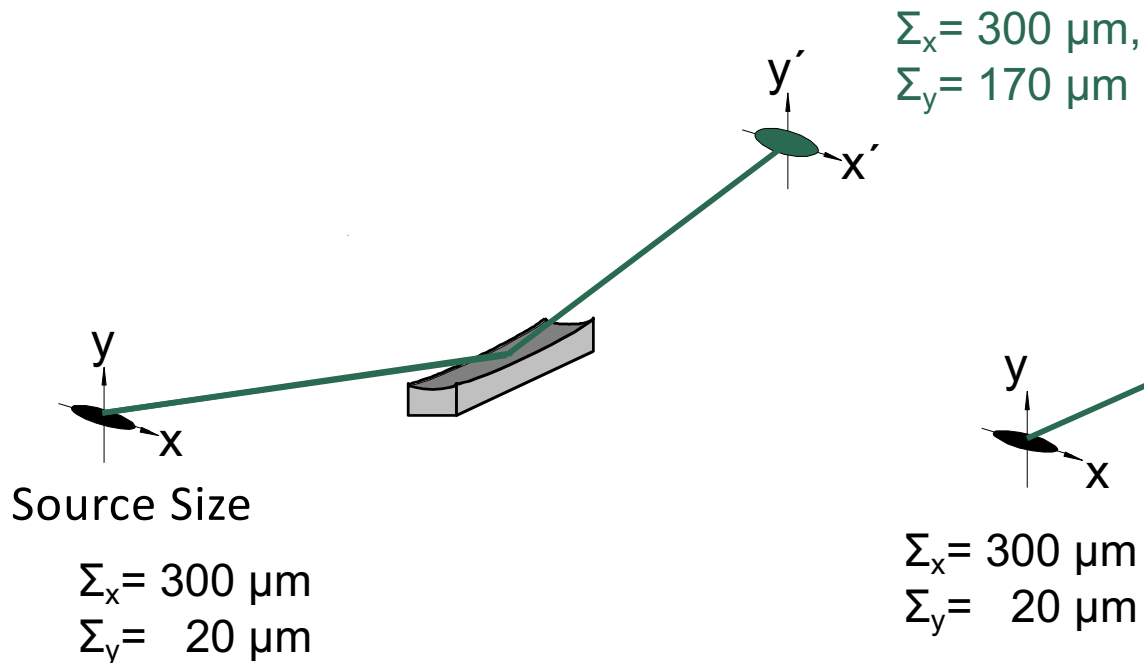


Sagittal vs. Meridional focusing (Example)

Incident angle 3° , 17m :17m imaging, **slope error 1 arcsec**

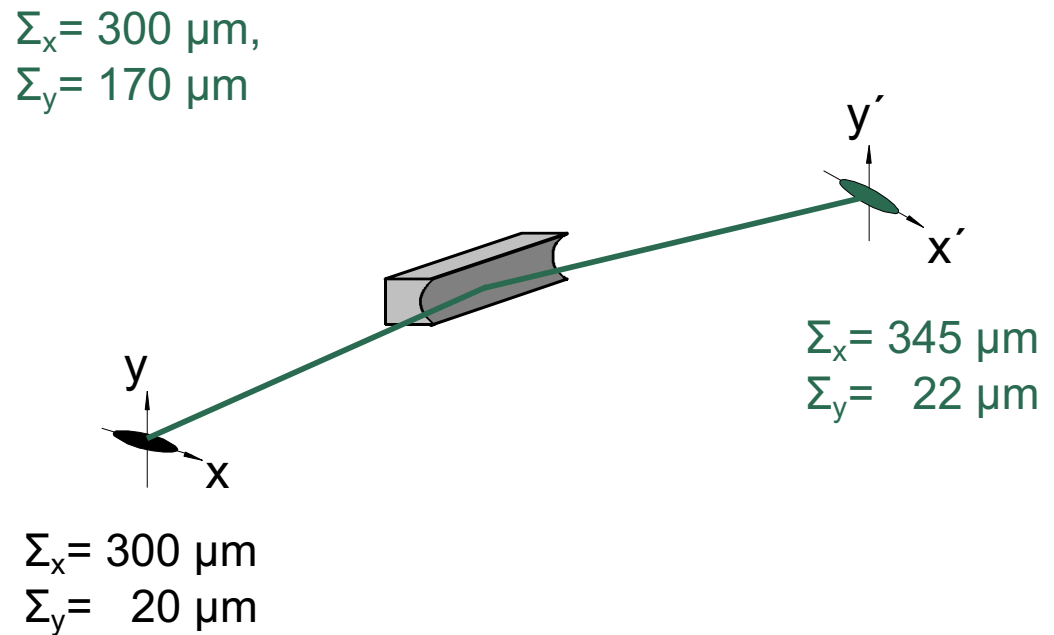
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meridional focusing



Increase in area: 8.5

sagittal focusing



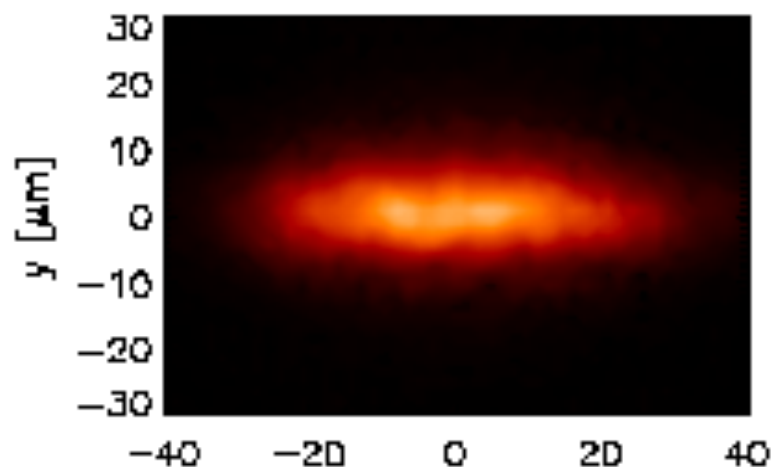
Increase in area: 1.3

sagittal focusing preserves brilliance at 3rd generation SR

Put dispersion plane perpendicular to deflection of mirrors!

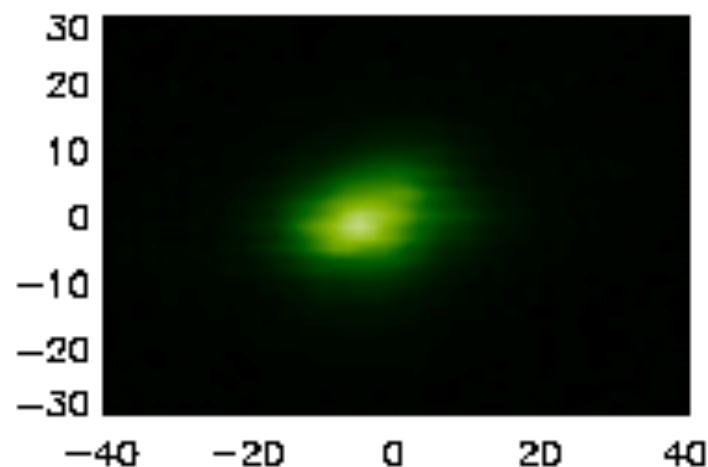
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old mirror (1,5 arcsec)



hor. focus
43 μm

new mirror (0,14 arcsec)

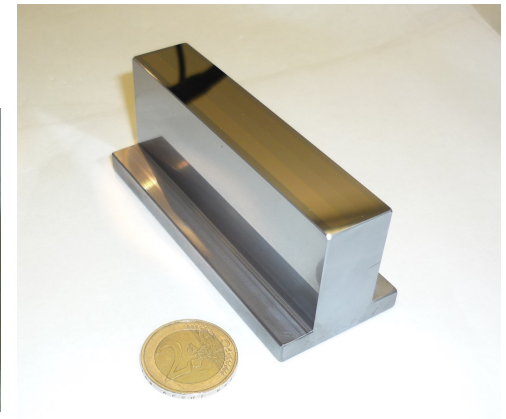
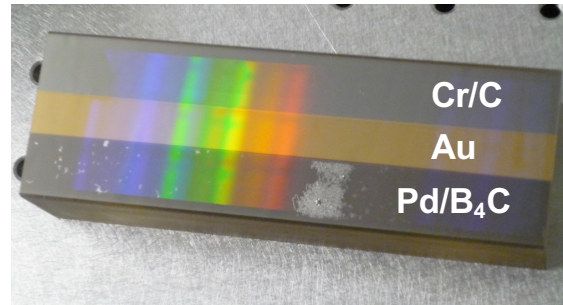


hor. focus
17 μm
(source limited)

Gratings

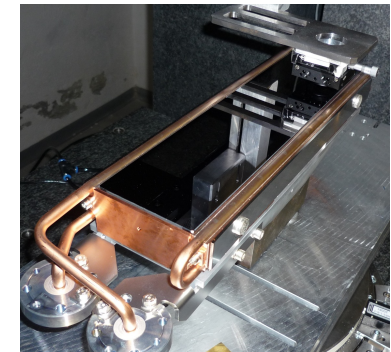
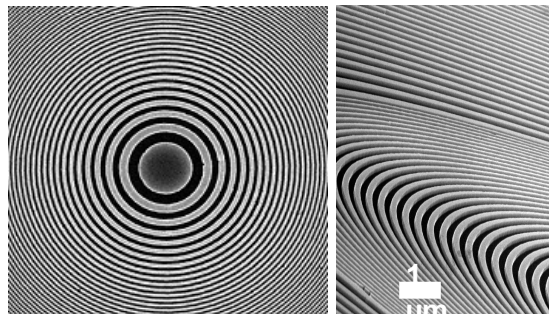
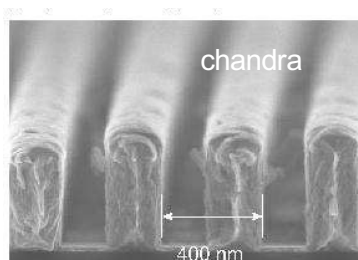
Majority of soft X-ray beamlines use reflection gratings

- High resolving power (100 000)
- Wide spectral range (one decade)
- Stability
- Efficient cooling of substrate
- Single crystal silicon



Alternatives

- Transmission gratings
- Zone plates
- Multilayer mirrors

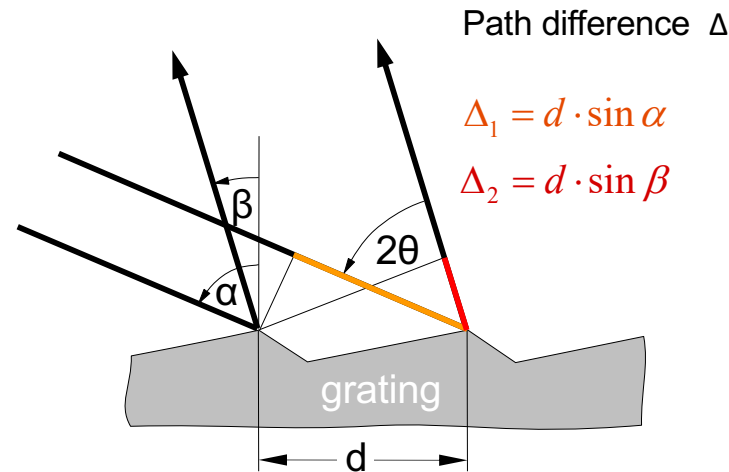


Courtesy BESSY II

Grating equation

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$N=1/d$: Line density
 α : incidence angle
 β : diffraction angle
 $2\theta=\alpha+\beta$: deflection angle



$$\Delta = \Delta_1 + \Delta_2 = d(\sin \alpha + \sin \beta)$$

Constructive Interference

$$\Delta = m \cdot \lambda$$

m : diffraction order (any integer)

Grating equation:

$$m\lambda = d(\sin \alpha + \sin \beta)$$

$$Nm\lambda = \sin \alpha + \sin \beta$$

$$Nm\lambda = 2 \cos \theta \sin(\theta + \beta)$$

From path function

Grating equation

$$F_{10}| = m \frac{\lambda}{d} - (\sin \alpha + \sin \beta) = 0$$

$$m \frac{\lambda}{d} = mN\lambda = \sin \alpha + \sin \beta \quad (\text{grating equation})$$

$$\frac{\partial \beta}{\partial \alpha} = -\frac{\cos \alpha}{\cos \beta} \equiv -\frac{1}{c} \quad (\text{angular magnification})$$

Meridional focus condition ($R=\infty$)

$$F_{20} = \frac{\cos^2 \alpha}{r} + \frac{\cos^2 \beta}{r_M'} = 0 \quad \Rightarrow \frac{r_M'}{r} = -\frac{\cos^2 \beta}{\cos^2 \alpha} = -c^2$$

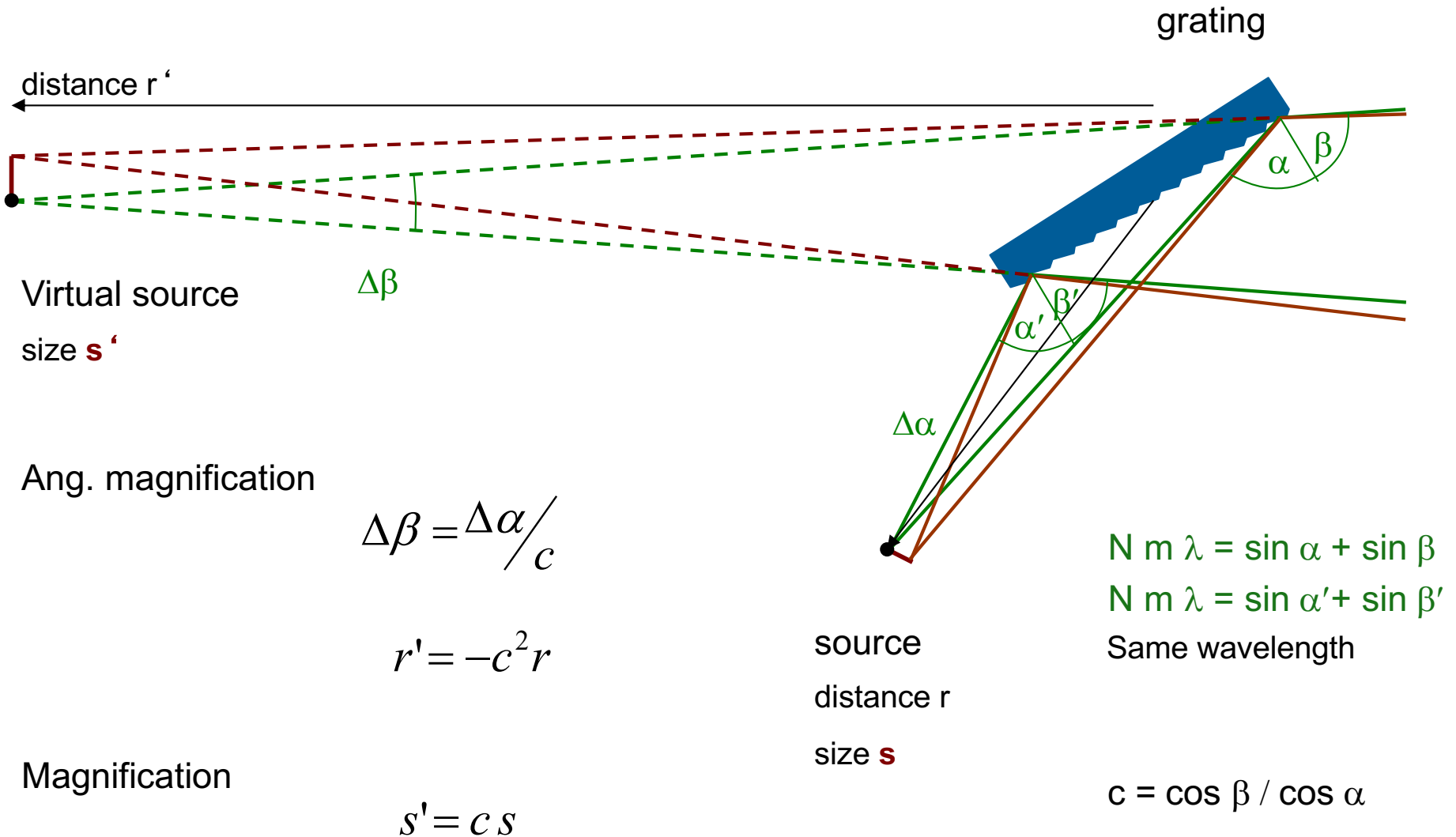
Sagittal focus condition ($R=\infty, a_{02}=0$)

$$F_{02} = \frac{1}{r} + \frac{1}{r_S'} = 0 \quad \Rightarrow r_S' = -r$$

Even plan gratings have focusing properties (Murphy 1956)

Grating equation and magnification

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The **grating equation** connects two free variables (α and β) to only one dependent, λ . This allows to fulfill an additional condition.

$$Nm\lambda = \sin \alpha + \sin \beta$$

Constant c-value $c = \cos \beta / \cos \alpha$:

$$\beta = -\arcsin\left(B + \sqrt{B^2 - 1}\right) \quad \text{with} \quad B = \frac{mN\lambda c}{1 - c^2}$$

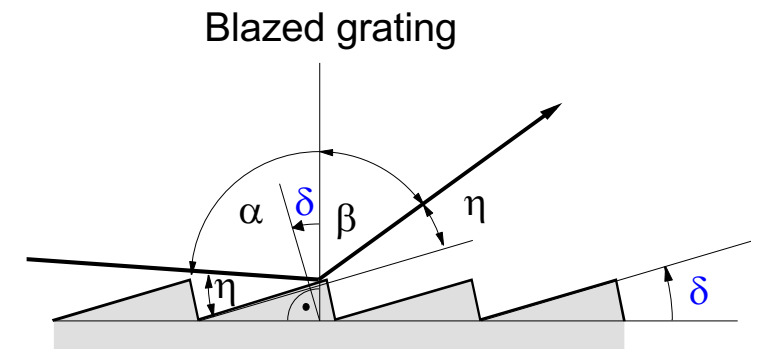
Fixed deviation $2\theta = \alpha - \beta$

$$\beta = \arcsin\left(\frac{mN\lambda}{\sin \theta}\right) - \theta$$

On blaze mode, $2\delta = \alpha + \beta$ is fixed ($\alpha - \delta = -\beta + \delta$)

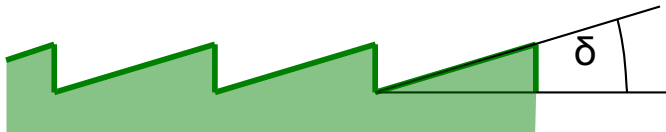
$$\beta = -\arccos\left(\frac{mN\lambda}{2 \sin \delta}\right) + \delta$$

Other focusing conditions (SGM, VLS-monochromators,...)

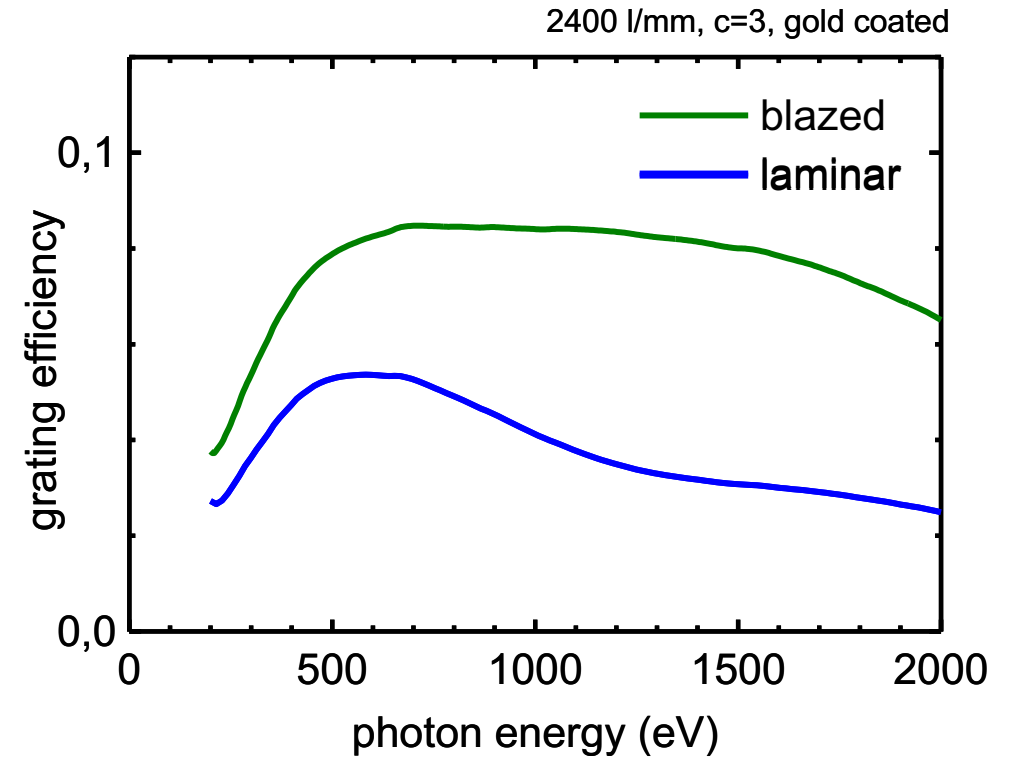
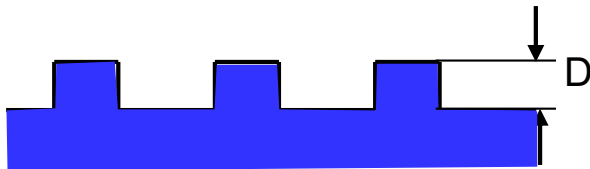


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blazed profile



Laminar profile



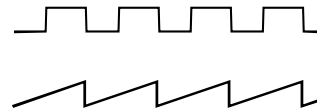
**Blazed profile with significantly higher grating efficiency
but only a few suppliers can make blazed gratings**

Guidelines for grating parameters

- Profile

Laminar : high spectral purity

Blaze : high flux



- Line density N (Energy range: In grating equation only dimensionless product $m \cdot N \cdot \lambda$)

High : High photon energies, high resolution (1200 - 2400 l/mm)

Low : high grating efficiency (150-300 l/mm)

- Diffraction order m

Inside : high demagnification, insensitive to source position variations

Outside : large acceptance

- Groove depth D and valley to groove width w , blaze angle δ

- $D = 5 - 40$ nm, $w = 0.5-0.7$, $\delta = 0.8^\circ - 4^\circ$

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Higher order light perturbs

- Reflectometry
- Determination of cross sections
- Non linear optics
- ...

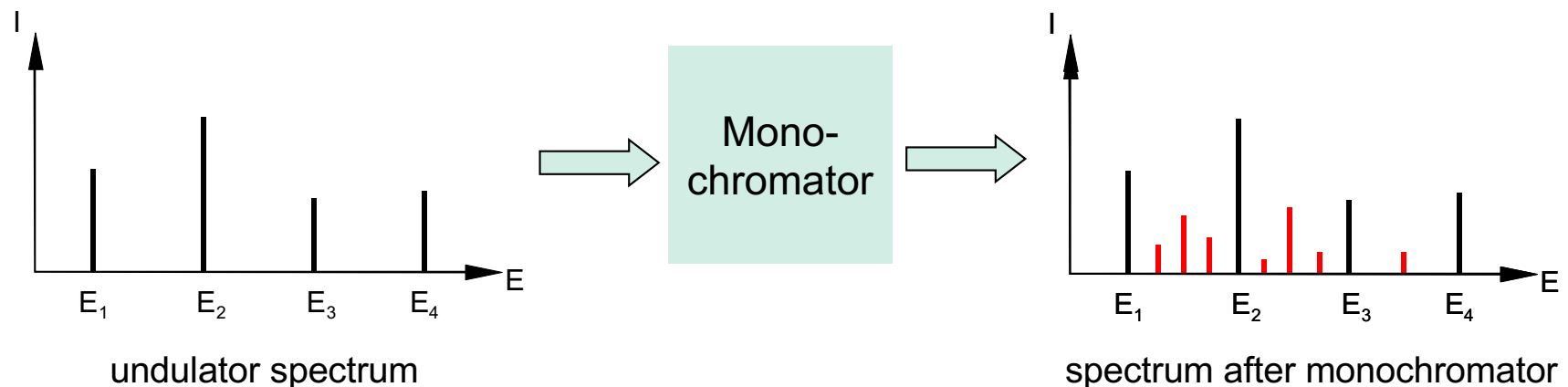
Determination of higher order

Quantitative:

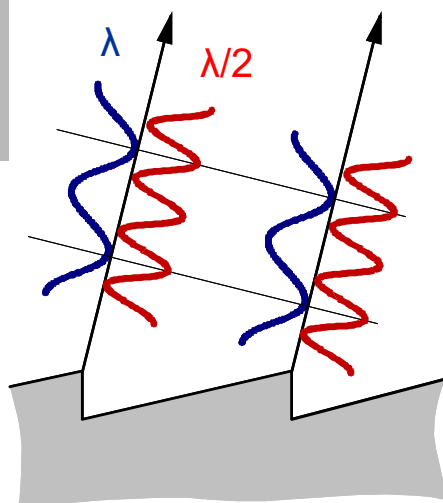
Secondary spectrometer for selected beamline energies

Qualitative :

Measure beamline output for fixed undulator gap



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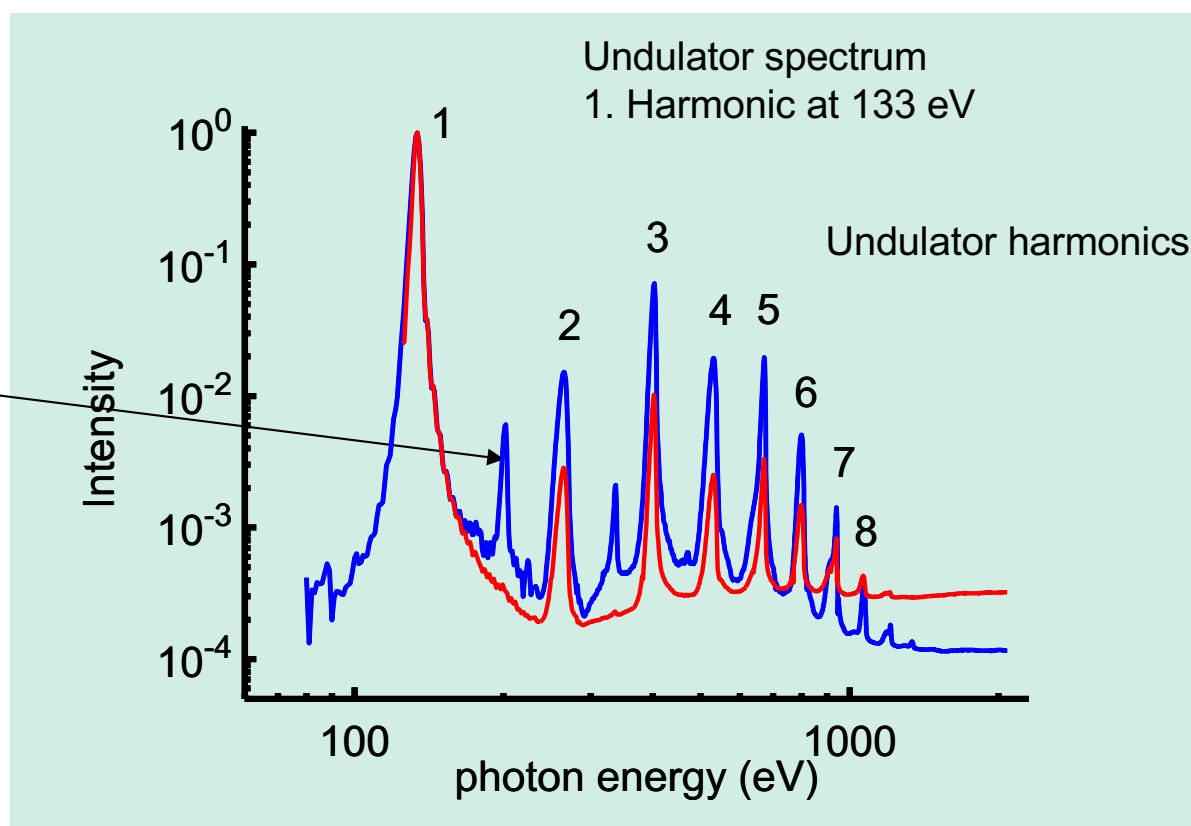
This is no 200 eV light
It is 400 eV!

Can be suppressed by
deflection angle or c-value
($c=2,25$ / $c=1.4$)

If wavelength λ shows constructive interference
then also $\lambda/2$, $\lambda/3$, ...

Although you tune the monochromator to a
specific photon energy, you probably get a
totally different one

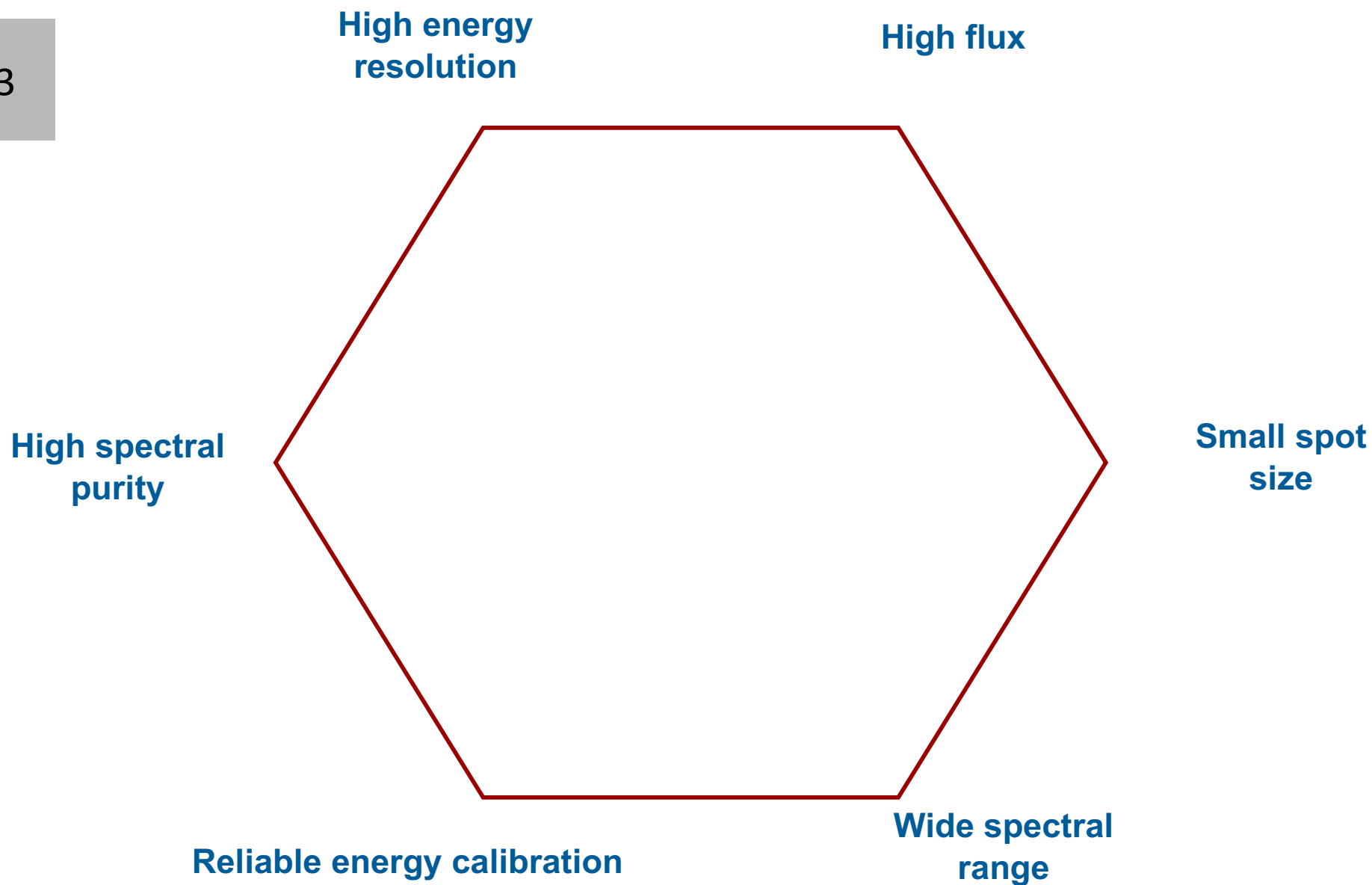
FALSE LIGHT



Grating Monochromators

Optimization goals

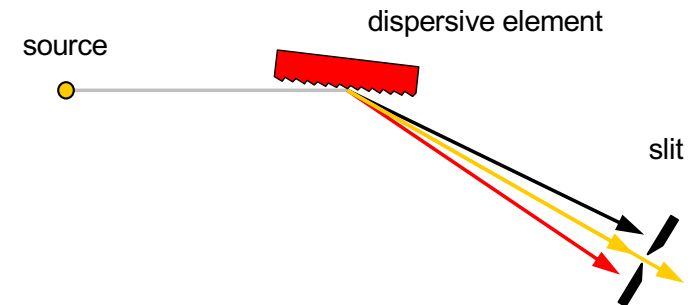
43



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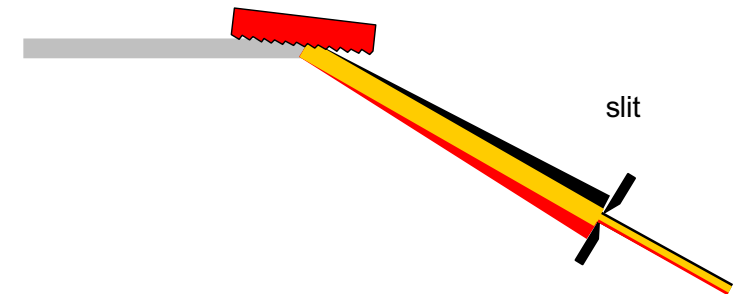
• Dispersive element

- Point source emits pencil of white light.
- Dispersive element separates wavelength.
- Slit selects one wavelength.



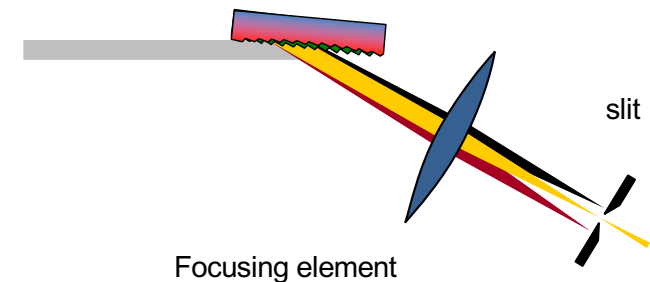
• Finite beam cross section

- Light of different colours transmit through the slit.



• Use focusing element

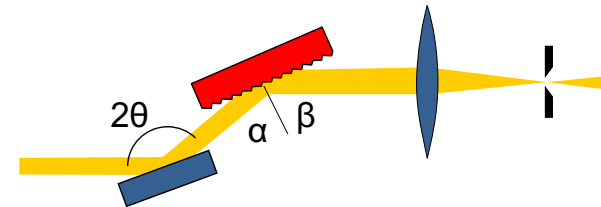
- Focusing element / slit select angular directions. Slit selects single wavelength.
- Focusing and dispersive element can be merged into one element.



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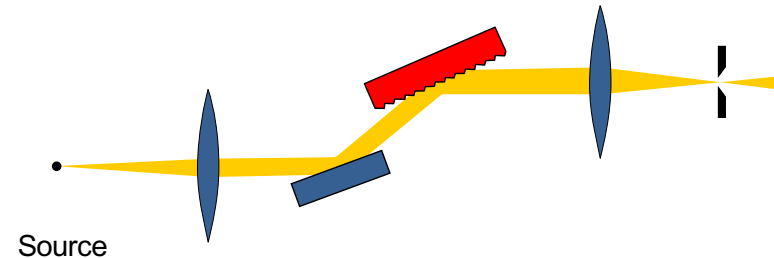
- **Additional plane mirror**

- Independent setting of α and β .



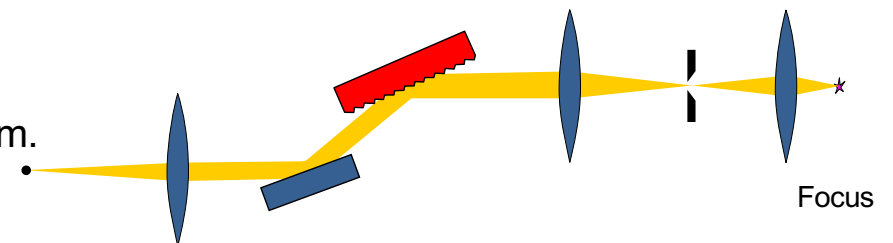
- **Source point is at finite distance**

- Preoptic matches source to the beamline.
- Collimates the light.



- **Experiment cannot be placed at the slit**

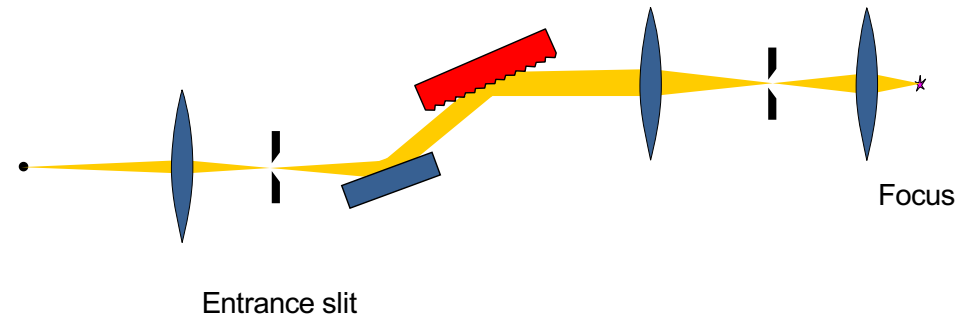
- Refocusing optics brings light to the experiment.
- Small spot $\approx 30 \mu\text{m}$ in a distance of 800 - 1500 mm.



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• Entrance slit

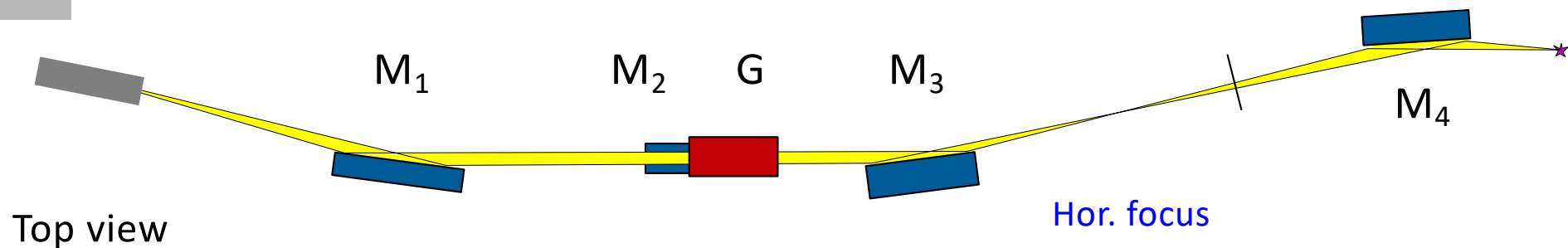
- Defines source point independent of the electron beam of the storage ring.



General guidelines

- Few optical surfaces.
- Reduce number of moving components.
- Horizontal beam trajectories facilitates alignment.

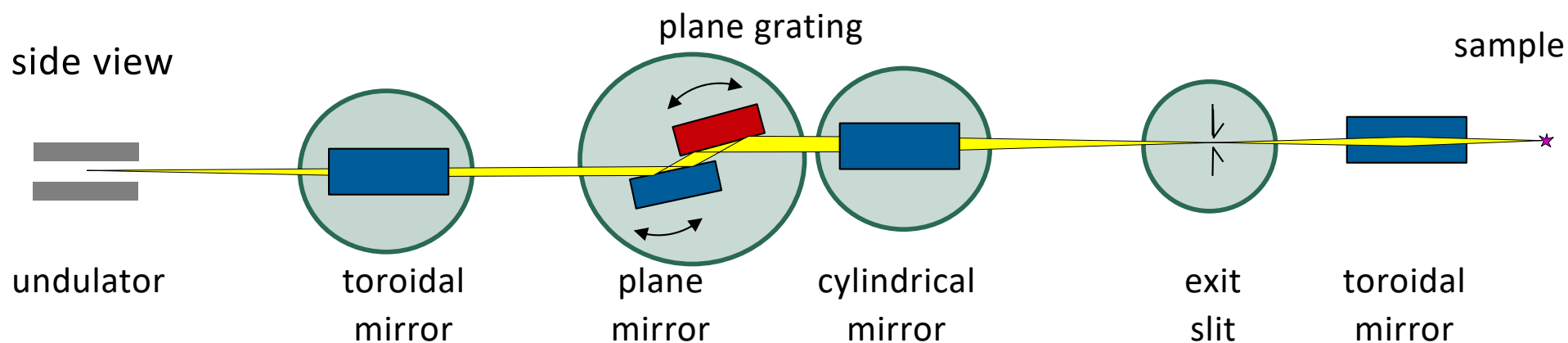
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Sagittal focusing

Variable magnification

Vertical dispersion



Typical length ~ 35 m

Undulator beamline at BESSY

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Pre optics

Grating chamber

Focusing chamber

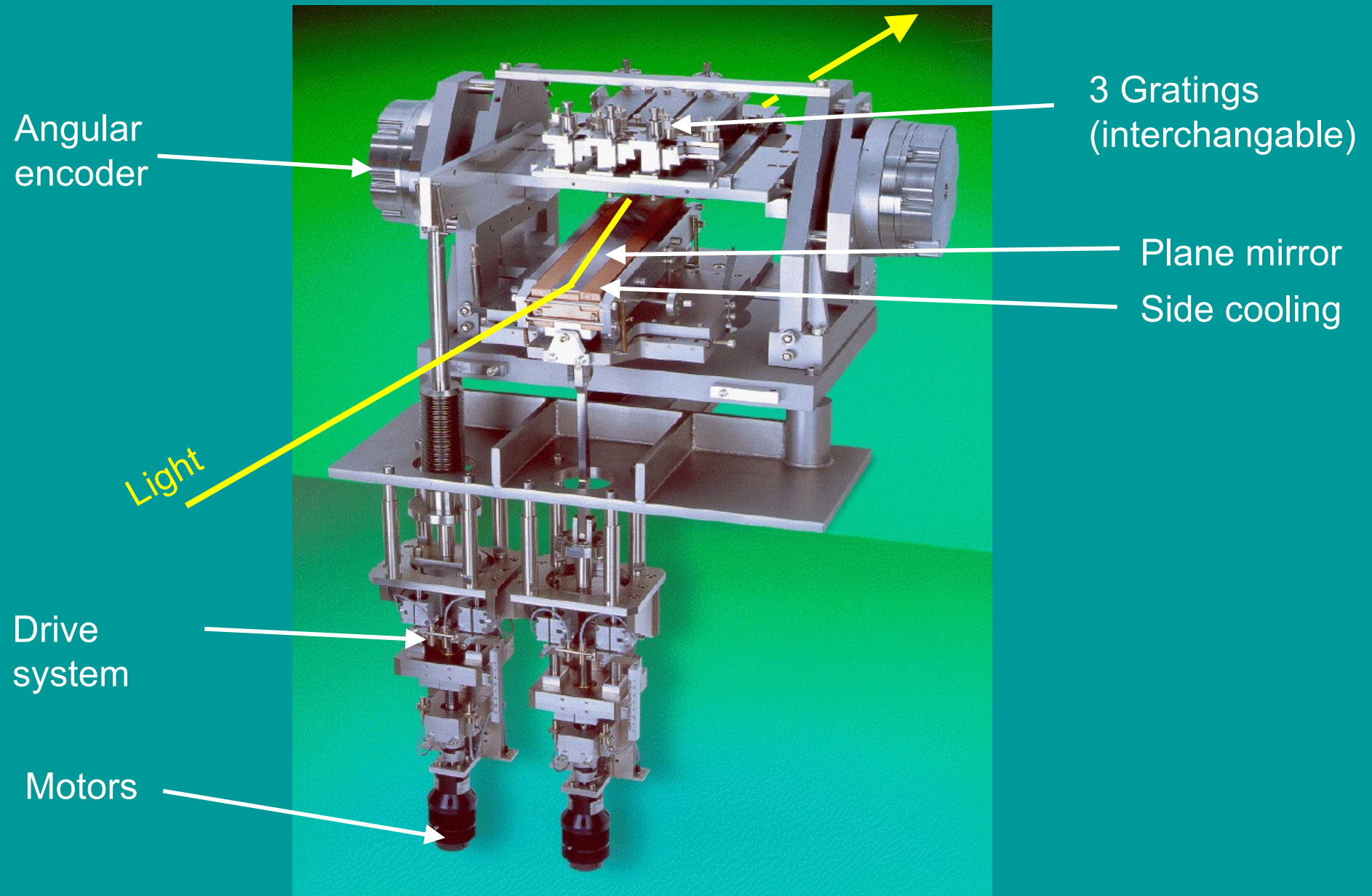
Exit slit

Beamline scientists

Polarimeter

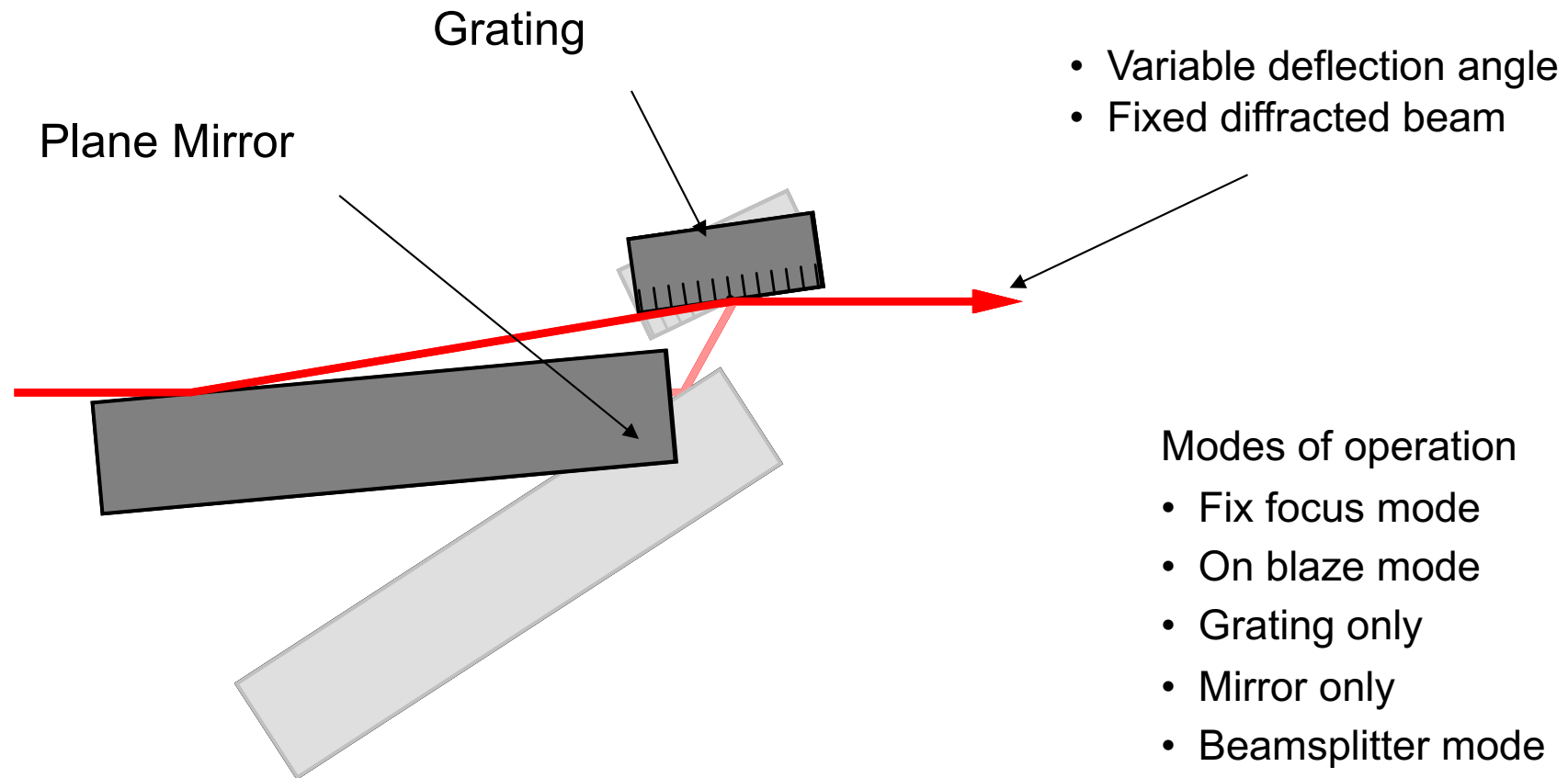
6/5/1999

Grating chamber mechanic



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SX700: First plane grating monochromator with tilting premirror

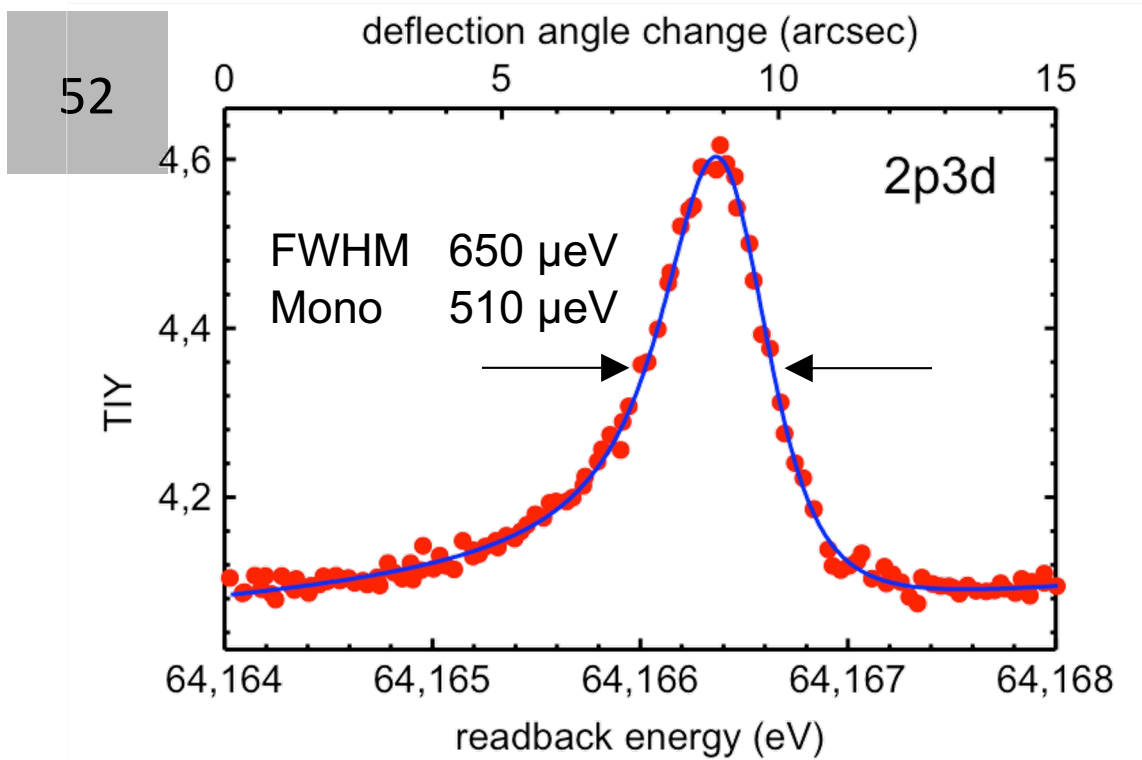


Incident (α) and diffraction angle (β) at the grating can be set independently

H. Petersen, Opt. Comm. **40**, 402 (1982)

F. Riemer & R.Torge, Nucl. Instr. and Meth. **208**, 313 (1984)

- Vertical dispersion plane set up by the grating
- Sagittal focusing: horizontally deflecting, vertically focusing
- Plane grating monochromator with variable deflection angle
- Illumination of grating with collimated light allows free choice of demagnification c
- Heat load effects on M_1 do not deteriorate the performance
- Typical length of 3rd generation beamlines up to 35 m
- Long exit arm for highest resolving power
- Use high c -value for high energy resolution, low c -value for high spectral purity



Helium

$$E/\Delta E \approx 125\,000$$

2007: Highest resolving power in EUV/ soft X-ray range

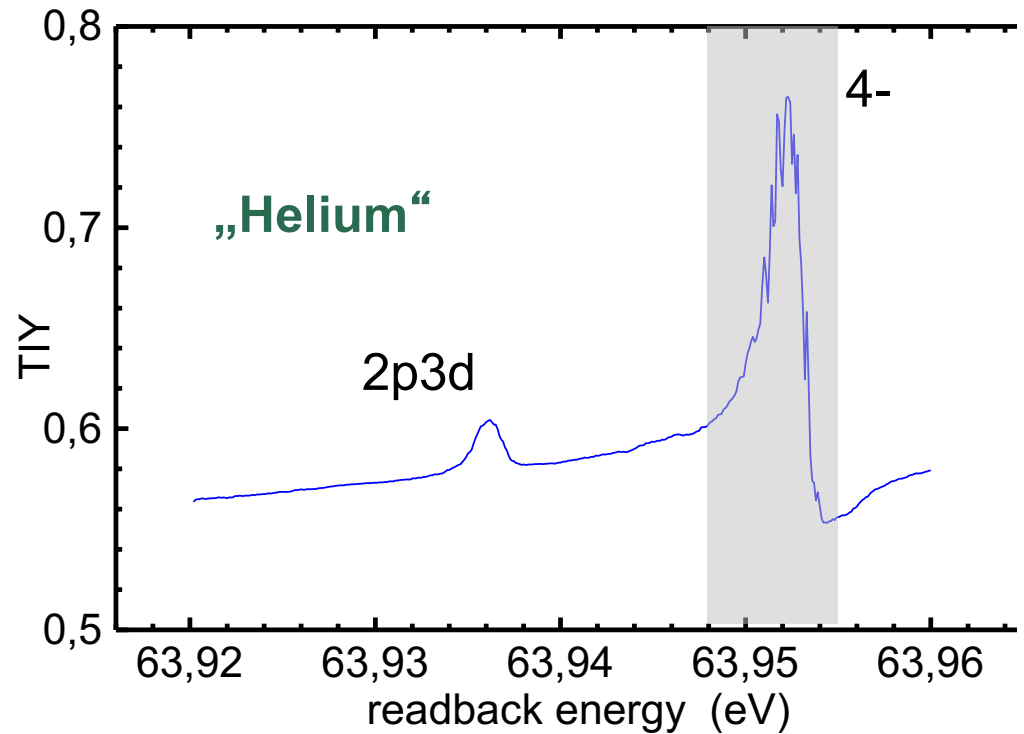
2400 l/mm $c=15$

What can go wrong?

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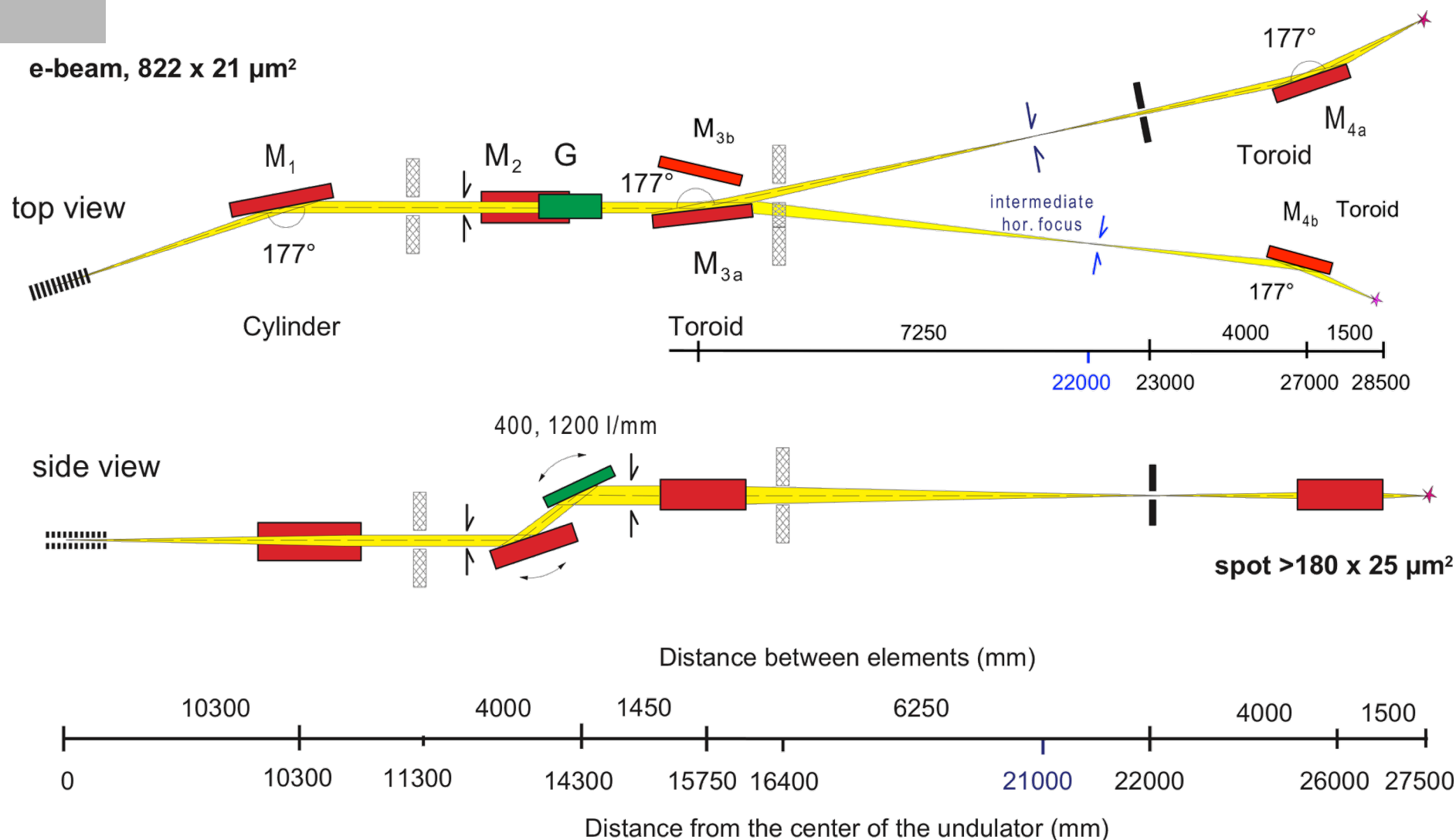
Crane moves over beamline



Ist not allowed to operate the crane during measurements

- Branch a in phase 1, branch b postponed

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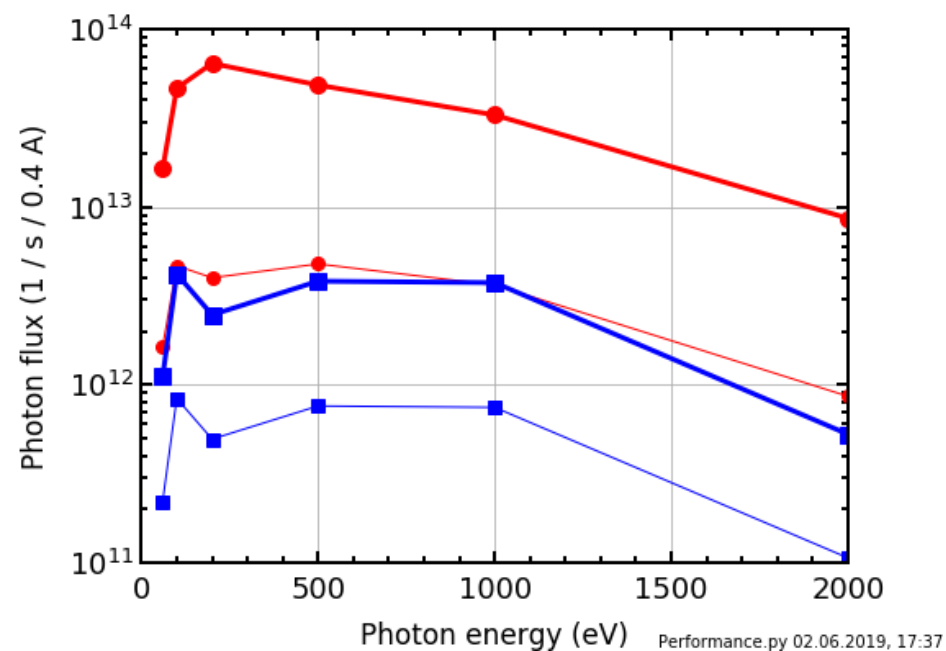
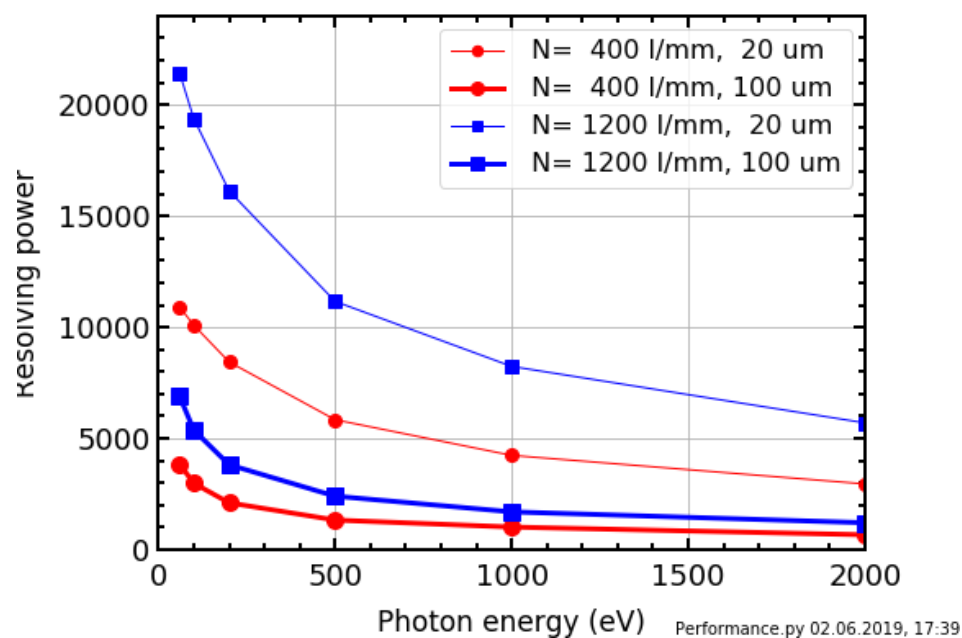


Photon Energy	unit	M1	M2	M3a	M3b	M4a/b	G-1	G-2
Shape		Cylindrical	Plane	Toroidal	Toroidal	Toroidal	Plane	Plane
Geometrical surface	mm ²	310 x 25	360 x 40*	310 x 40	310 x 40	410 x 50	100 x 20	100 x 20
Optical surface	mm ²	300 x 20	350 x 20	300 x 30	300	400 x 20	95 x 15	95 x 15
Slope error (m/s)	arcsec	0.5"/1"	0.1"	0.5"/1"	0.5"/1"	0.5"/1"	0.1"	0.1"
Source distance (m/s)	m	10.3	-	15.75 / ∞	15.75 / ∞	5 / 4	-	-
Image distance (m/s)	m	∞	-	5.25/6.25	6.25/7.25	1.5	-	-
Incidence angle		1.5°	1° - 8°	1.5°	1.5°	1.5°	1° - 13°	1° - 13°
Radius	mm	ρ=539	∞	ρ=327 R=300800	ρ=380 R=341900	ρ=57 R= 88150		
Line density	1/mm						400	1200
Blaze angle							0.8°±0.1°	1.4°±0.1°

* M2 width 30 mm in Specification

- Branch a

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- Refurbished undulator from BESSY II

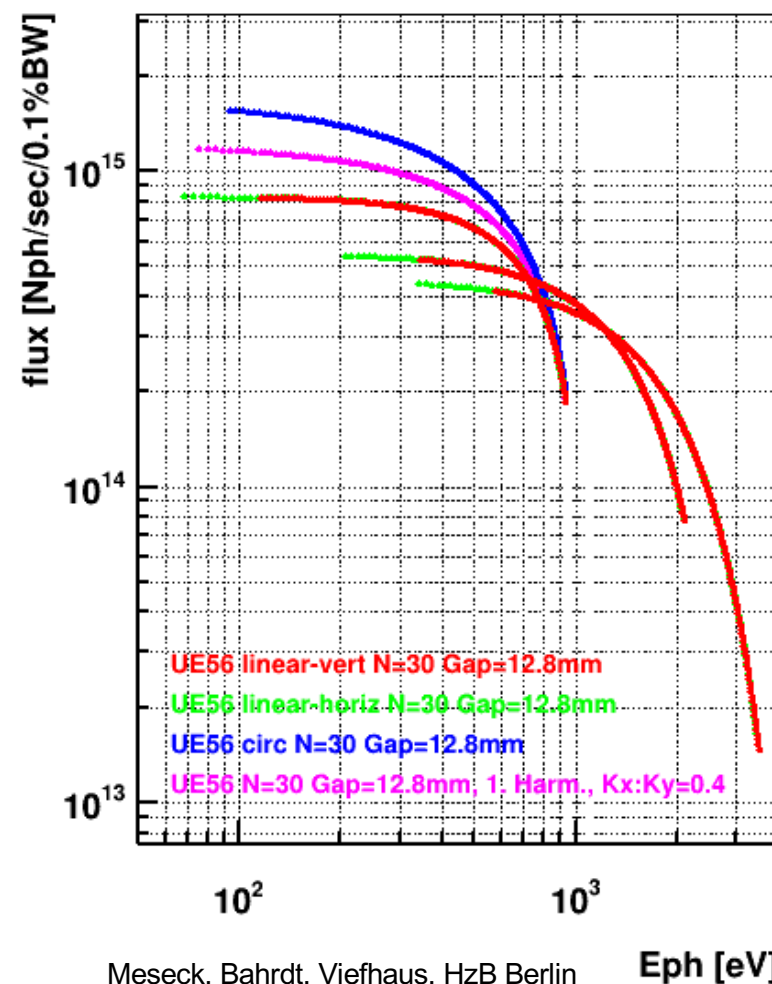
		UE 56
Periodlength	(mm)	56
Periods		30
1. Harmonic	(eV)	70 - 350
$k_{\max}$		5.3 - 2.0
P	(kW)	2.7 - 0.4

Sesame: $E_e = 2.5$ GeV, $I = 400$ mA

BESSY II: $E_e = 1.7$ GeV, $I = 400$ mA

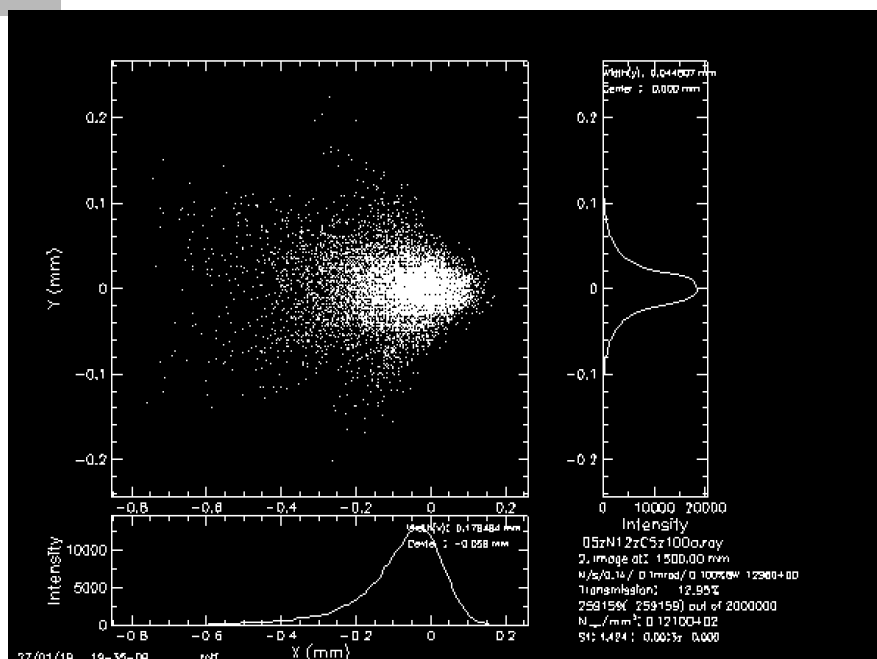
$K_{\max} = 5.3$ (3.7)
 $P = 2700$ W (600 W)
 $p = 5100$ W/mrad² (765 W/mrad²)

Flux, 2.5 GeV, 400 mA

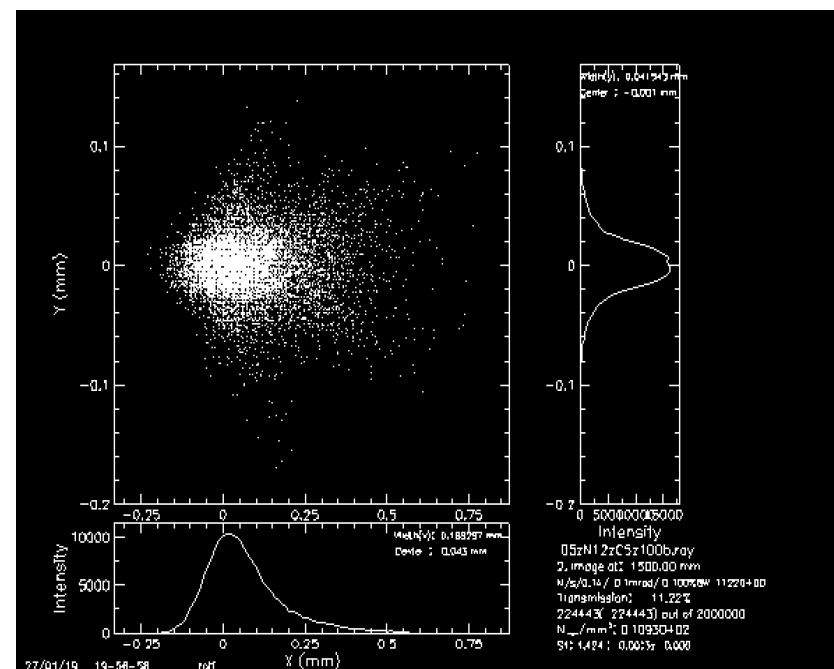


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Branch **a**, 100 μm exit slit 100 eV



Branch **b**, 100 μm exit slit 100 eV



Depending on exit slit size (20 – 100 μm and photon energy 100 eV – 2000 eV

Spotsize

Hor: 120 – 180 μm

Vert: 10 – 50 μm

Spotsize

Hor: 140 – 200 μm

Vert: 10 – 50 μm

- J.A. Samson, D.L. Ederer : Vacuum ultraviolet spectroscopy, Academic press (2000)
- D. Attwood : Soft x-rays and extreme ultraviolet radiation, Cambridge university press (1999)
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Wir schaffen Wissen – heute für morgen



Thank you for your attention