Rolf Follath:: SwissFEL Photonics :: Paul Scherrer Institut

Beamlines Design for Synchrotron Radiation

HESEB Soft X-ray Lecture & Training Course
8.5.2023

Properties of synchrotron radiation

SESAME, 2.5 GeV

133 m circumference

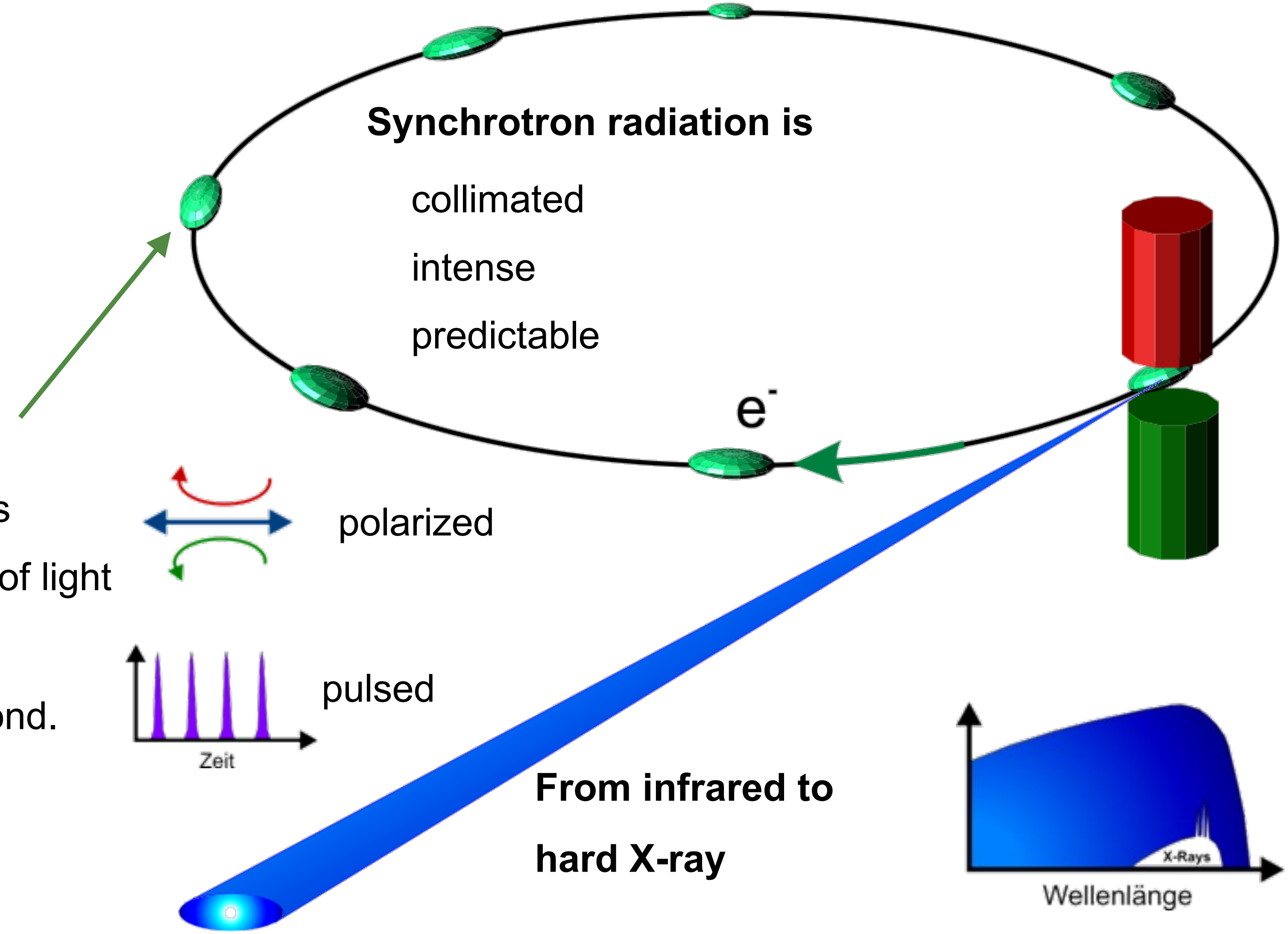
222 buckets

200 electron bunches

Stroboscopic flashes of light

50 ps flashes

500 000 000 per second.



Courtesy BESSY II

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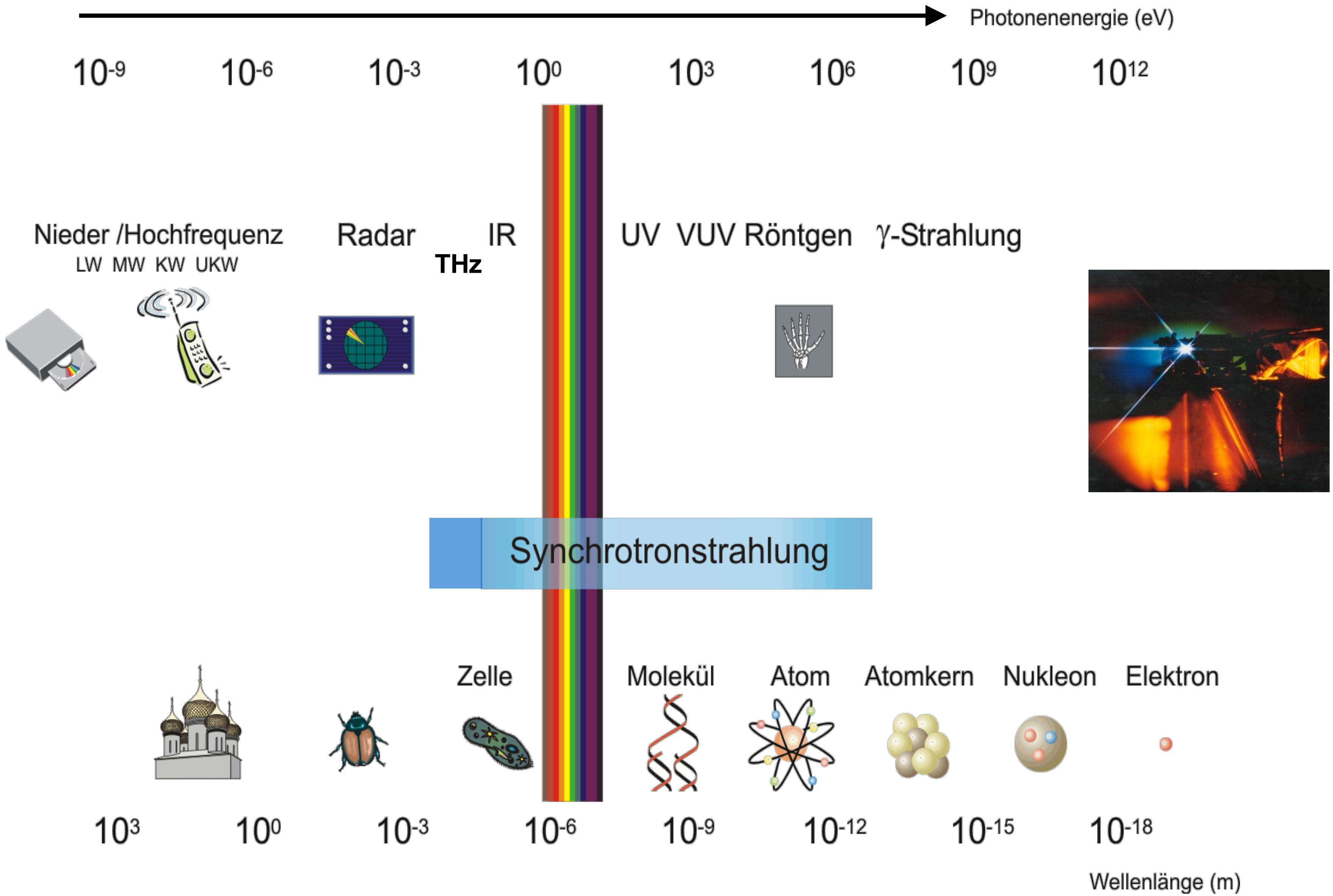
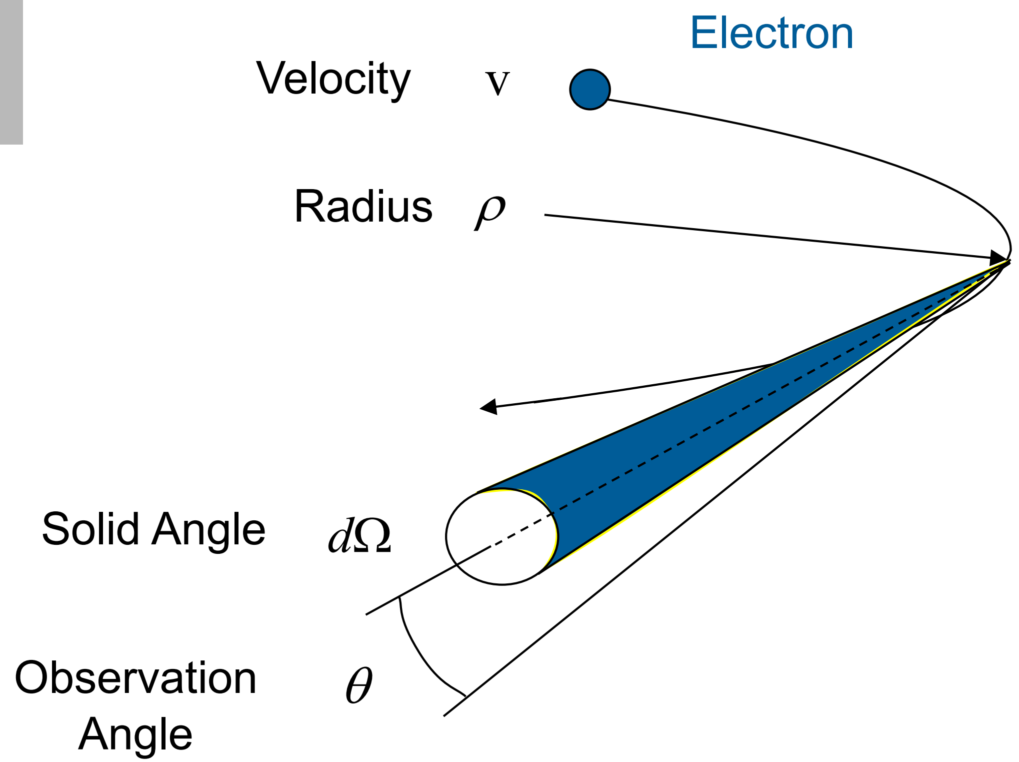
Wavelength of synchrotron radiation



Courtesy BESSY II

Predictability of synchrotron radiation



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

ω : frequency

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

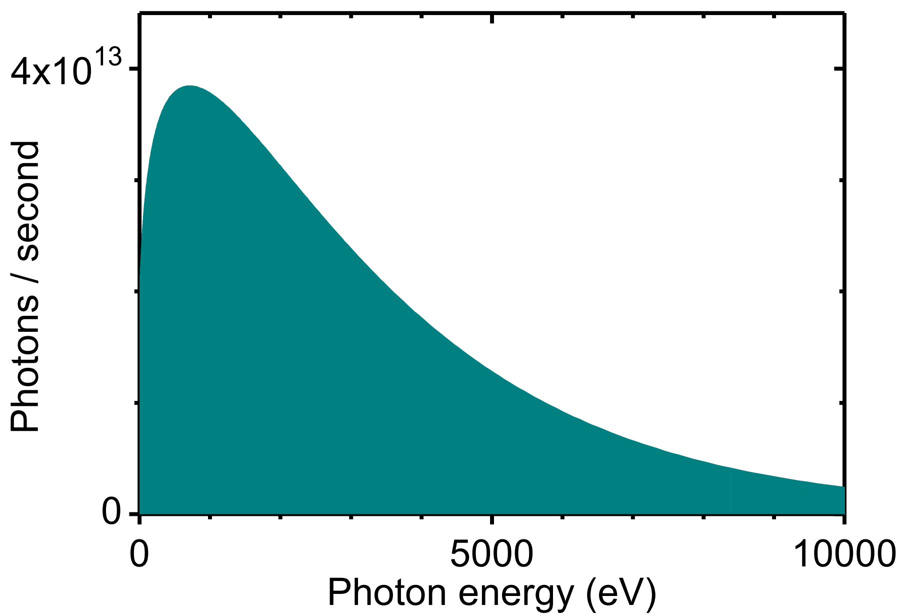
K : mod. Bessel functions

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

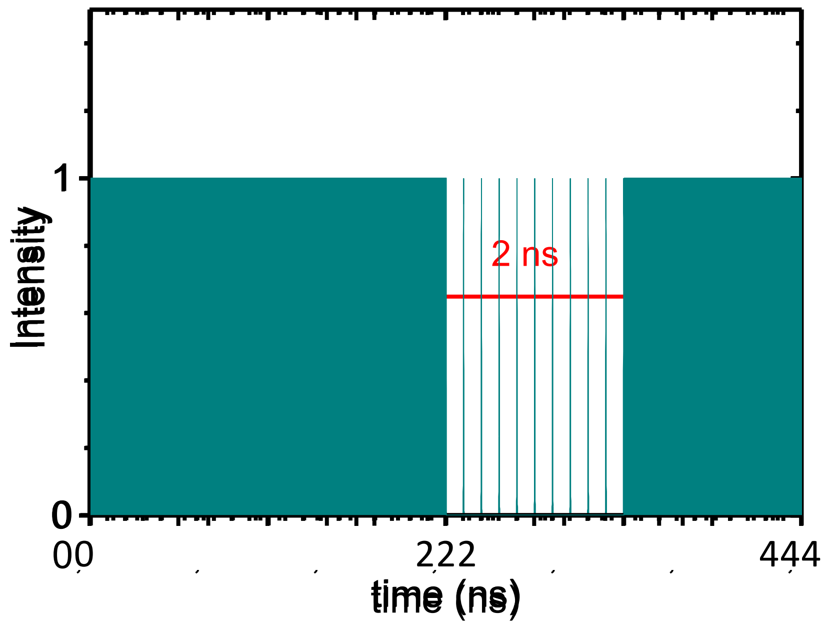
Exactly predictable -> Used as radiation standard in national metrology labs

Dipol radiation

spectrum



Time domain

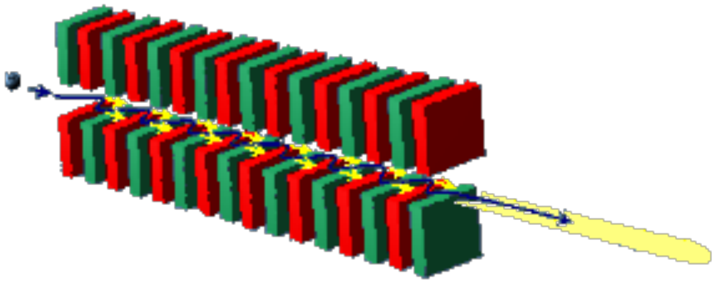


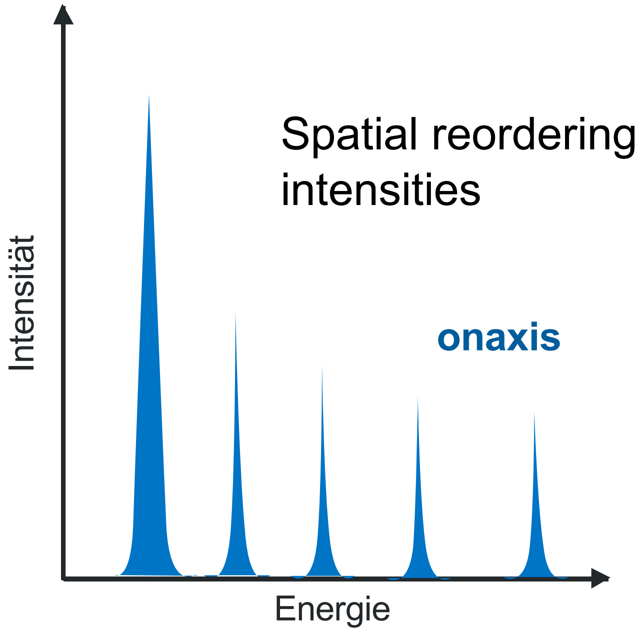
1 revolution
(gap to increase live time)

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

Undulators

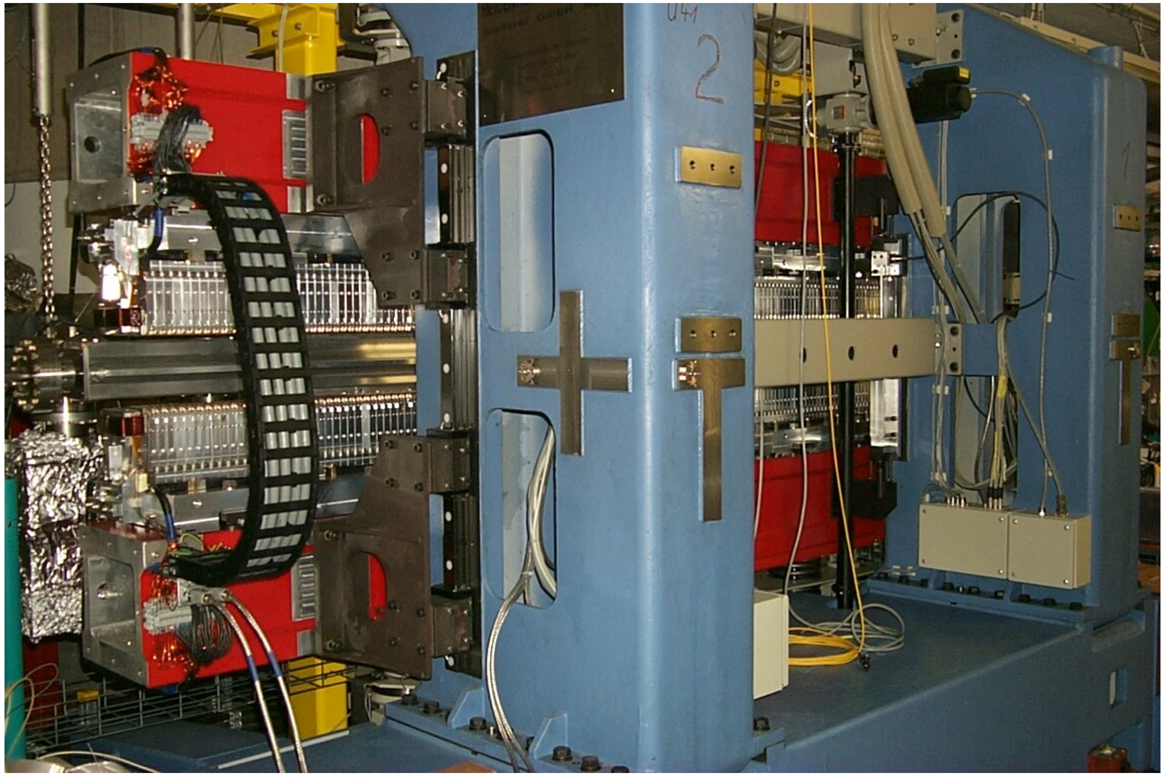
Magnetic array





Spatial reordering of intensities

onaxis



Typical values

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

Courtesy BESSY II

Undulator equation

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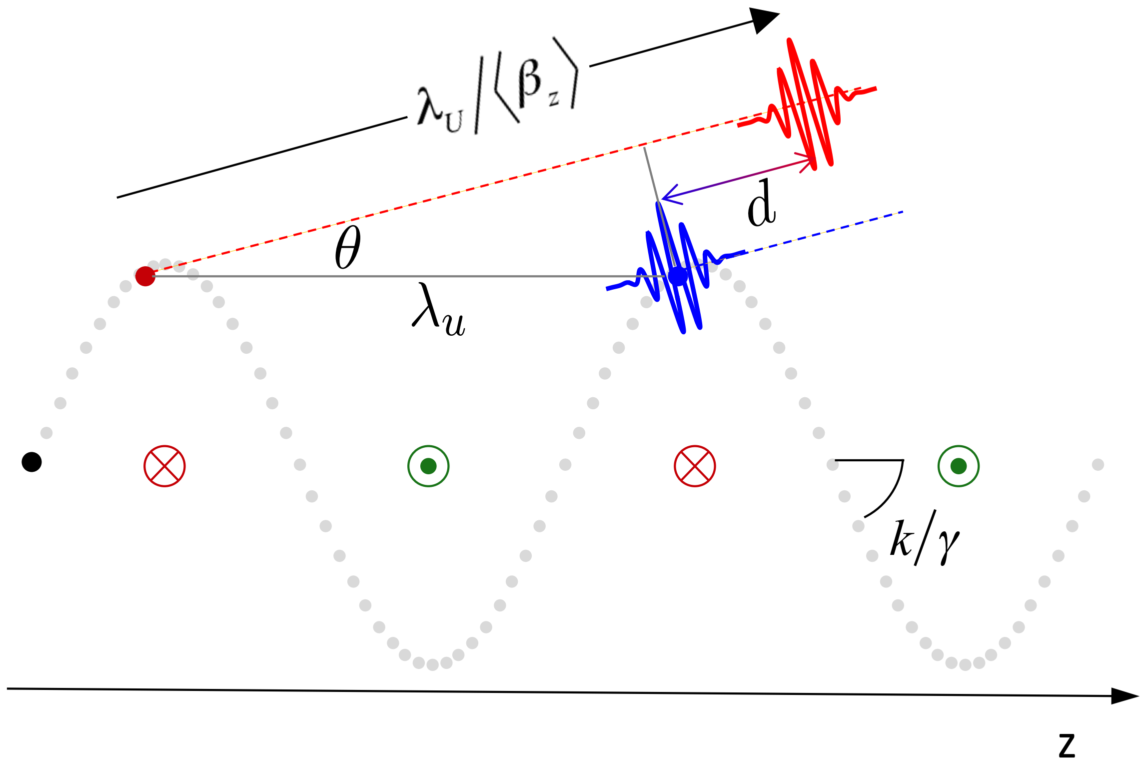
Sinusoidal magnetic field, amplitude B_0, periodicity λ_U
Electron with speed $\boldsymbol{v}=(v_x,v_z)$,
Mean speed $<v_z>$

Looking from above onto the magnetic field



Time for electron to proceed from red to blue position

$T = \lambda_U / <v_z>$

Light travels distance

$c\,T = c\,\lambda_U/<v_z> = \lambda_U/<\beta_z>$

Path difference between flashes

d

$$<\beta_z> \approx 1 - \frac{1}{2\gamma^2} - \frac{K^2}{2\beta\gamma^2}$$

Constructive interference for light with wavelength λ

Resonance-condition

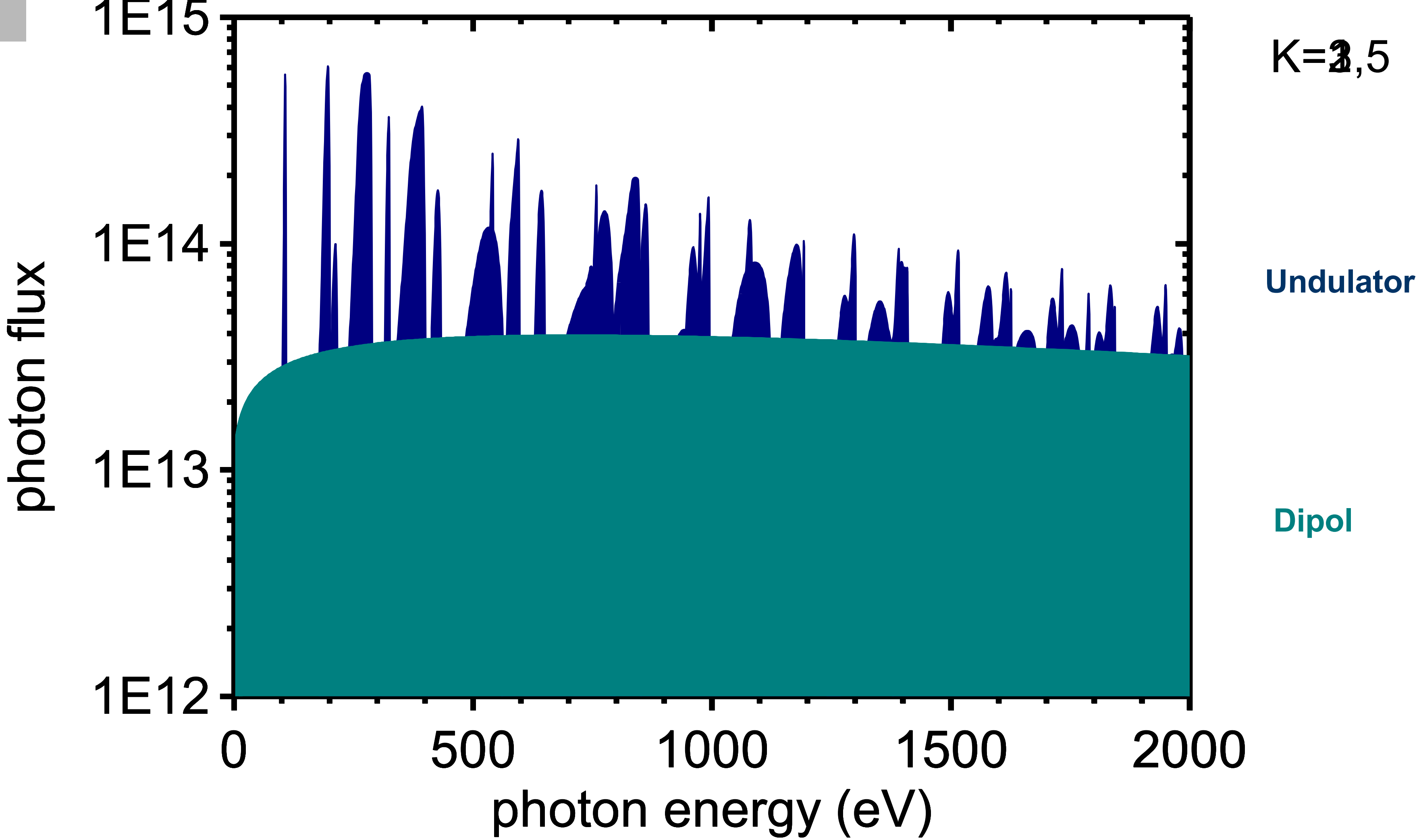
$$\lambda = \frac{\lambda_U}{2n\gamma^2}\left(1+\tfrac{1}{2}K^2+\theta^2\gamma^2\right)$$

Undulator-Parameter K

$$K = \frac{B_0 e}{mc}\frac{\lambda_U}{2\pi}$$

Courtesy Marco Calvi, PSI

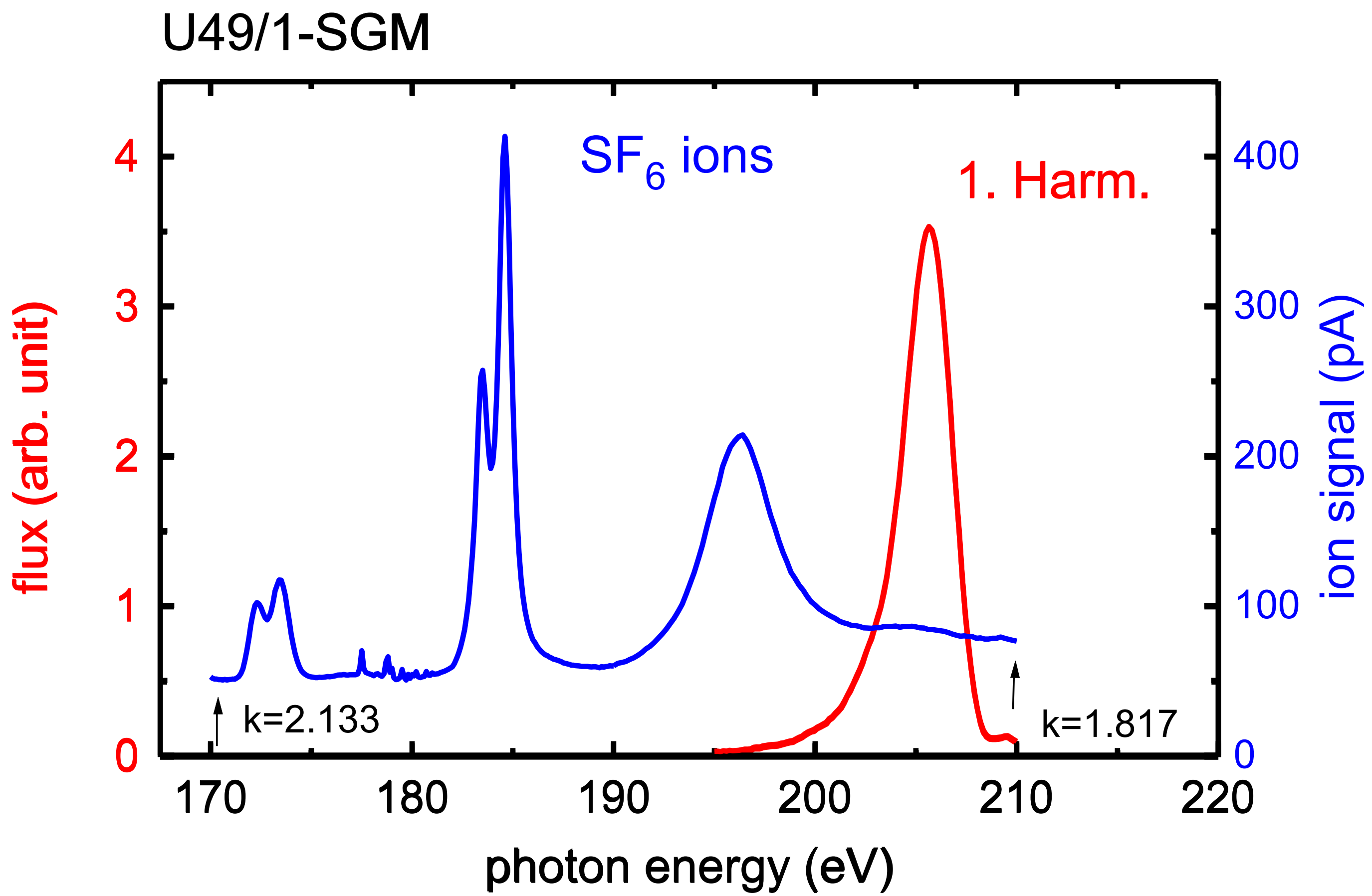
Undulators



Scan k-value to extend the photon energy range.

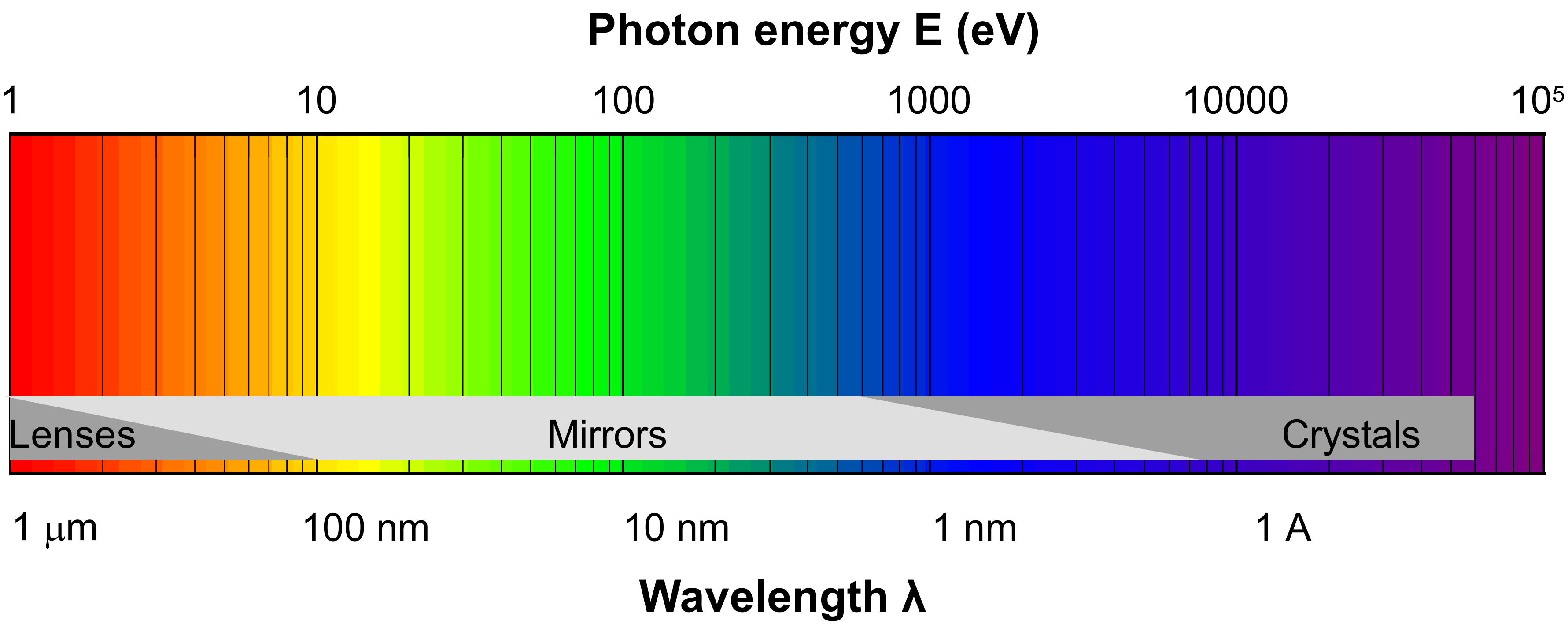
Undulator harmonic

Photoabsorption of SF_6 gas



- Undulatorharmonic too broad for spectral features, need for monochromator.
- But too small to cover complete spectrum simultaneos scanning of ID and mono

Spectral range at Synchrotrons



Normal incidence monos

Grazing Incidence monos

Crystal monochromators

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

Reflectance

Matter is almost opaque for soft X-ray radiation

Spectral range of interest

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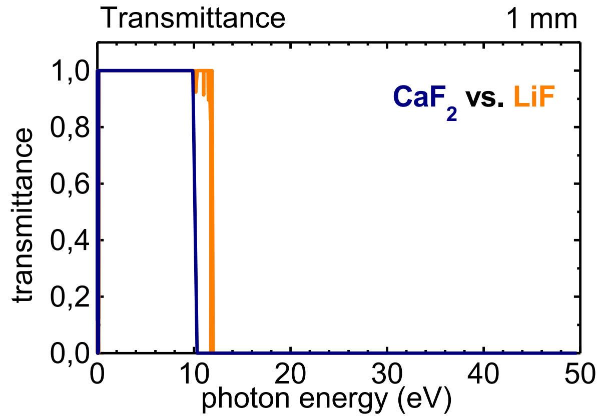
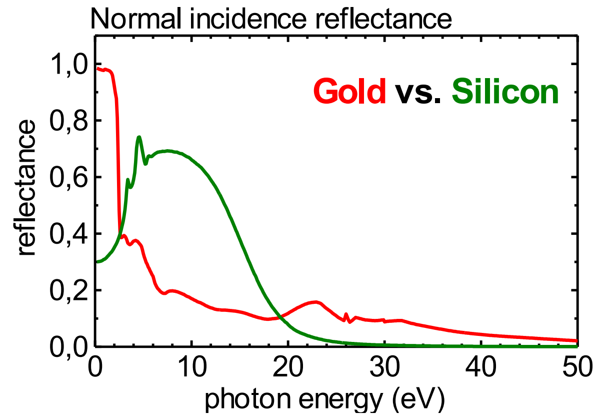
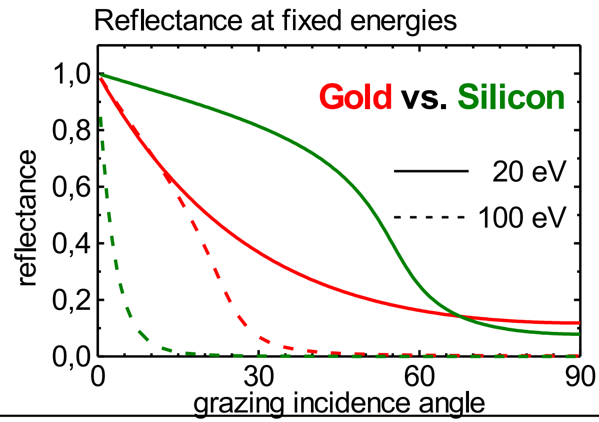
Photon energy

- **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



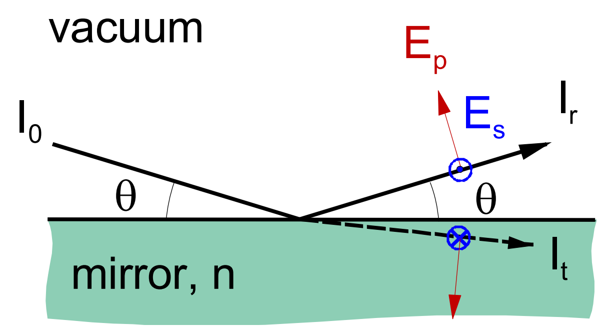




Reflectance

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



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

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 $n = n + ik$

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

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

V_A : Atomic volume = 1 / n_A

r_e : classical electron radius (2.82×10^{-15} m)

f_1, f_2 : atomic scattering factors

$\left(f_1, f_2\right)$ in the Henke tables $\left(n, k\right)$ in the book of Palik

Reflectance

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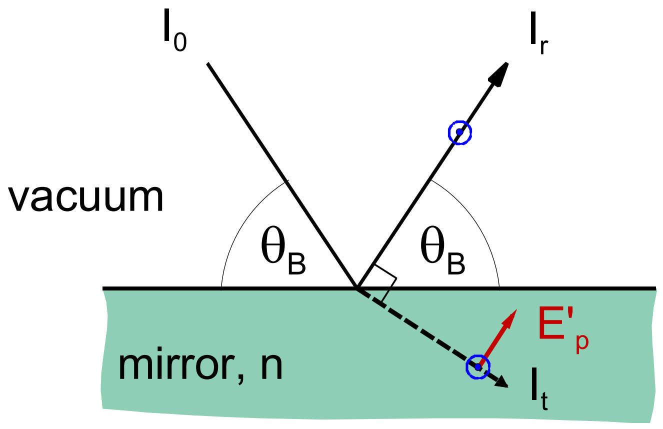
Brewster angle

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

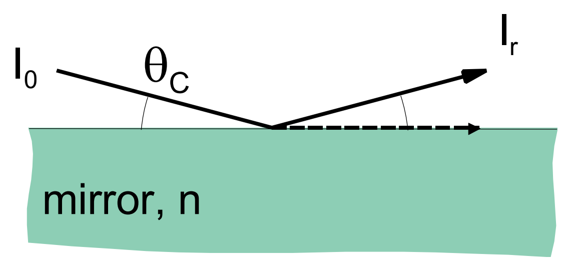


The electrons oscillate always along an axis parallel to the electric field of the transmitted light.

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



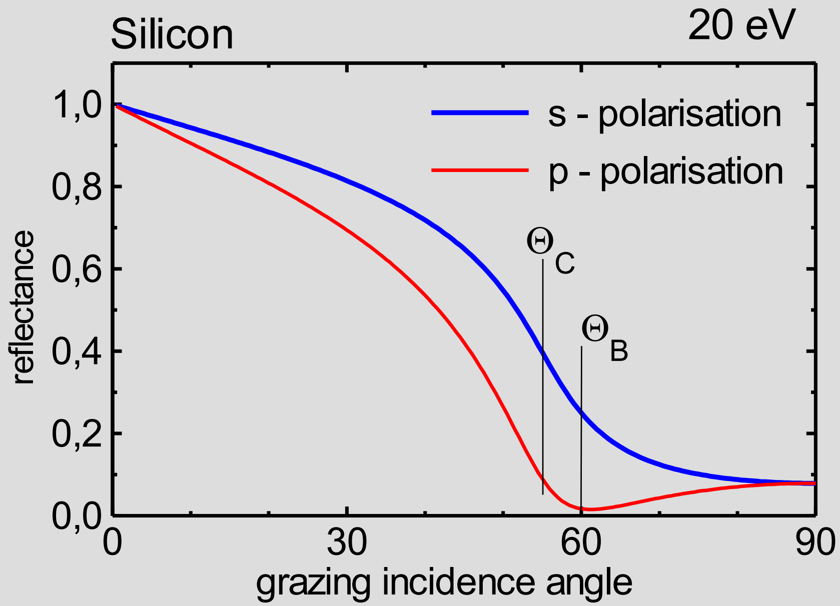
If the light comes from the optical denser side of the boundary surface, total reflection can occur (e.g. from under water to air).
In the soft x-ray regime **vacuum is optical denser** than matter. Total reflection occurs when the angle of the transmitted light equals zero.

$$\Theta_C = \arccos n$$

Reflectance

Example 1

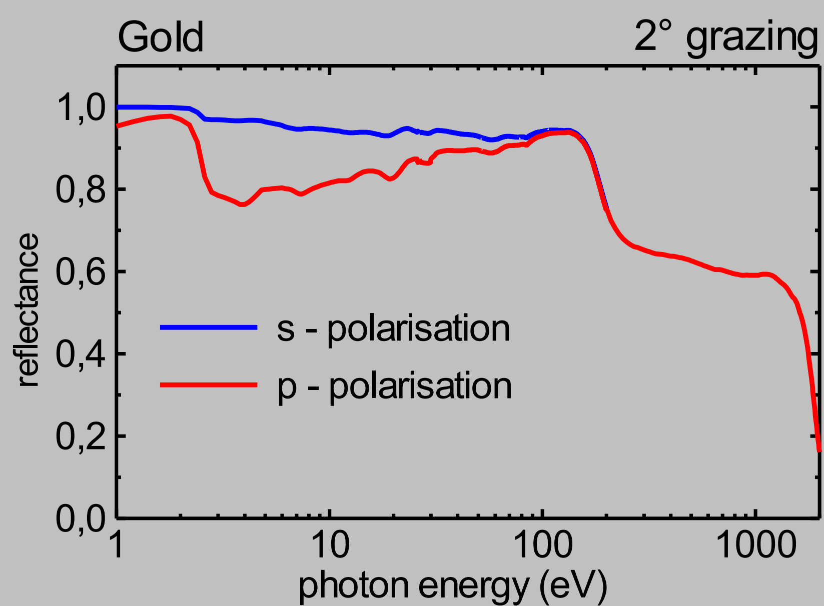
- silicon at 20 eV
- n = 0.567, k = 0.0835
- critical angle θ_C = 55°
- Brewster angle θ_B = 60°



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

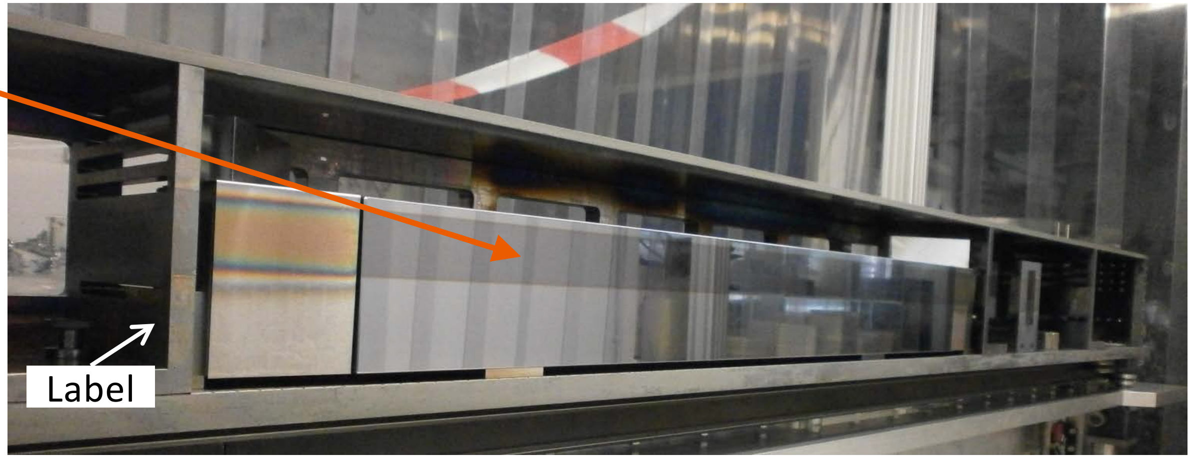
Mirrors

Offset Mirror of SwissFEL

First stripe: SiC + top B_4C

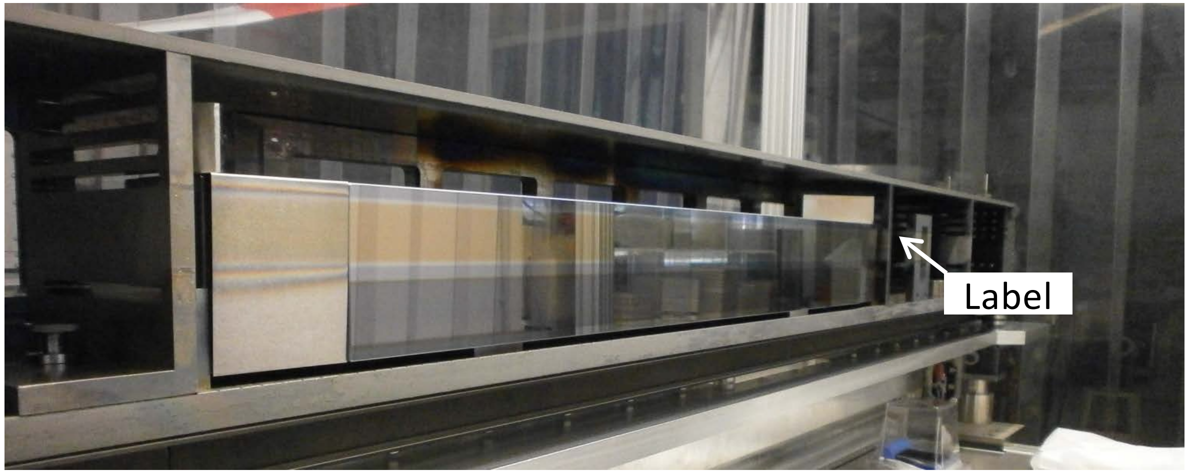
End of June 2016
Run ID T664

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



Second stripe: Mo + top B_4C

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

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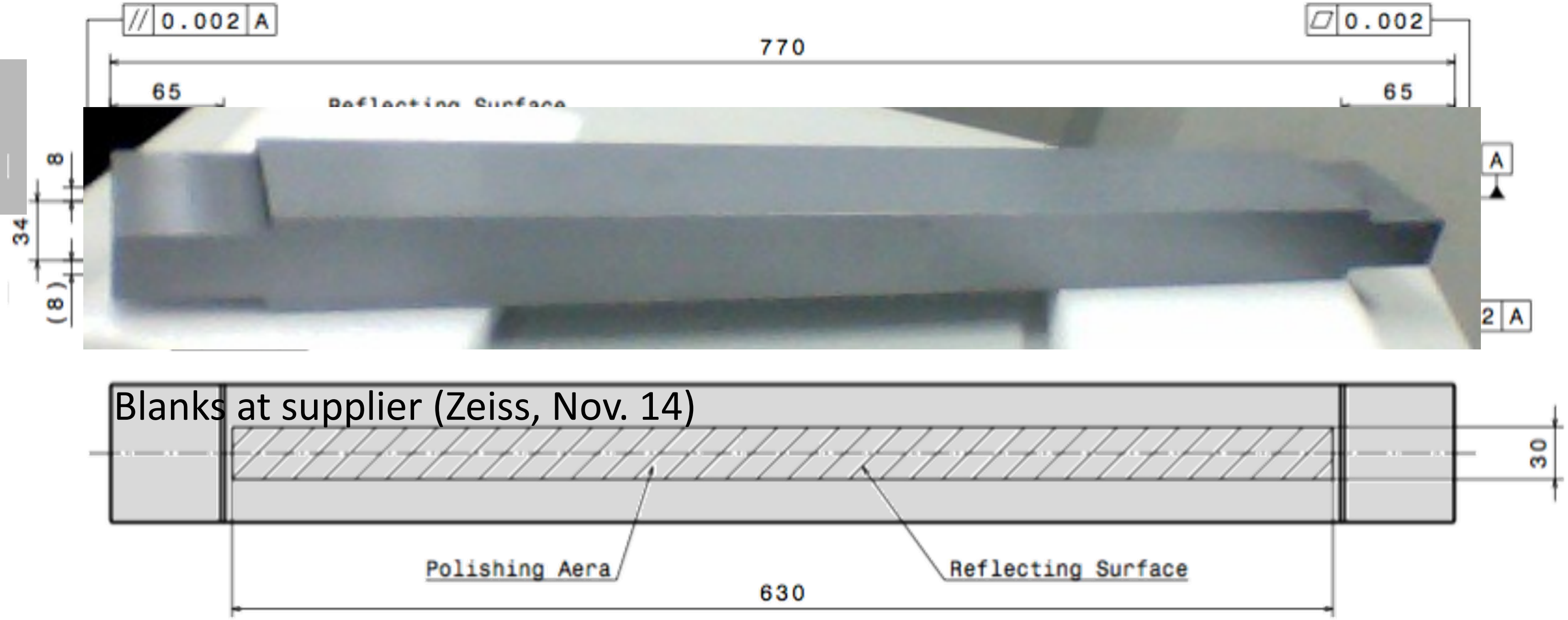
Offset Mirror specification



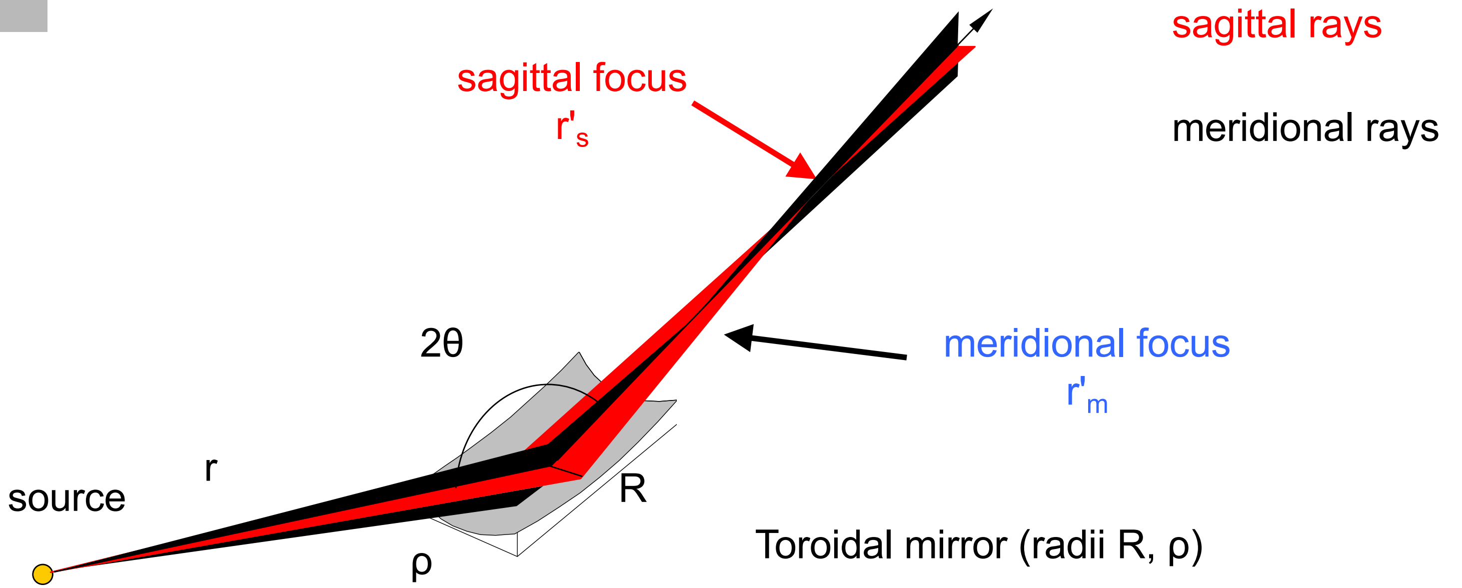
Blanks at supplier (Zeiss, Nov. 14)

- Bulk : Si (100)
- Height error : < 0.6 nm rms
  : < 3 nm PV
- Microroughness : < 0.2 nm rms
- Dimensions : 770 x 80 x 50 (80) mm^3
- Optical surface : 630 x 30 mm^2
- Coatings : SiC/B_4C, Si , Mo/B_4C

- Ordered : Jul. 2014, Zeiss and JTEC
- Delivery : Jul. 2015
- Coating : Start Aug. 2016 (HZ Geesthacht)

Focusing with mirrors

We must use grazing incidence to enhance reflectance.

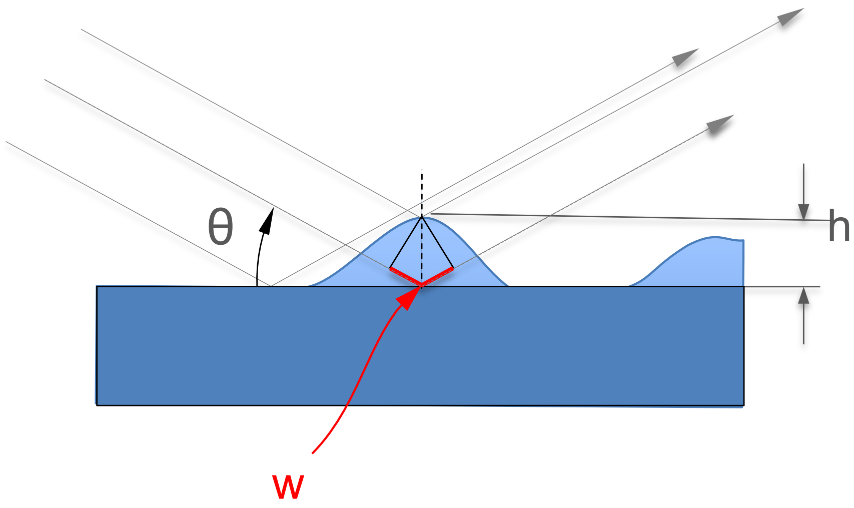


$$\frac{1}{r}+\frac{1}{r_S'}=\frac{2\cos\theta}{\rho}$$ sagittal focus

„Astigmatic image" because focii do not coincide

„Stigmatic image" match parameters R, ρ

What means ideal optics (1)

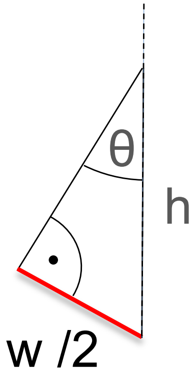


Path difference **w**

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

Phase error φ

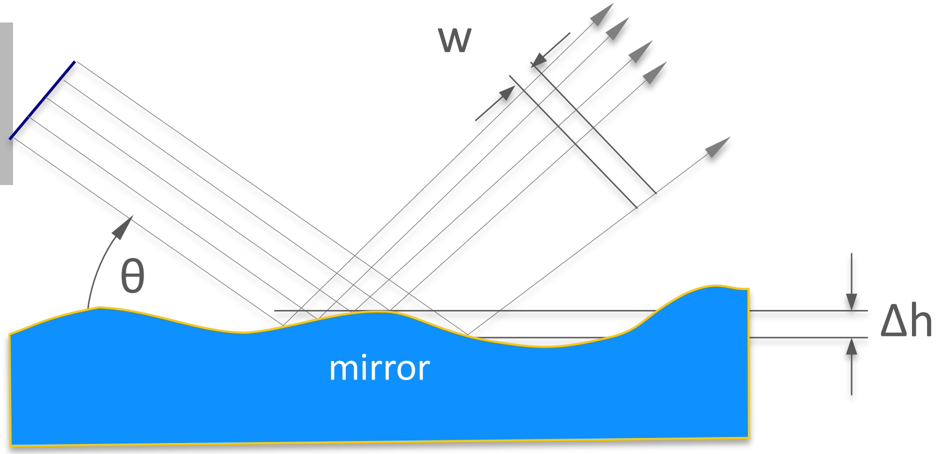
$$\varphi = 2\pi \cdot \frac{2h\sin\theta}{\lambda}$$



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

- Abberations reduce with smaller incidence angle
- Abberations stay constant when sinθ / λ = constant

What means ideal optics (2)



Height error Δh-> 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:

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

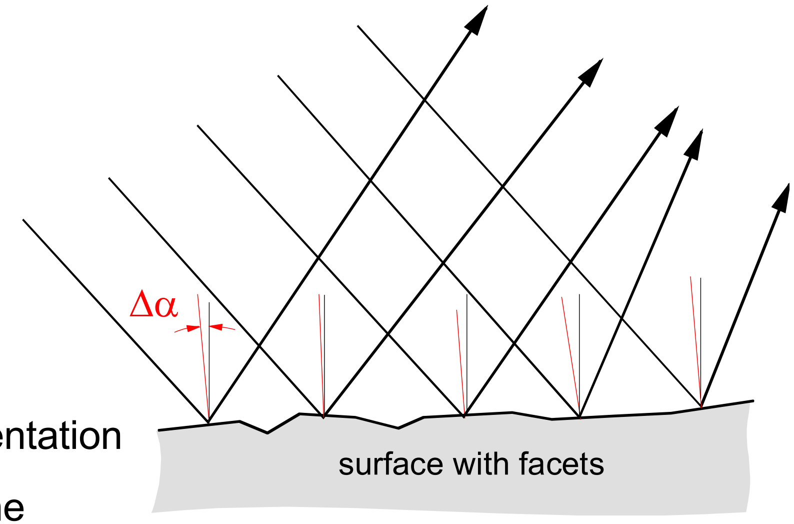
N=4, θ= 0.75° (13 mrad)

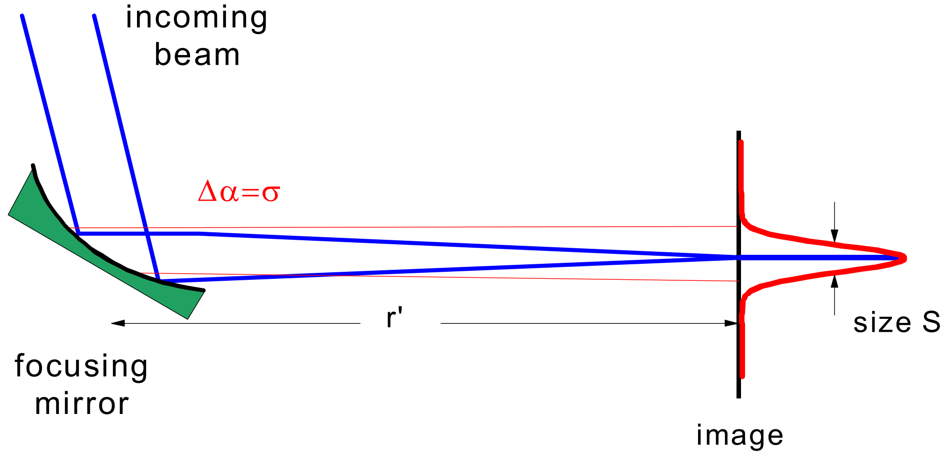
1800 eV (0.7nm) → σ_{rms} = 1 nm
600 eV (2 nm) → σ_{rms} = 2.7 nm
250 eV (5 nm) → σ_{rms} = 6.8 nm

Strongly curved (ρ = 1.0.. 1.4 m) mirrors
Zeiss σ_{rms} = 10 nm

Slope errors

- Consider the surface to be composed of facets
- Each surface normal having an individual angle $\Delta\alpha_i$ with respect to the mean surface plane.
- The initially parallel incident beams are deflected by $2\cdot\Delta\alpha_i$
- Assume a gaussian probability distribution of the facets orientation
- The rms-value of the angular distribution is usually called the slope error σ of the surface.
- The slope errors give rise to a blurring of the image by $S = 2\cdot\sigma\cdot r'$





Typical values of σ for various mirror shapes

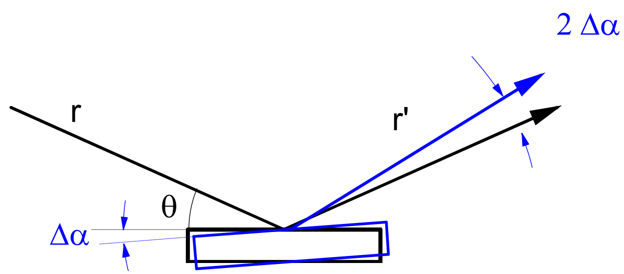
plane and spheres	< 0.1 arcsec
toroids	< 0.5 arcsec
elliptical, paraboloidal	< 2 arcsec

Note that FWHM = $2.3\cdot\sigma$

Forgiveness factor

Meridional focusing

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



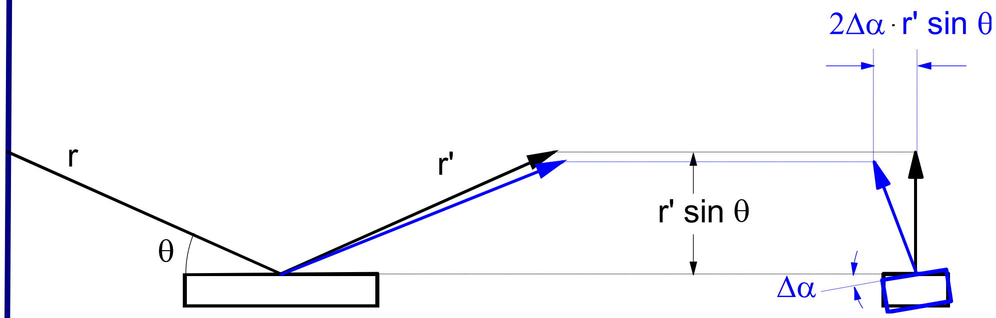
side view

- Supose the surface is tilted in the plane of deflection (which is the focusing plane) by $\Delta\alpha$
- the incident beam is then deflected by $2 \cdot \Delta\alpha$ d
- 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



side view

front view

- Surface tilts in the plane of deflection do not affe the image size in the focusing plane.
- A surface tilt in the focusing plane cause the

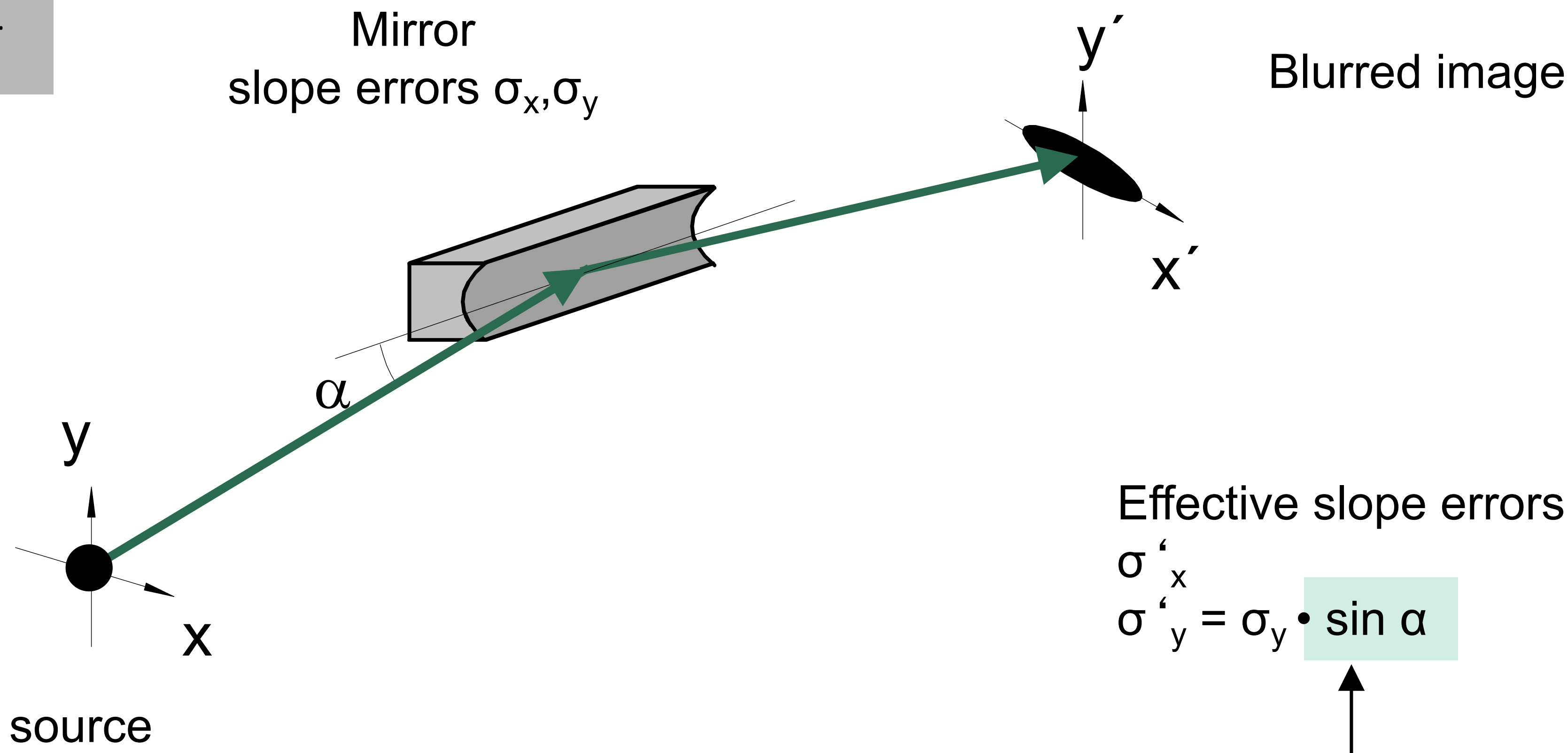
  ncident beam to be deflected by $2 \cdot \Delta\alpha$,
- and the image size in the focusing plane is

  increased by $\Delta S = 2\, r' \,\Delta\alpha \sin\theta$

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

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

Sagittal focusing



Effective slope errors

σ'_x

$\sigma'_y = \sigma_y \bullet \sin\alpha$

Forgiveness factor

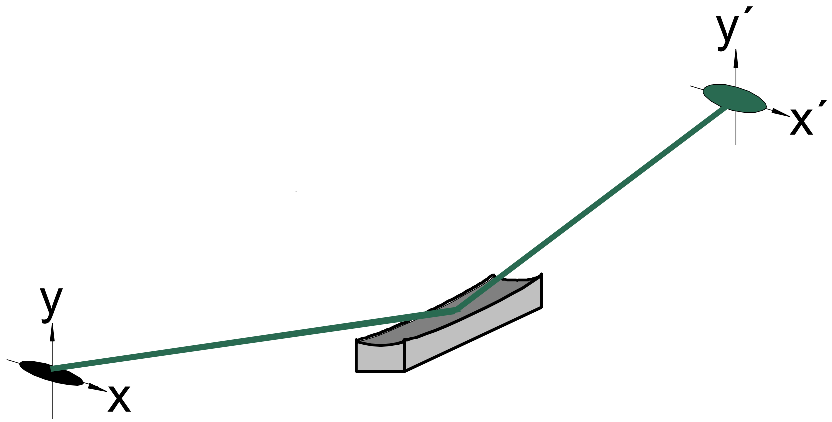
Deflection plane(x,x')

Focusing plane (y,y')

Sagittal vs. Meridional focusing (Example)

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

meridional focusing

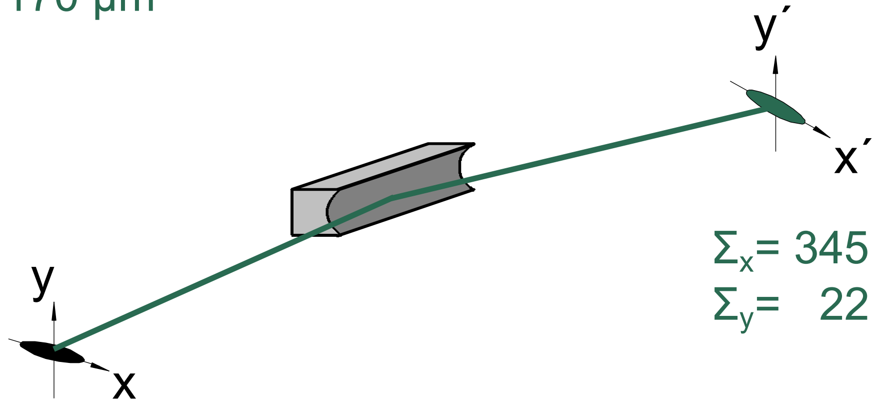


Σ_x= 300 µm,
Σ_y= 170 µm

Σ_x= 300 µm
Σ_y= 20 µm

Increase in area: 8.5

sagittal focusing



Σ_x= 345 µm
Σ_y= 22 µm

Σ_x= 300 µm
Σ_y= 20 µm

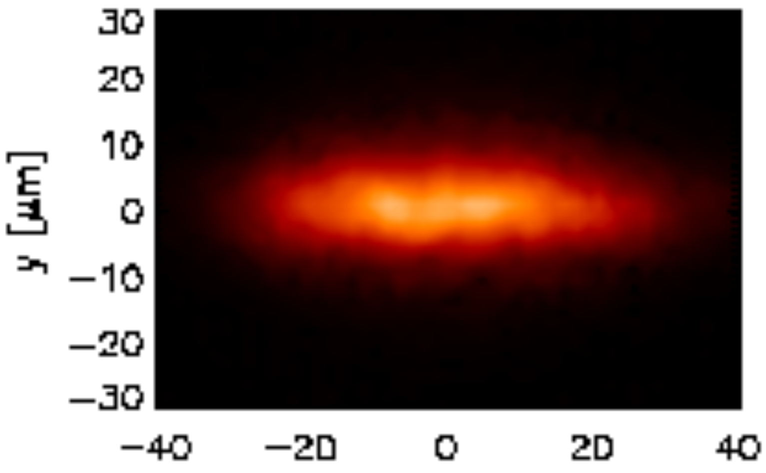
Increase in area: 1.3

sagittal focusing preserves brillance at 3rd generation SR

Put dispersion plane perpendicular to deflection of mirrors!

Focus of UE52-SGM beamline at BESSY II

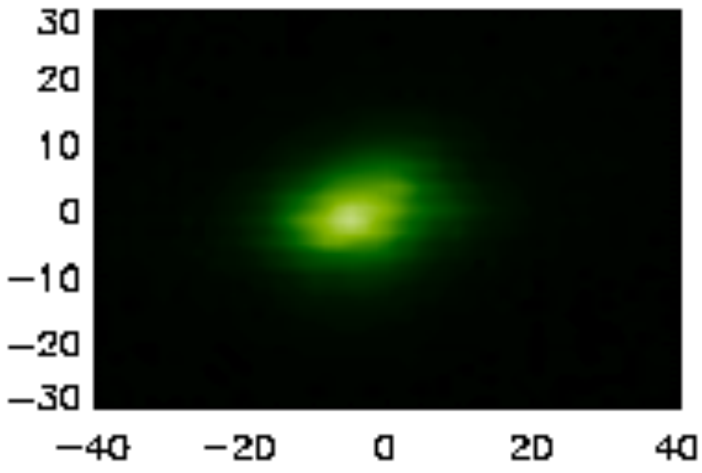
old mirror (1,5 arcsec)



hor. focus

43 µm

new mirror (0,14 arcsec)



hor. focus

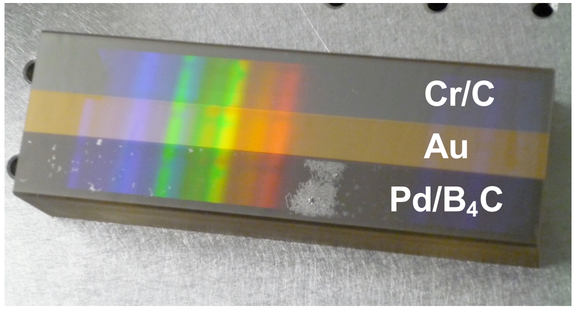
17 µm

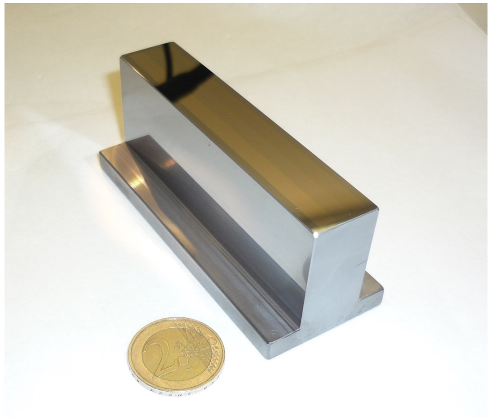
(source limited)

Gratings

Majority of soft X-ray beamlines use reflection gratings

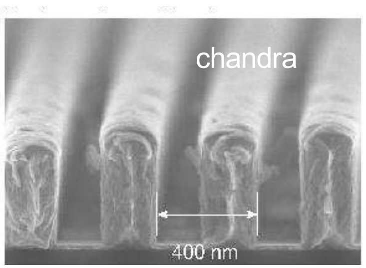
- High resolving power (100 000)
- Wide spectral range (one decade)
- Stability
- Efficient cooling of substrate
- Single crystal silicon

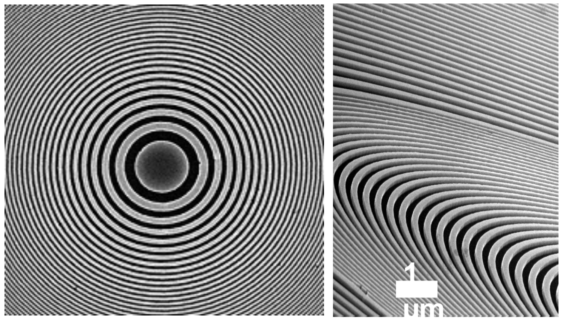


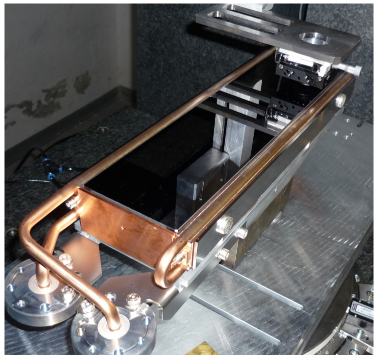


Alternatives

- Transmission gratings
- Zone plates
- Multilayer mirrors



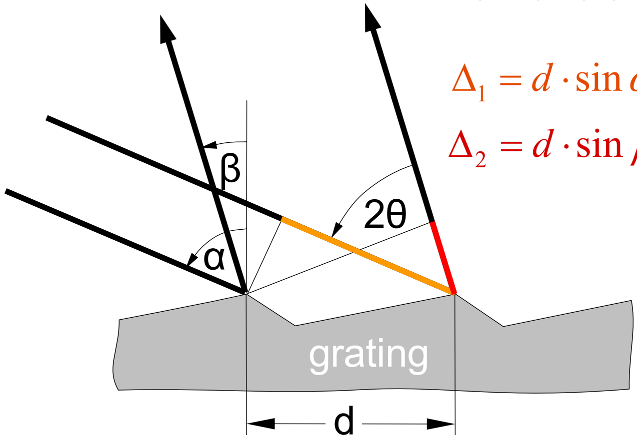




Courtesy BESSY II

Grating equation

N=1/d : Line density
α : incidence angle
β : diffraction angle
2θ=α-β : deflection angle



Path difference Δ

$\Delta_1 = d \cdot \sin\alpha$

$\Delta_2 = d \cdot \sin\beta$

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

Constructive Interference

$\Delta = m \cdot \lambda$

m: diffraction order (any integer)

Grating equation: $m\lambda = d(\sin\alpha + \sin\beta)$ $\quad Nm\lambda = \sin\alpha + \sin\beta$ $\quad Nm\lambda = 2\cos\theta\sin(\theta+\beta)$

From path function

Grating equation

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

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

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

Meridional focus condition (R=∞)

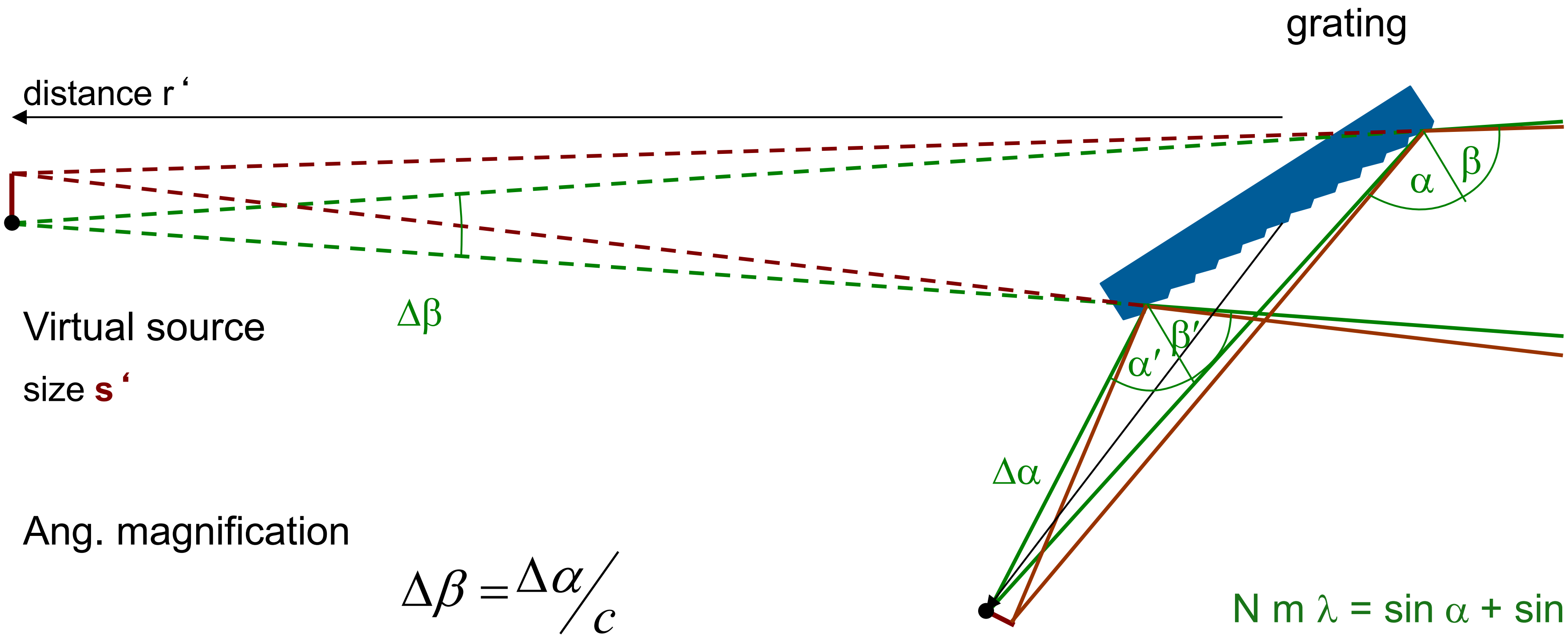
$$F_{20} = \frac{\cos^2\alpha}{r} + \frac{\cos^2\beta}{r_M'} = 0 \qquad \Rightarrow \frac{r_M'}{r} = -\frac{\cos^2\beta}{\cos^2\alpha} = -c^2$$

Sagittal focus condition (R=∞,a_{02}=0)

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

Even plan gratings have focusing properties (Murphy 1956)

Grating equation and magnification



Ang. magnification

$$\Delta\beta = \Delta\alpha / c$$

$$r' = -c^2 r$$

Magnification

$$s' = c\, s$$

source

distance r

size **s**

N m λ = sin α + sin β

N m λ = sin α′+ sin β′

Same wavelength

c = cos β / cos α

Modes of operation

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 β / cos α:

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

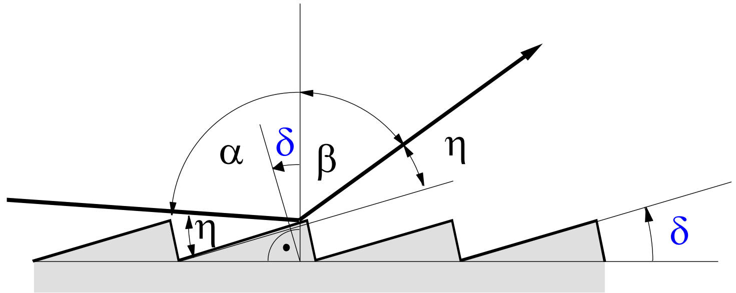
Fixed deviation 2θ=α-β

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

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

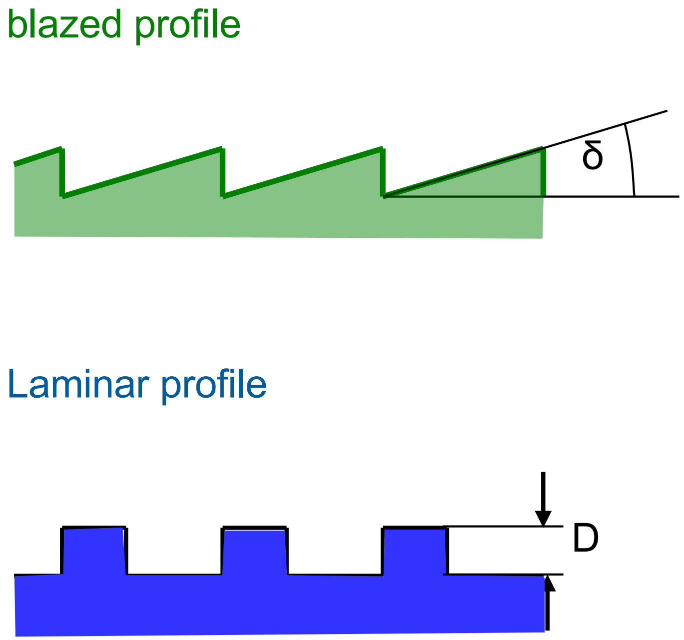
$$\beta = -\arccos\left(\frac{mN\lambda}{2\sin\delta}\right) + \delta$$

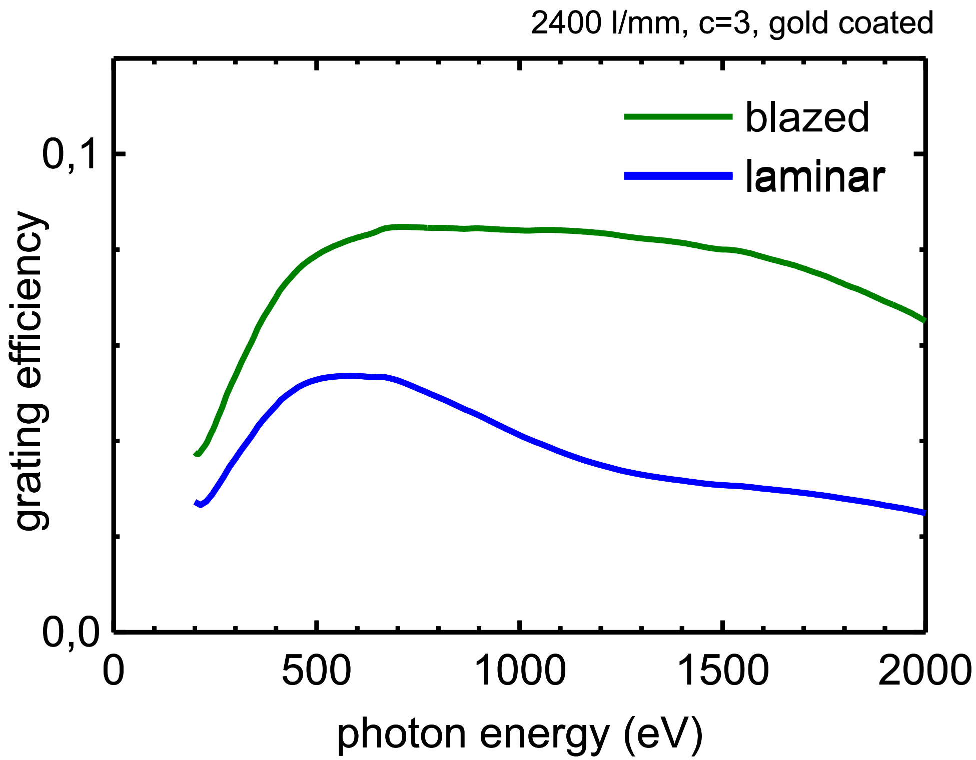
Blazed grating



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

Grating profile





Blazed profile with significantly higher grating efficiency

but only a few suppliers for blazed gratings

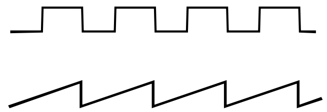
Grating parameters

Guidlines for grating parameters

- **Profile**

  Laminar : high spectral purity

  Blaze : high flux



- **Line density N** (Energy range: In grating equation only dimensionless product m·N·λ)

  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, δ=0.8° – 4°

Higher order content

Higher order light perturbs

- Reflecometry
- Determination of cross sections
- Non liniear optics
- …

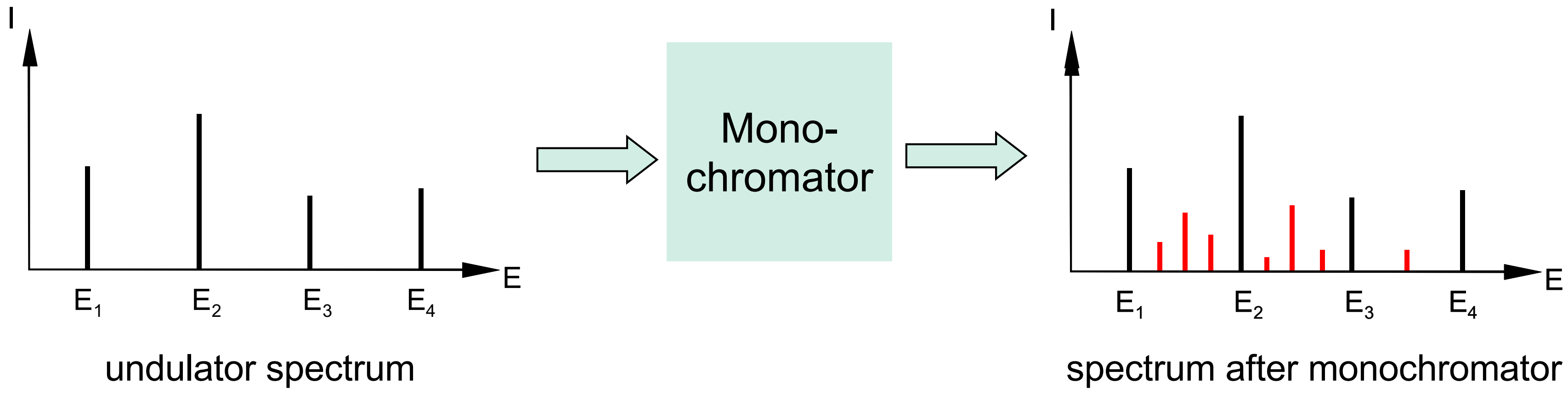
Determination of higher order

Quantitative:

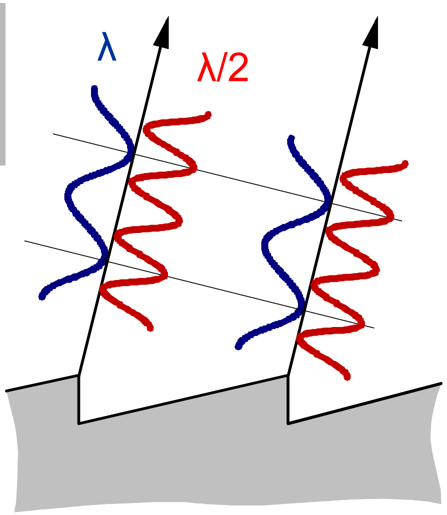
Secondary spectrometer for selected beamline energies

Qualitative :

Measure beamline output for fixed undulator gap



False light

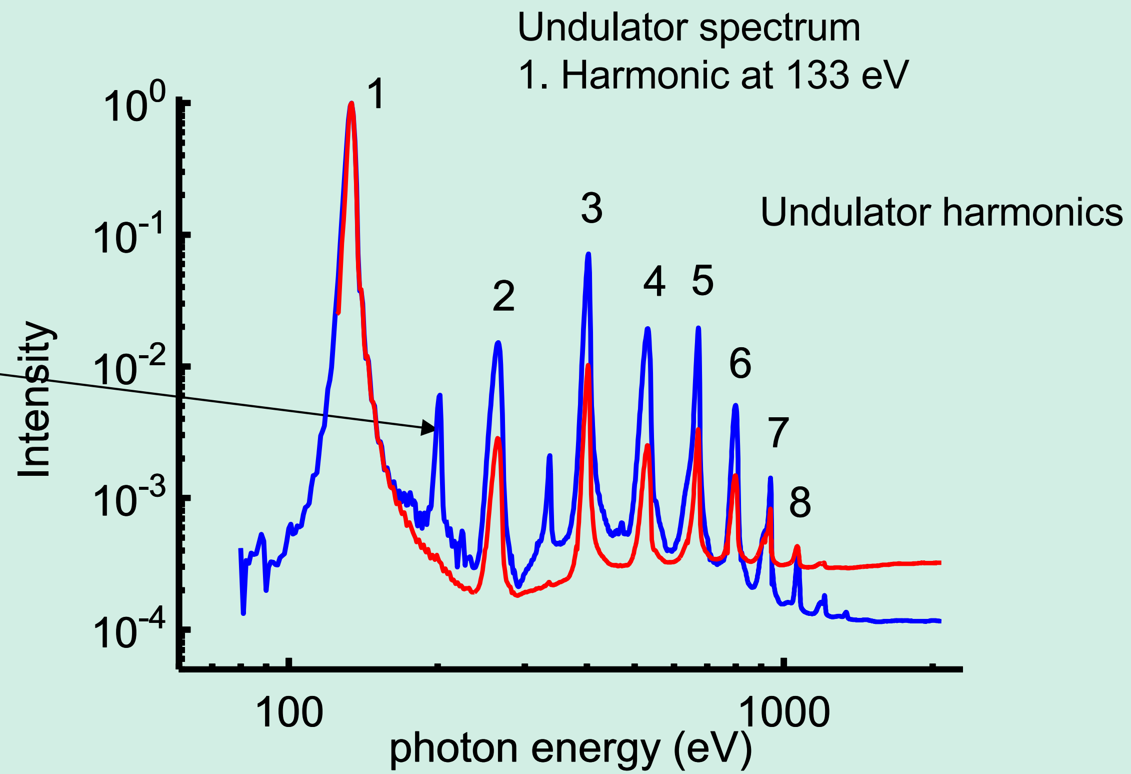


If wavelength **λ** shows constructive interference then also **λ/2**, **λ/3**, …

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

FALSE LIGHT

This is no 200 eV light
It is 400 eV!



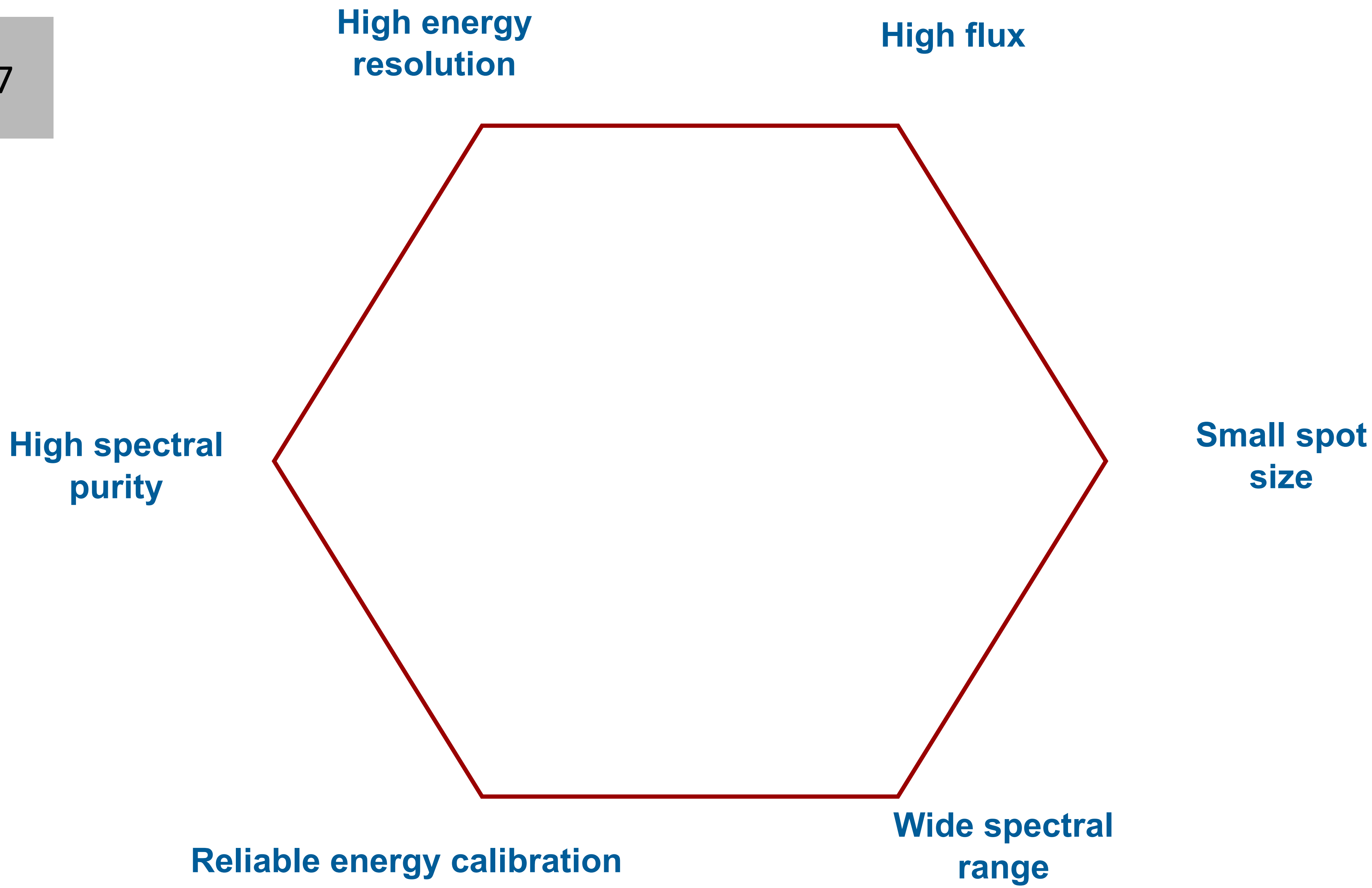
Can be suppressed by

deflection angle or c-value

(c=2,25 / c=1.4)

Grating Monochromators

Optimization goals

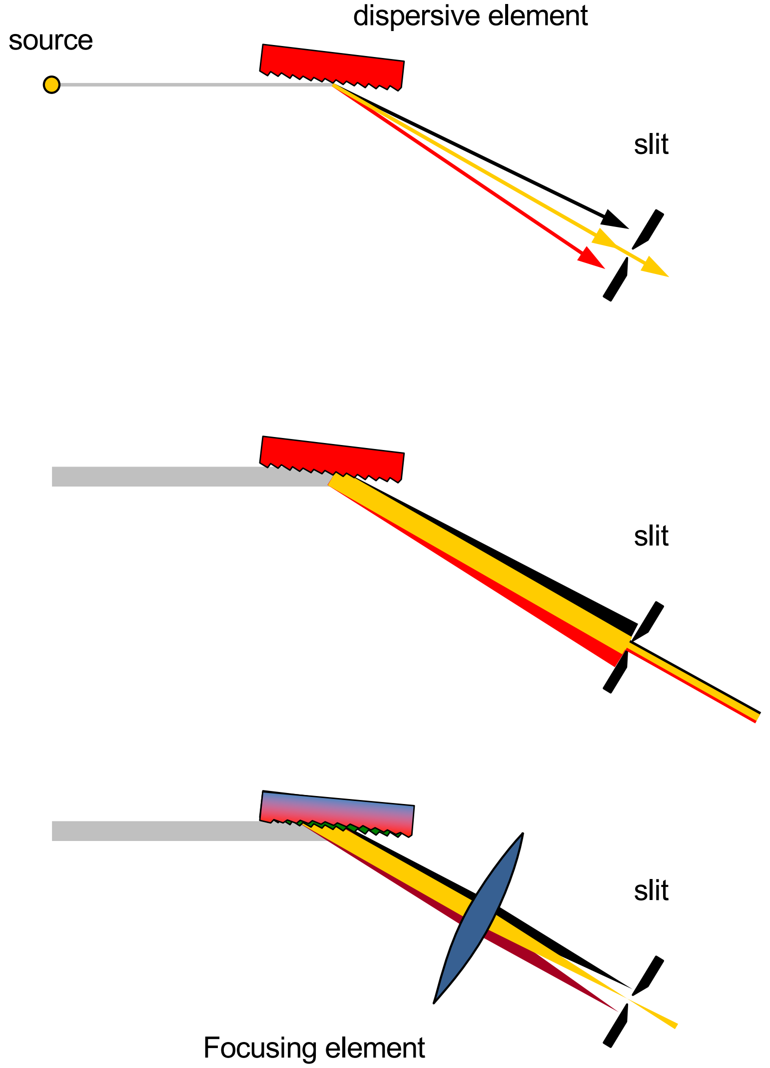


Function of beamline components

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

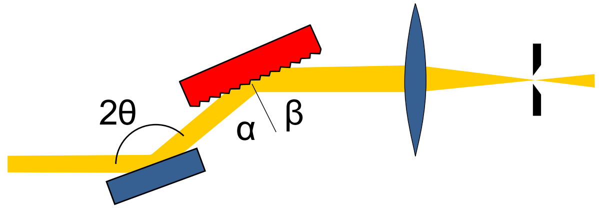
- **Finite beam cross section**
  - Light of different colours transmit through the slit.

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

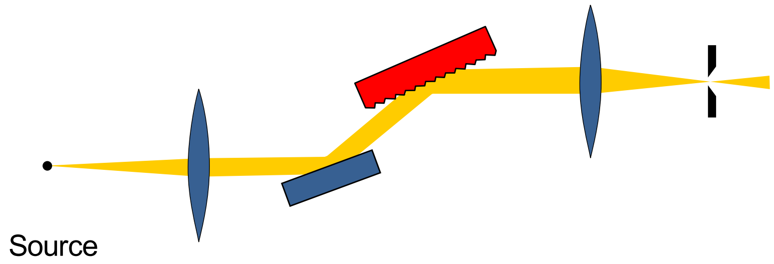


Function of beamline components

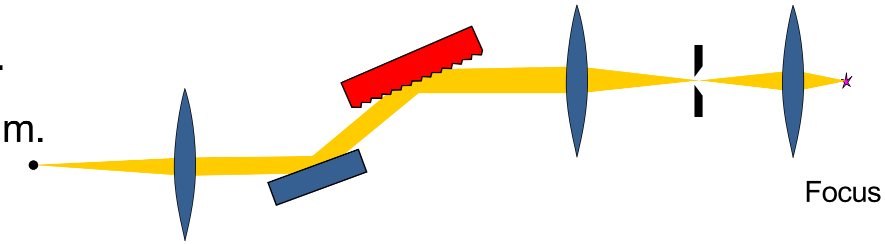
- **Additional plane mirror**
  - Independent setting of α and β.



- **Source point is at finite distance**
  - Preoptic matches source to the beamline.
  - Collimates the light.

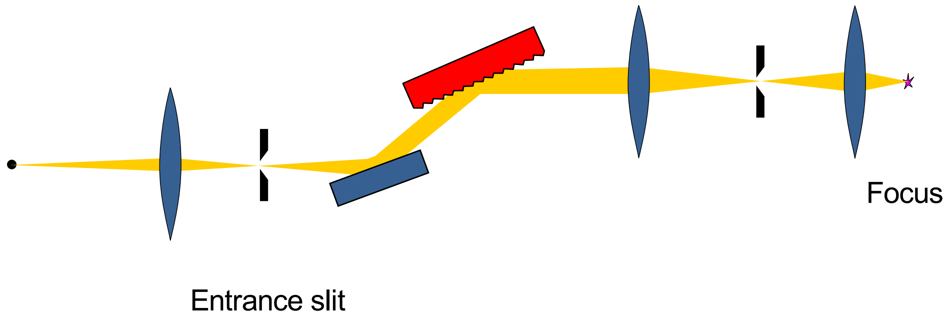


- **Experiment cannot placed at the slit**
  - Refocusing optics brings light to the experiment.
  - Small spot ≈30 μm in a distance of 800 -1500 mm.



Function of beamline components

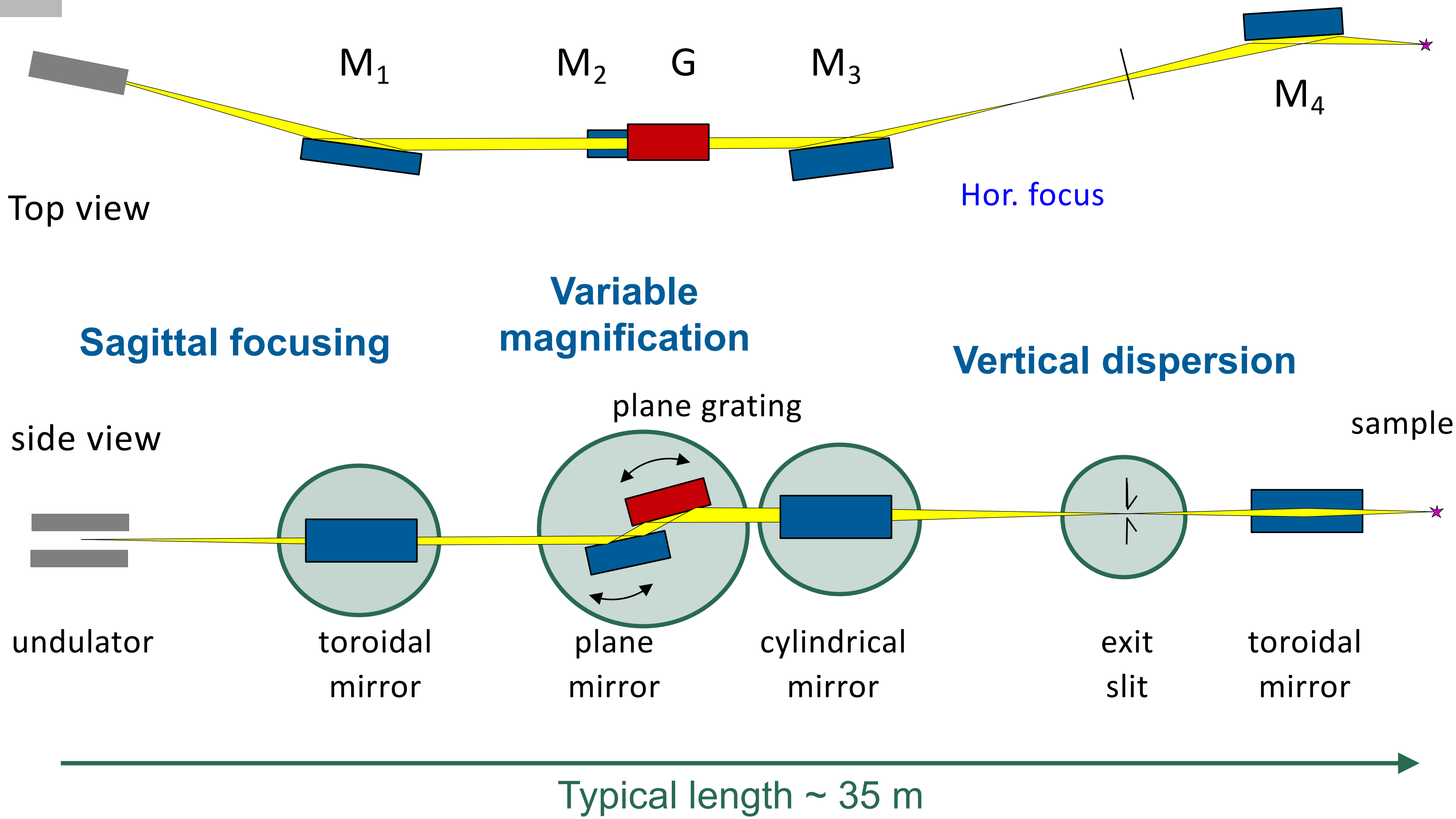
- **Entrance slit**
  - Defines source point independent of the electron beam of the storage ring.



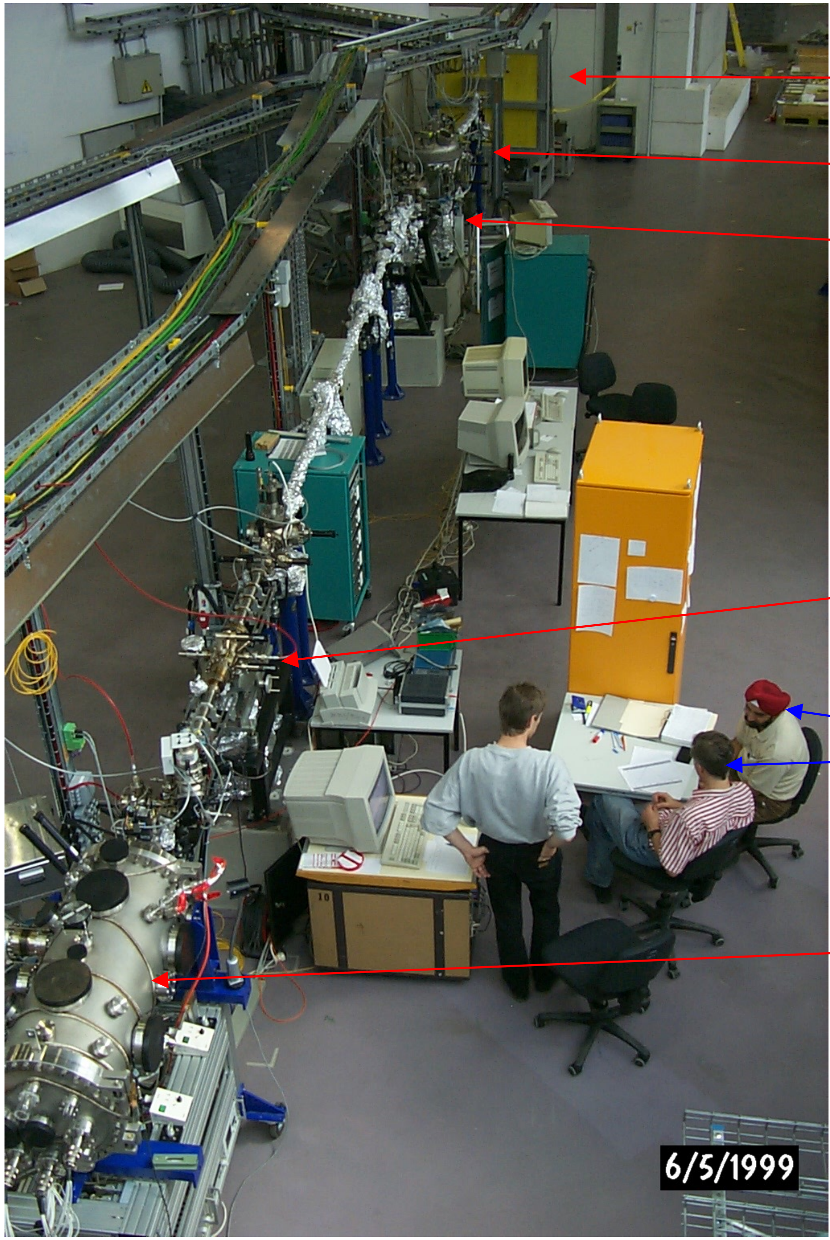
General guidelines

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

Collimated PGM



Undulator beamline at BESSY



Pre optics

Grating chamber

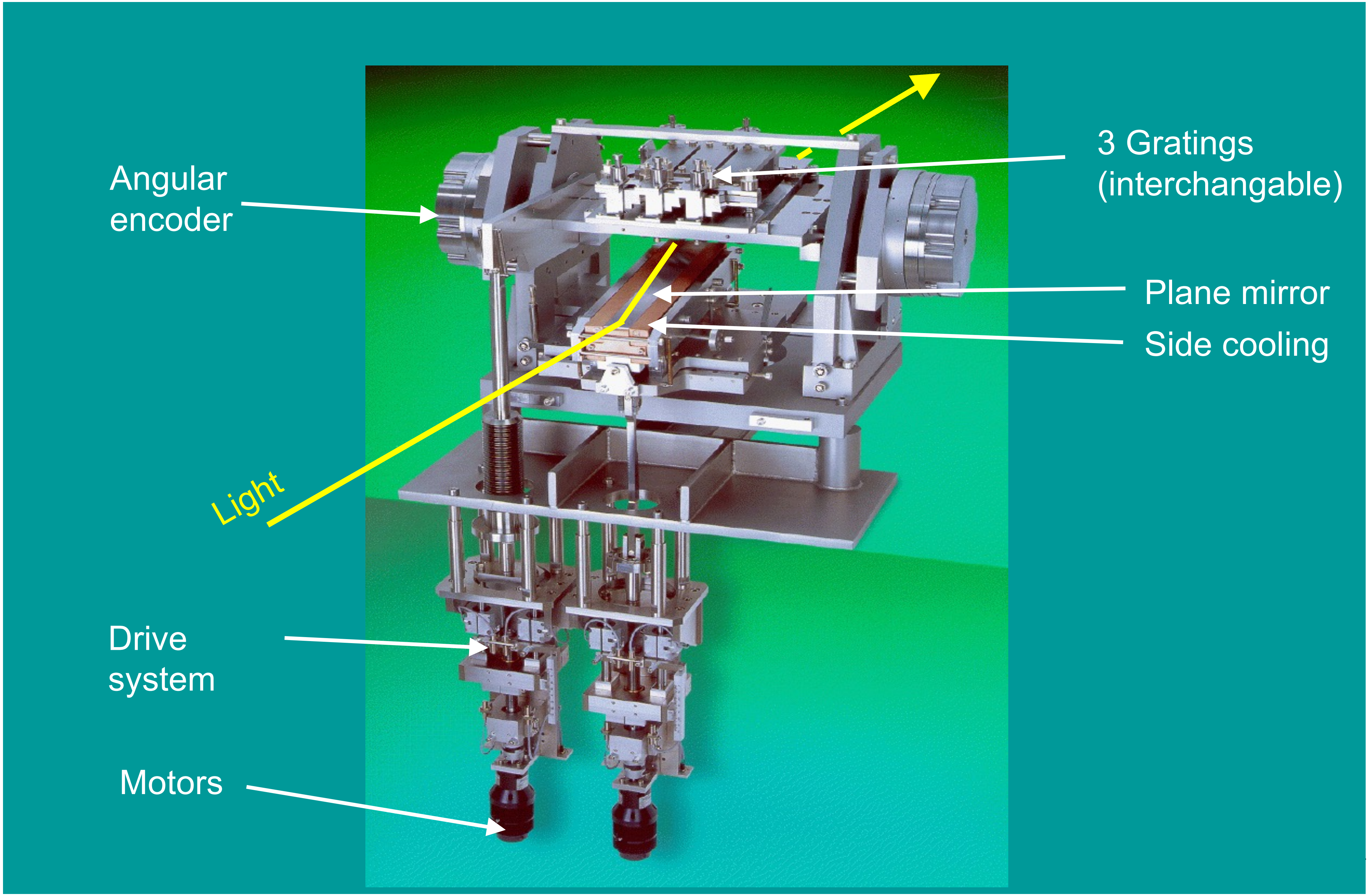
Focusing chamber

Exit slit

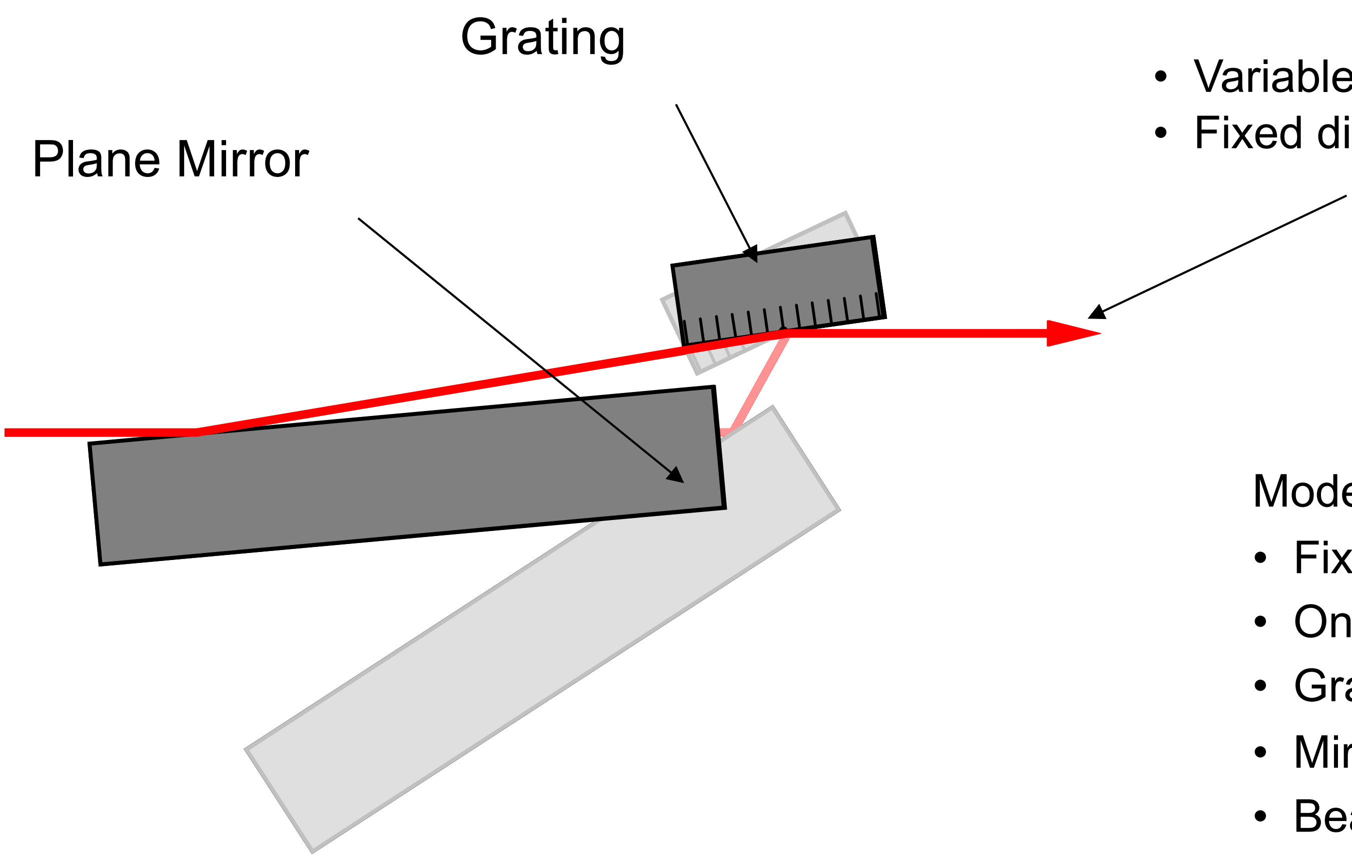
Beamline scientists

Polarimeter

Grating chamber mechanic



SX700: First plane grating monochromator with tilting premirror



- Variable deflection angle
- Fixed diffracted beam

Modes of operation

- Fix focus mode
- On blaze mode
- Grating only
- Mirror only
- Beamsplitter mode

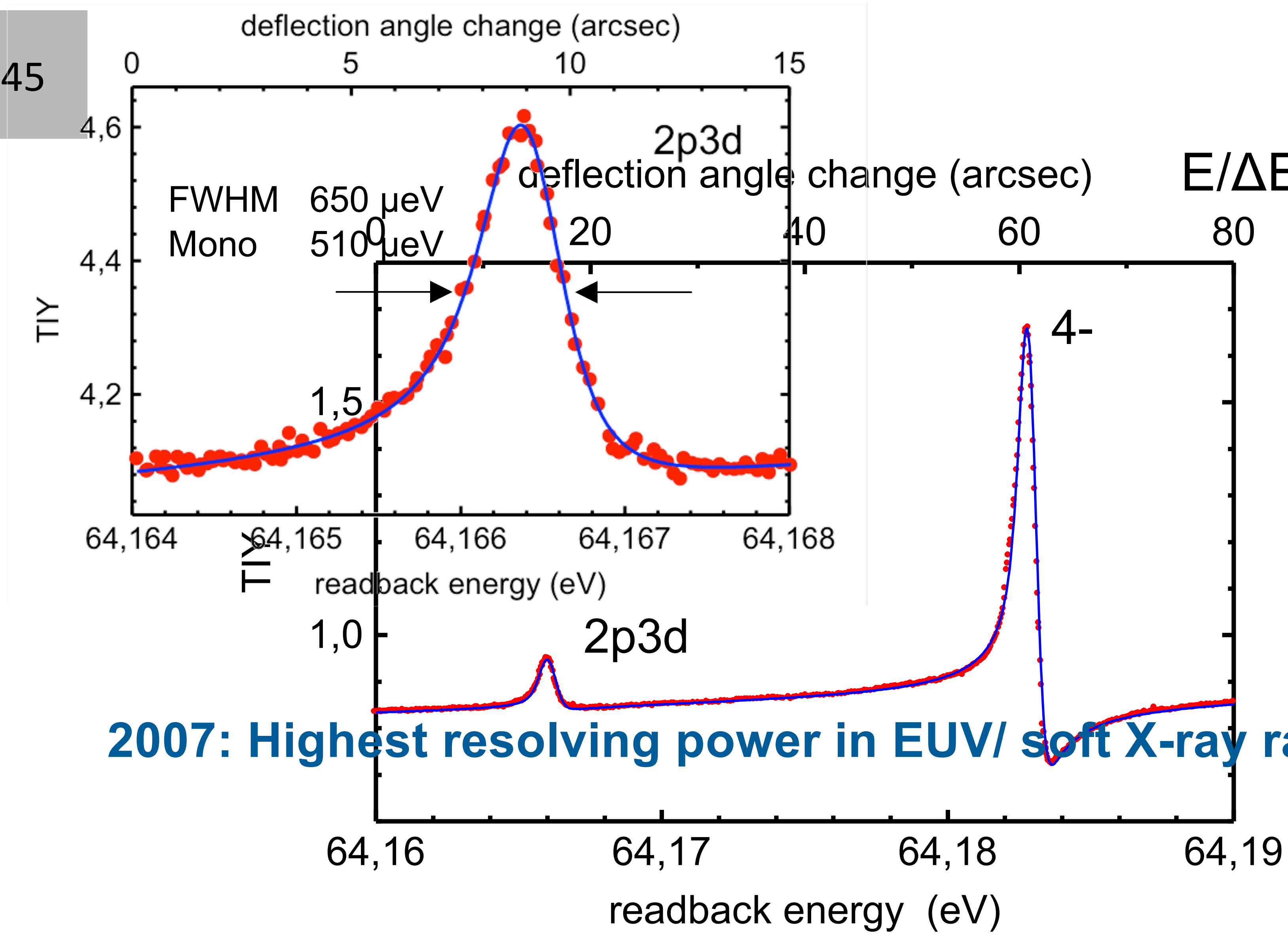
Incident (α) and diffraction angle (β) at the grating can be set independently

H. Petersen, Opt. Comm. **40**, 402 (1982)
F. Riemer & R.Torge, Nucl. Instr. and Meth. **208**, 313 (1984)

Ionization of noble gas

Helium

E/ΔE ≈ 125 000

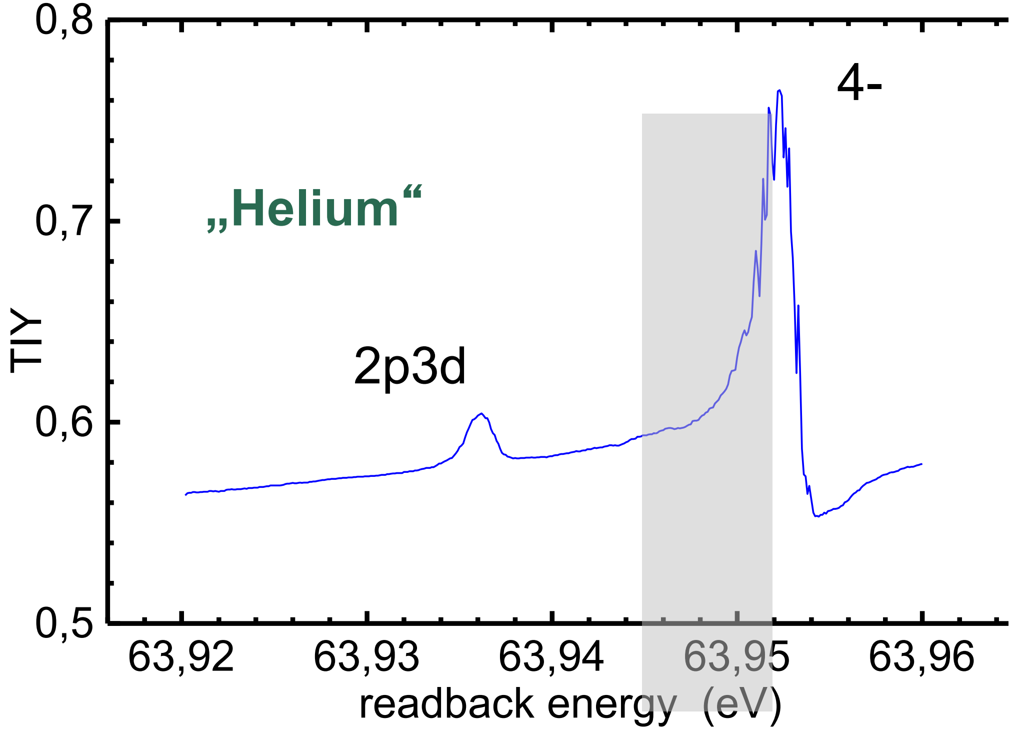


2007: Highest resolving power in EUV/ soft X-ray range

2400 l/mm c=15

What can go wrong?

Crane moves over beamline



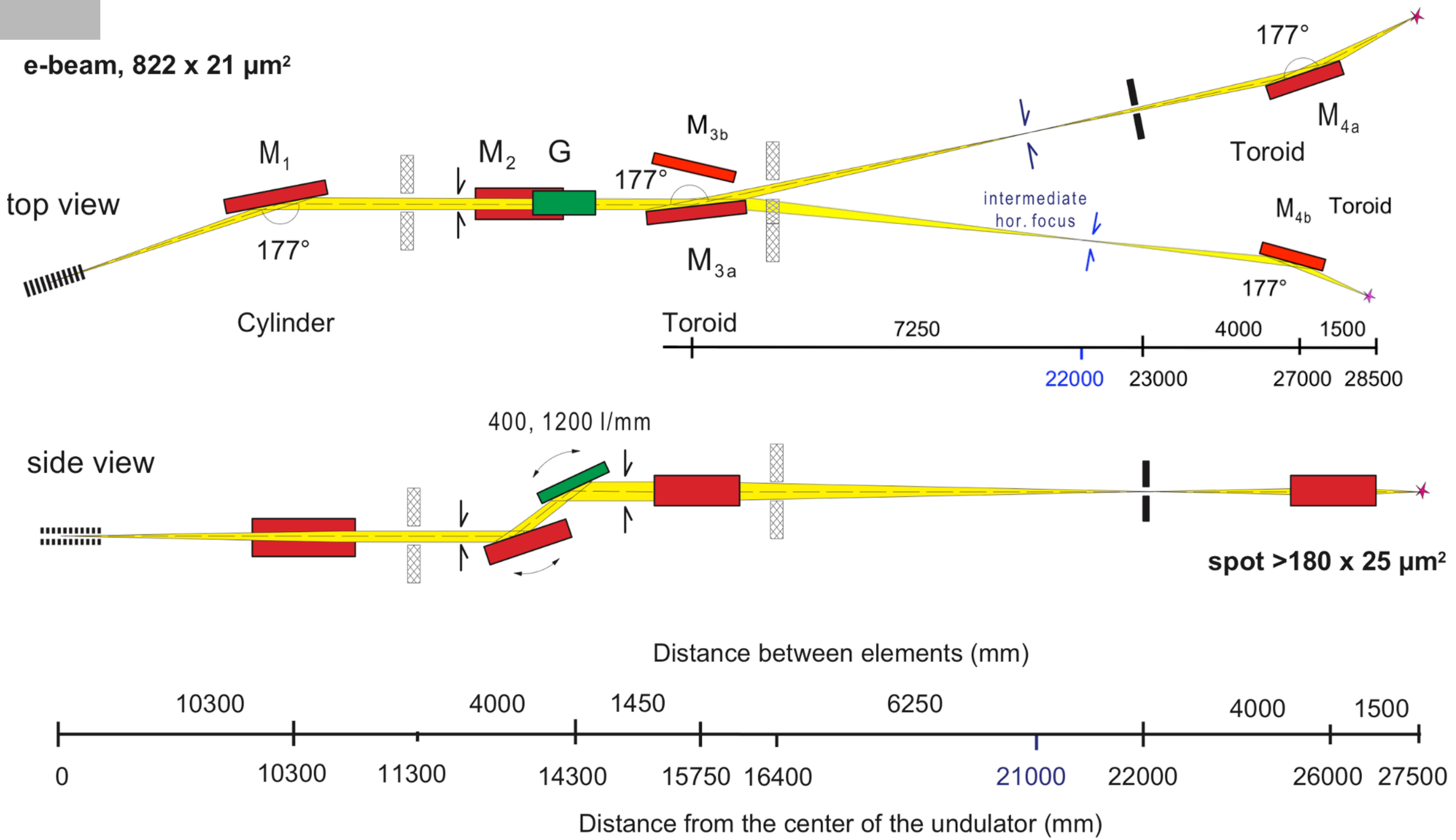
Ist not allowed to operate the crane during measurements

Plane grating monochromator

- 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

HESEB beamline

- Branch a in phase 1, branch b postponed



Mirror parameters

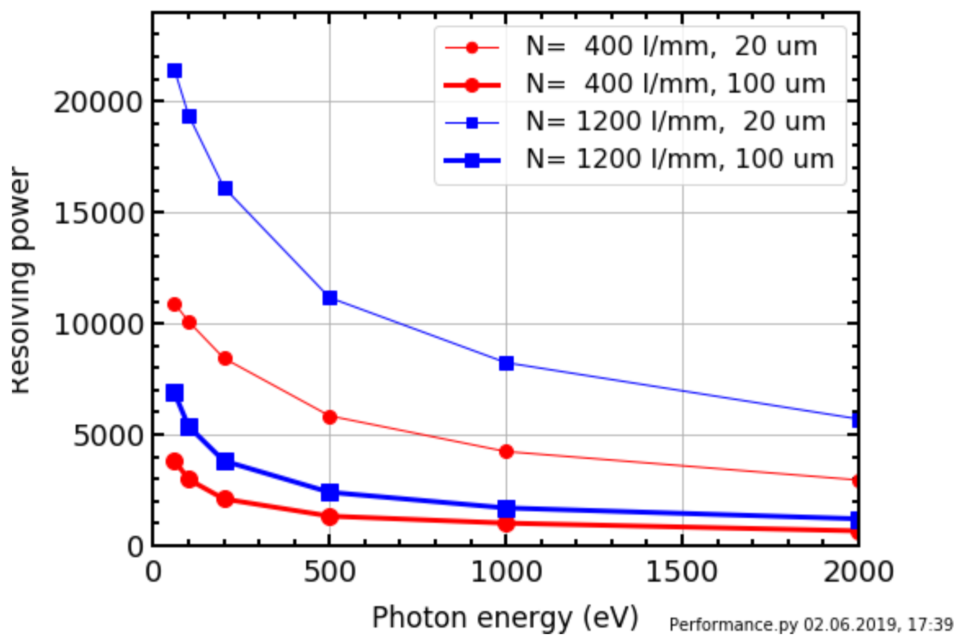
specifications

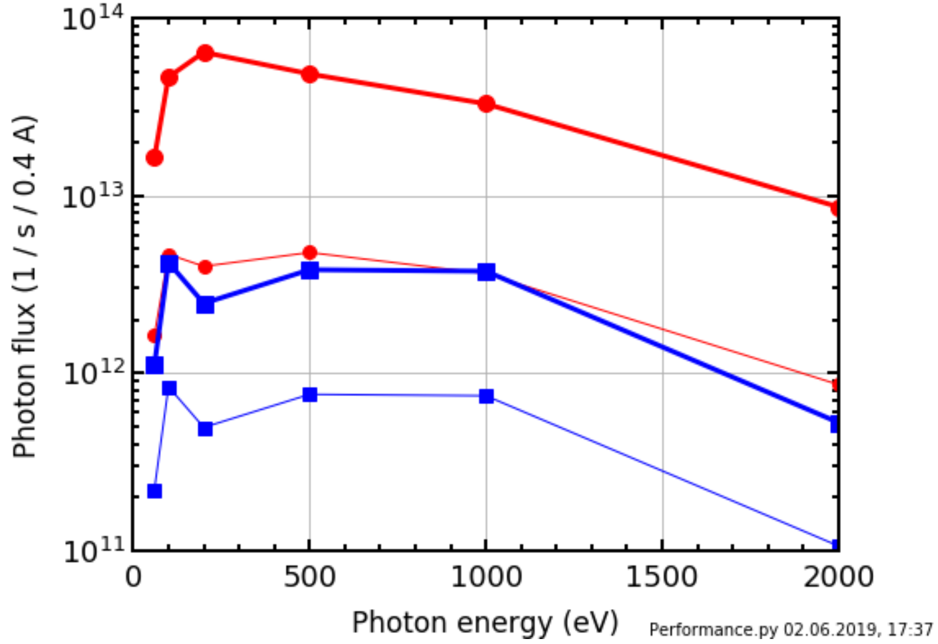
Photon Energy	unit	M1	M2	M3a	M3b	M4a/b	G-1	G-2
Shape		Cylindrical	Plane	Toroidal	Toroidal	Toroidal	Plane	Plane
Geometrical surface	mm^2	310 x 25	360 x 40*	310 x 40	310 x 40	410 x 50	100 x 20	100 x 20
Optical surface	mm^2	300 x 20	350 x 20	300 x 30	300	400 x 20	95 x 15	95 x 15
Slope error (m/s)	arcsec	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

HESEB beamline

- Branch a





HESEB beamline

- 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

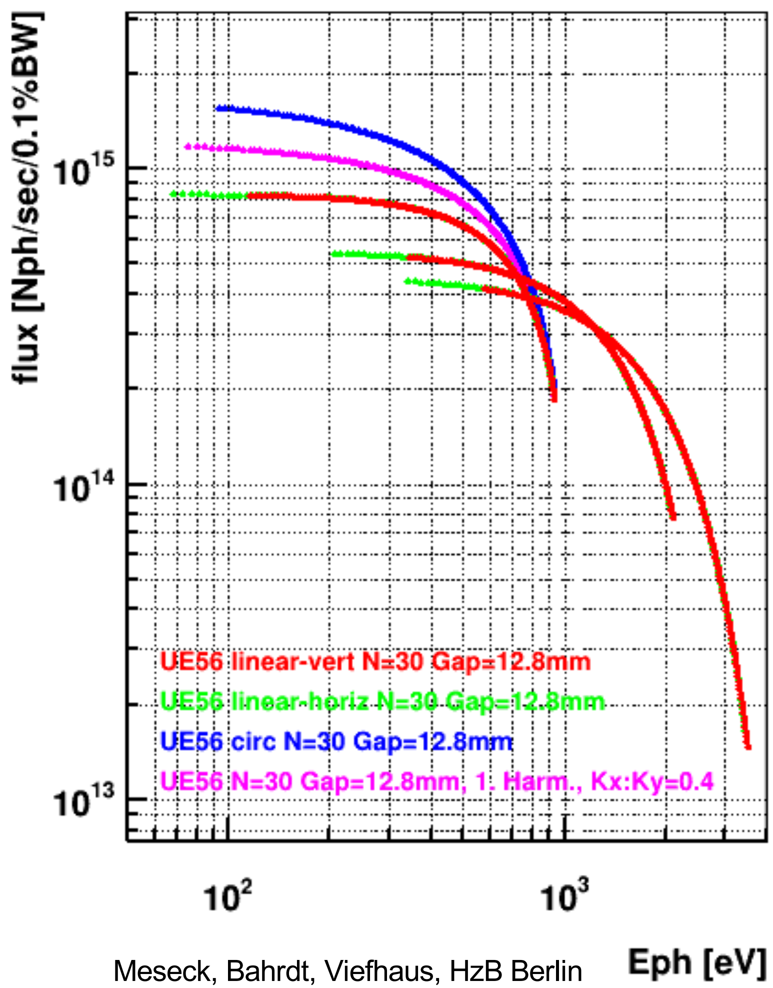
BESSY II: $E_{e=}$ 1.7 GeV, I = 400 mA

K_{max} = 5.3 (3.7)

P = 2700 W (600 W)

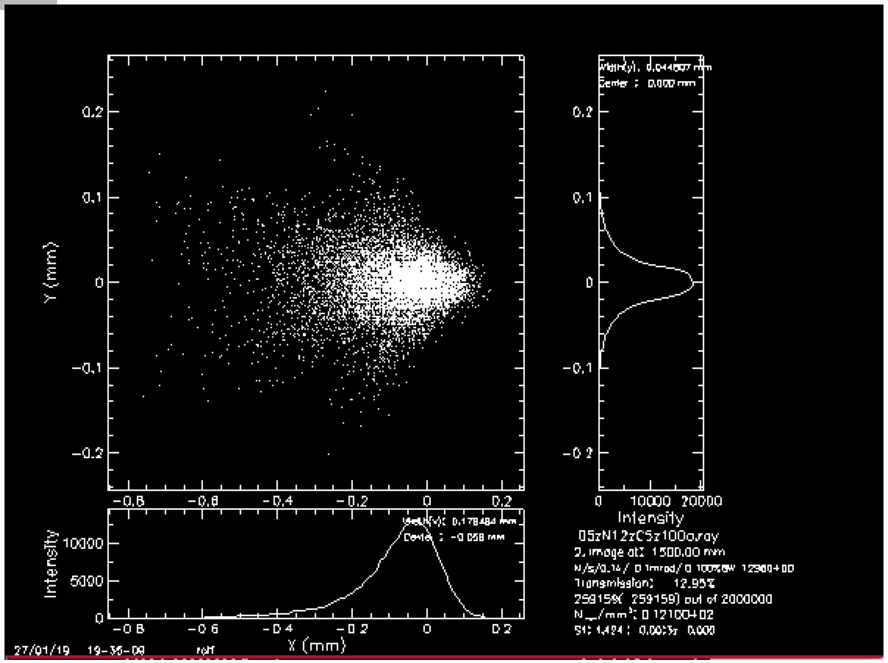
p = 5100 W/mrad² (765 W/mrad²)

Flux, 2.5 GeV, 400 mA

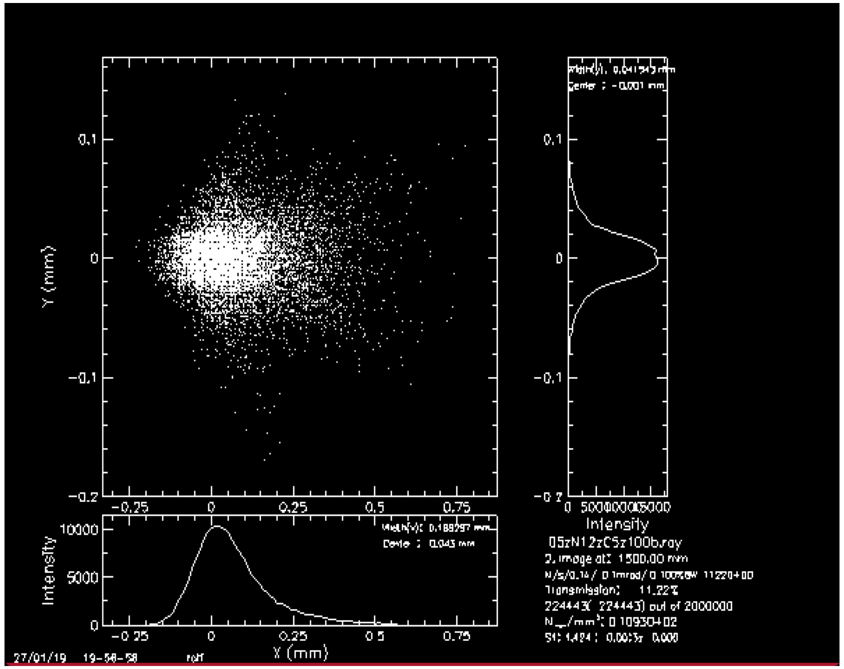


Meseck, Bahrdt, Viefhaus, HzB Berlin

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

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