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Beamline design

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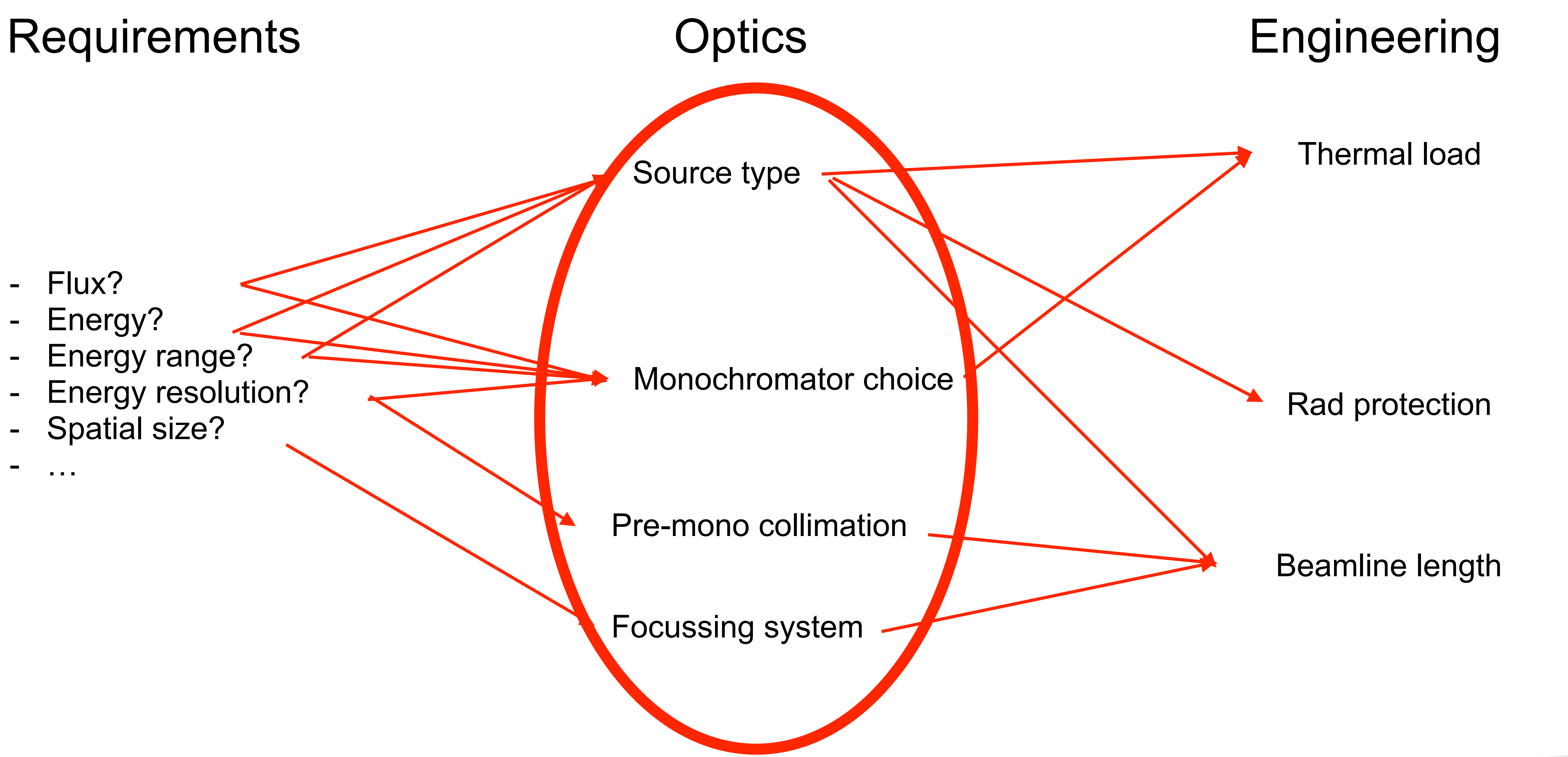
Goal of beamline design

Design a photon transport system connecting the light source to the experimental station within a set of specific parameters:

- Photon flux
- Photon energy
- Photon energy bandwidth
- Photon beam spatial size
- …

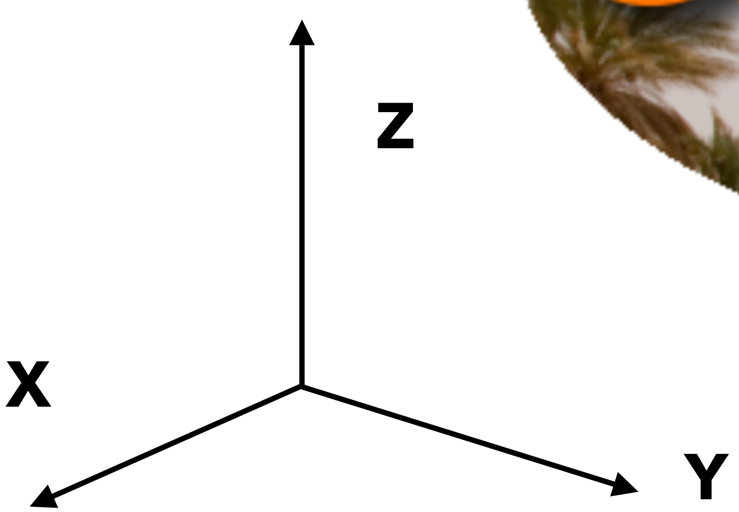
Beamline design process



Tools available

- Physical side: Photons' interactions with matter
  - Refraction
  - Reflection
  - Diffraction
- Design side: Simulators
  - Ray tracers
  - Wave optics
  - Finite Elements

Quick word about simulators



By SHADOW convention,
Y is the BEAM PROPAGATION DIRECTION

C. Welnak, P. Anderson, M. Khan, S. Singh, and F. Cerrina, "Recent developments in SHADOW," *Review of Scientific Instruments*, vol. 63, p. 865, 1992.
O. Chubar, P. E. P. O. T. E. Conference, 1998, "Accurate and efficient computation of synchrotron radiation in the near field region," *accelconf.web.cern.ch*
L. Rebuffi, M. Sanchez del Rio, "OASYS (OrAnge SYnchrotron Suite): an open-source graphical environment for x-ray virtual xperiments", Proc. SPIE 10388, 103880S (2017) . DOI: 10.1117/12.2274263

L. Rebuffi, M. Sanchez del Rio, "ShadowOui: A new visual environment for X-ray optics and synchrotron beamline simulations", J. Synchrotron Rad. 23 (2016). DOI:10.1107/S1600577516013837

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A quick recap

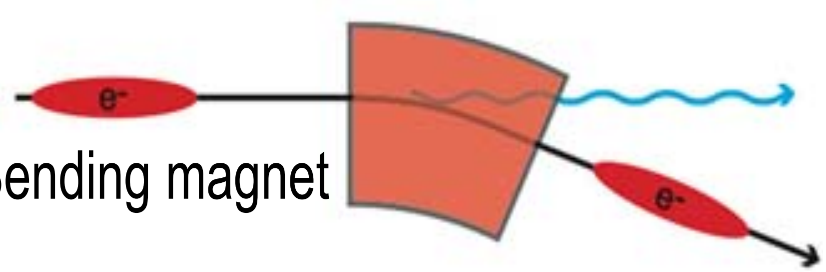
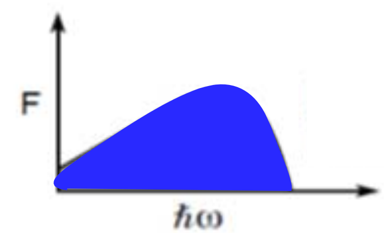
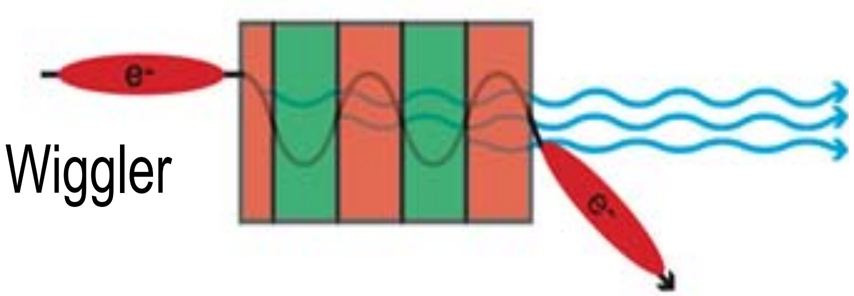
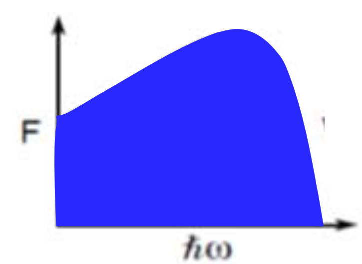
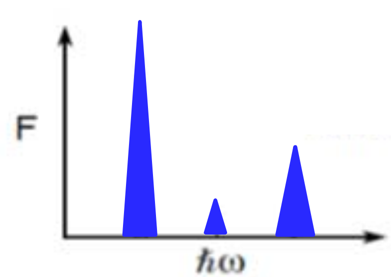
just to set the scene…

Handles available for "manipulating" x-ray photons

			Usage
Diffraction	$2d \cdot sin\theta = m\lambda$	$d \cong \lambda$	Monochromatization Focussing
Reflection	$sin\phi' = \frac{sin\phi}{n} \cong \frac{sin\phi}{1-\delta}$	$\theta_C \approx \sqrt{2\delta} \quad (rad)$ $\theta_C \approx 81\sqrt{\delta} \quad (degrees)$	Transport Divergence corrections Focussing Basic energy filtering
Refraction	$n = 1-\delta+i\beta$	$\delta = 10^{-1} \div 10^{-6}$ $\beta = 10^{-1} \div 10^{-8}$	Focussing

Synchrotron beam emitted by source

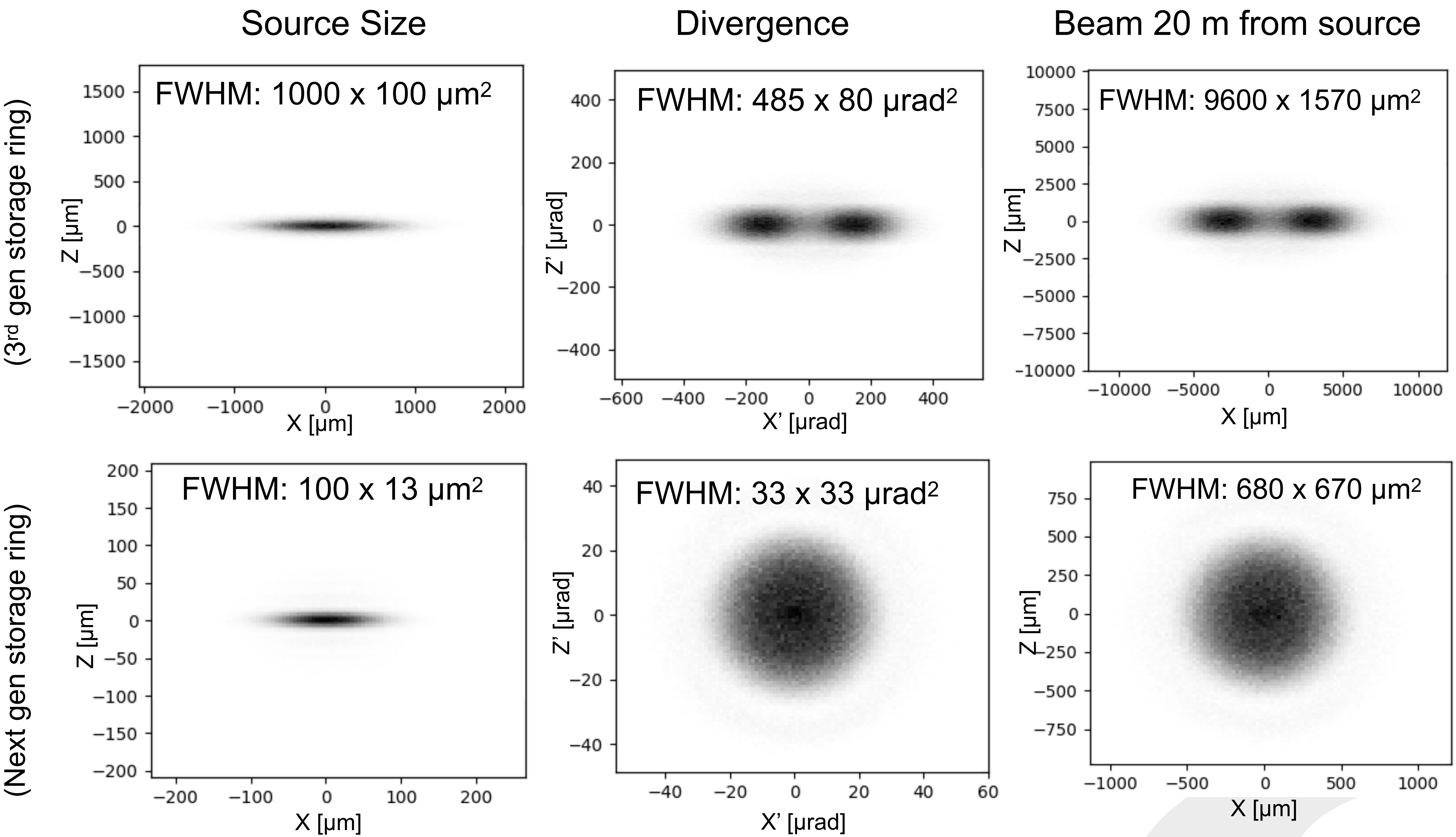
$\gamma = 1957\, E_e[\text{GeV}]$

Source	Spectrum	Divergence σ		Beam size @ 20 m
Bending magnet 		$\sim \frac{1}{\gamma}$	~ mrad	~ 1 - 10's mm
Wiggler 		$\sim \frac{1}{\gamma}$	~ mrad	~ 1 - 10's mm
Undulator 		$\sim \frac{1}{\gamma\sqrt{N}}$	~ 100's μrad	~ mm

For a typical experiment: required beam size ~ 0.1 to 10's of μm or more

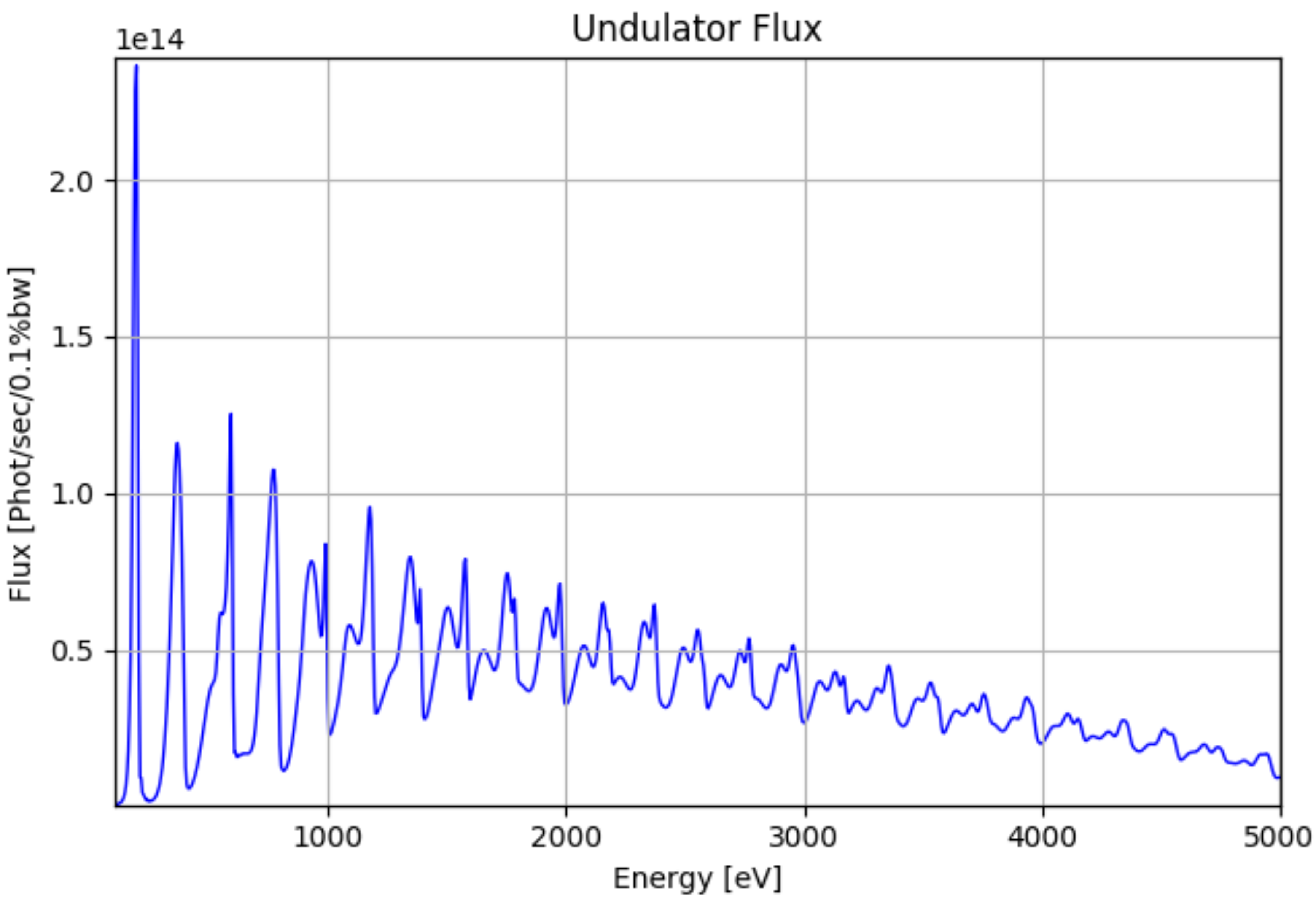
A couple of undulator simulations

E_e=2.4GeV, N = 17, period = 56mm, first harmonic only



It's even more complicated…

E_e=2.4GeV, N = 17, period = 56mm



Total flux ~ 10^{19} ph/s

So what am I going to talk about??

- Mirrors for X-rays
- Basics of diffracting elements
- Monochromators for X-rays
- The thermal load issue

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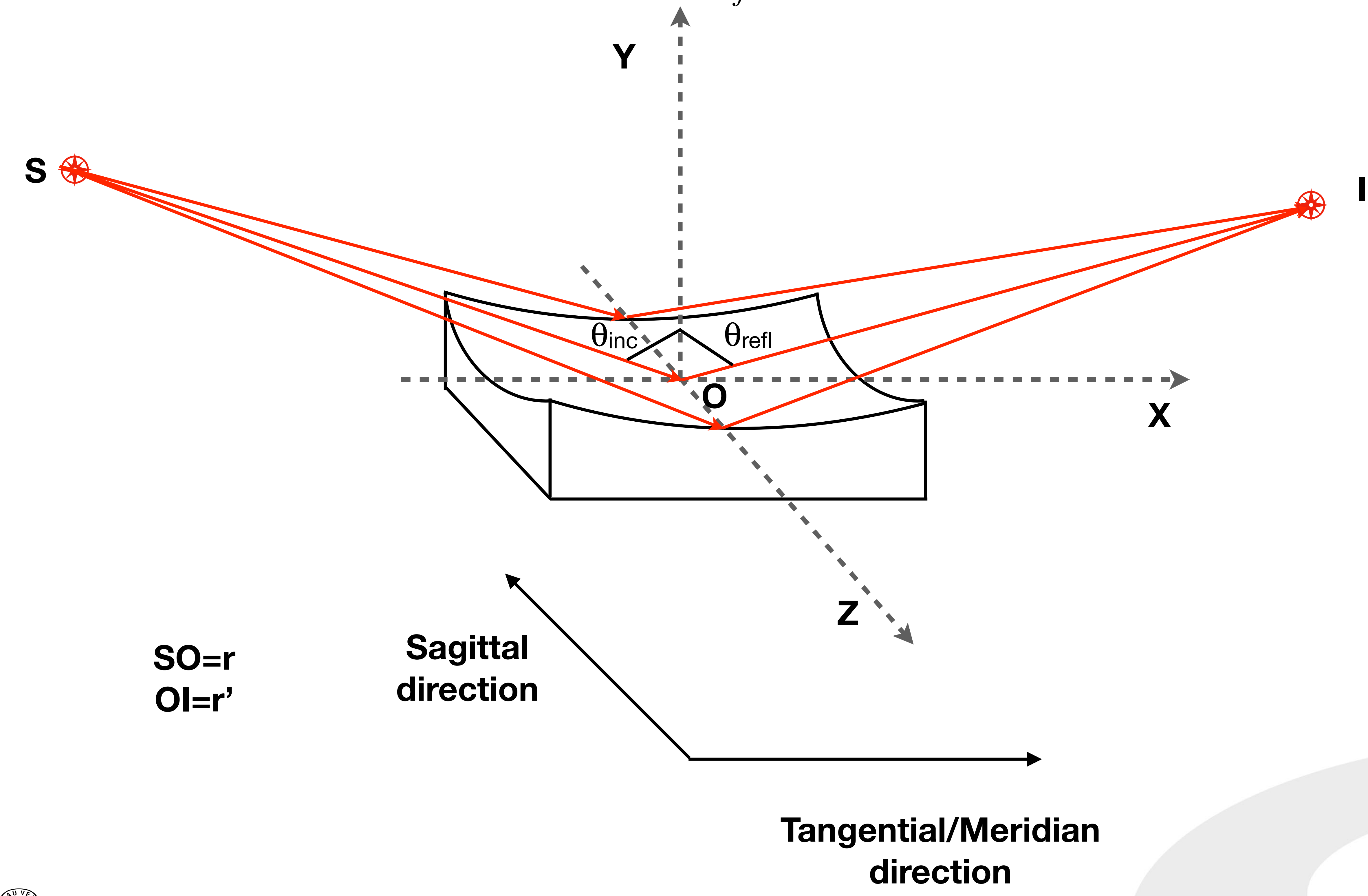
Mirrors for x-rays

Transport
Divergence corrections
Focussing
Basic energy filtering

Some nomenclature

$$\theta_{inc} = \theta_{refl}$$



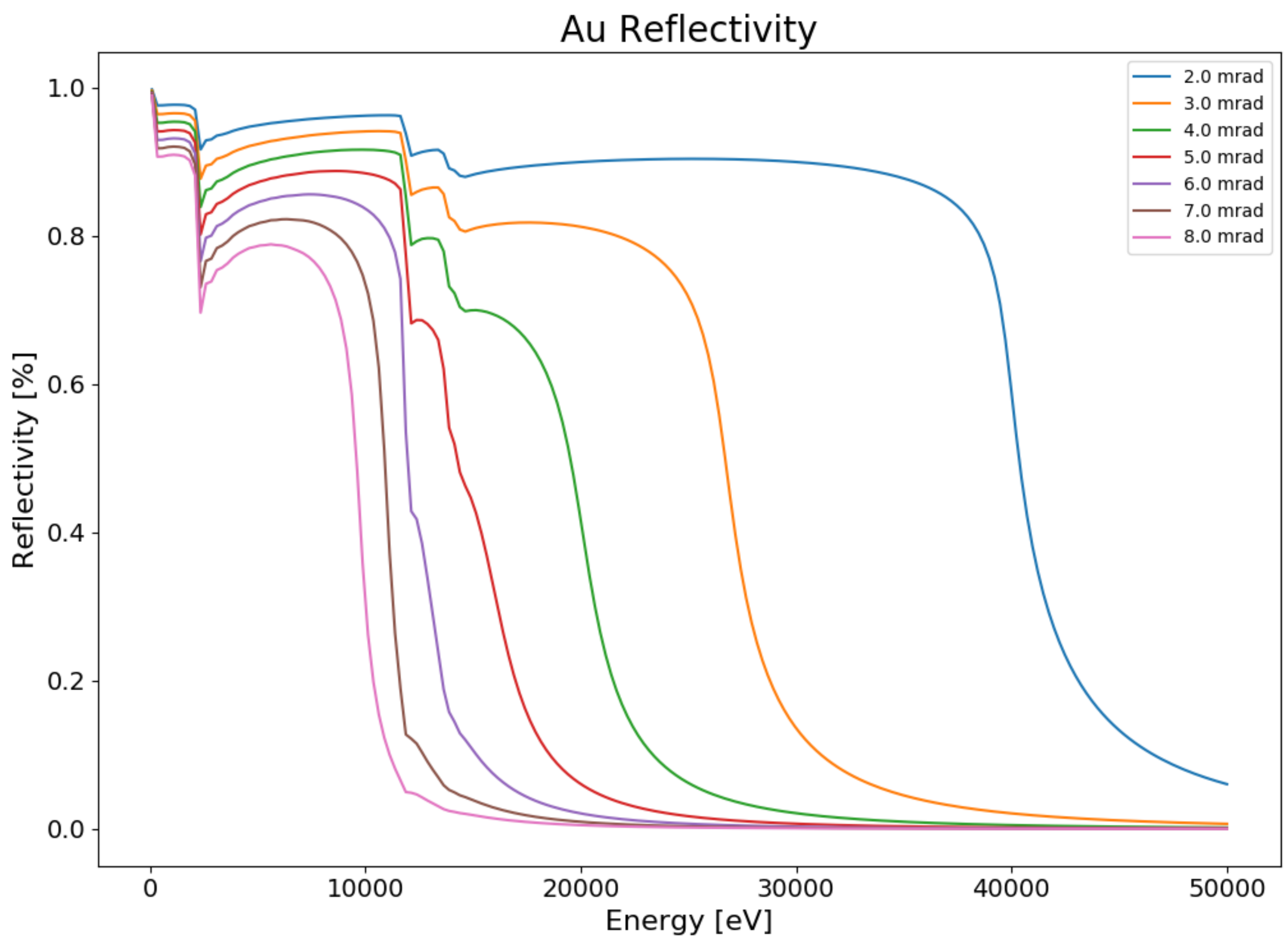
Mirror figures used in synchrotron beamlines

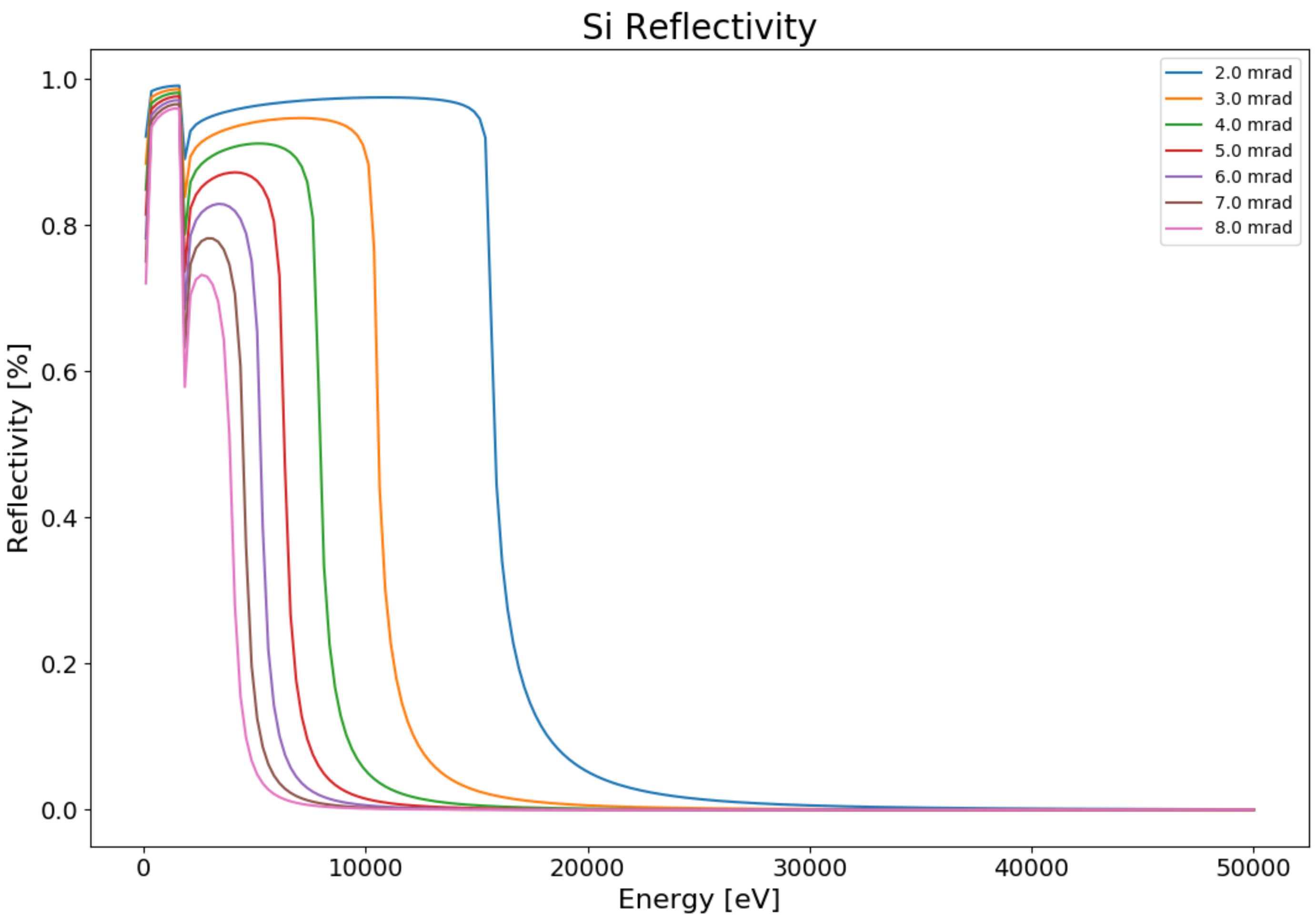
		Some numbers
Plane	Re-direction/filtering	R>100km
Cylindrical	1D focusing	R~ 100's m
Spherical	2D focusing	R~ 100's m
Paraboloid	Infinity to point (or viceversa)	a ~ cm, f ~ m
Elliptical	Point to point focusing	r>>r`
Toroidal	Astigmatic focusing	R ~ 100m, ρ ~ 10's cm

All this with an rms roughness ~ nm or less

A quick look at reflectivities

$$\theta_c = \sqrt{2\delta} \propto \lambda\sqrt{Z}$$





The higher the energy, the more grazing the incidence angle (1mrad = 0.057°, 1° = 17mrad)

Source for examples

Spatial Dimensions:

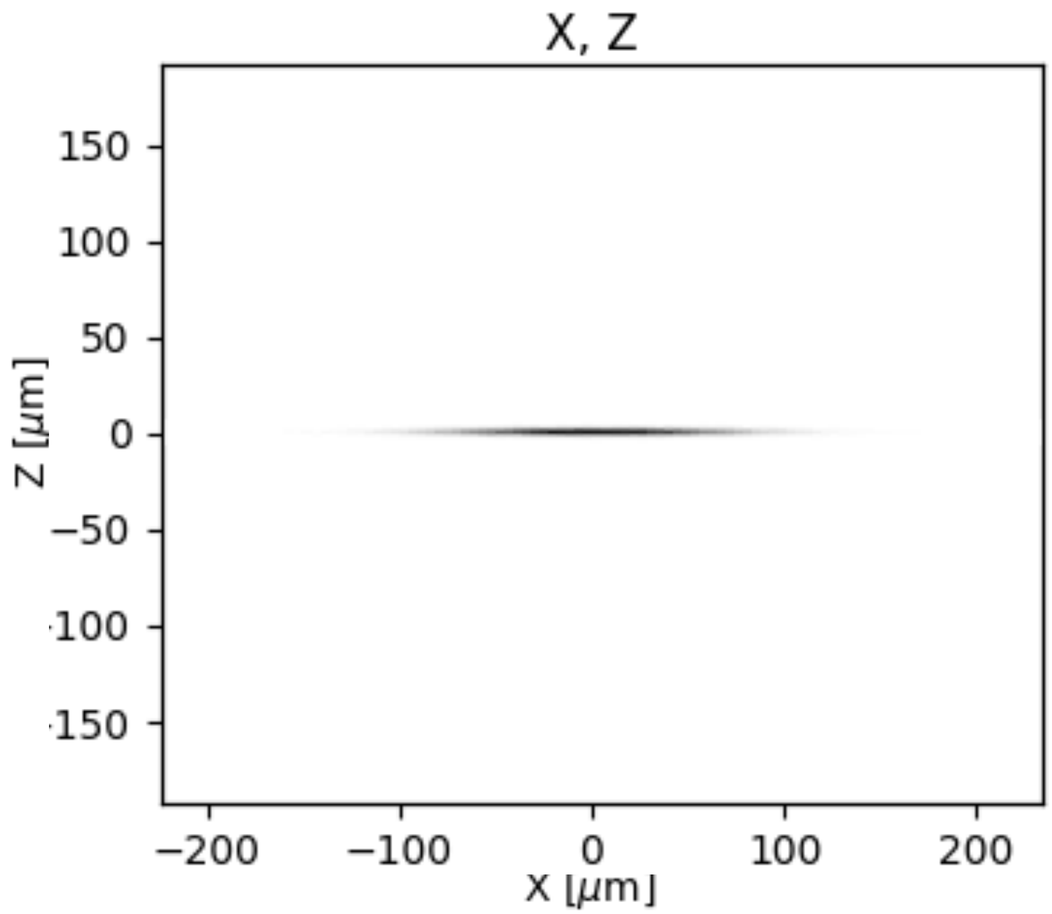
$$\sigma_x = 48\mu m \qquad \sigma_z = 1.3\mu m$$

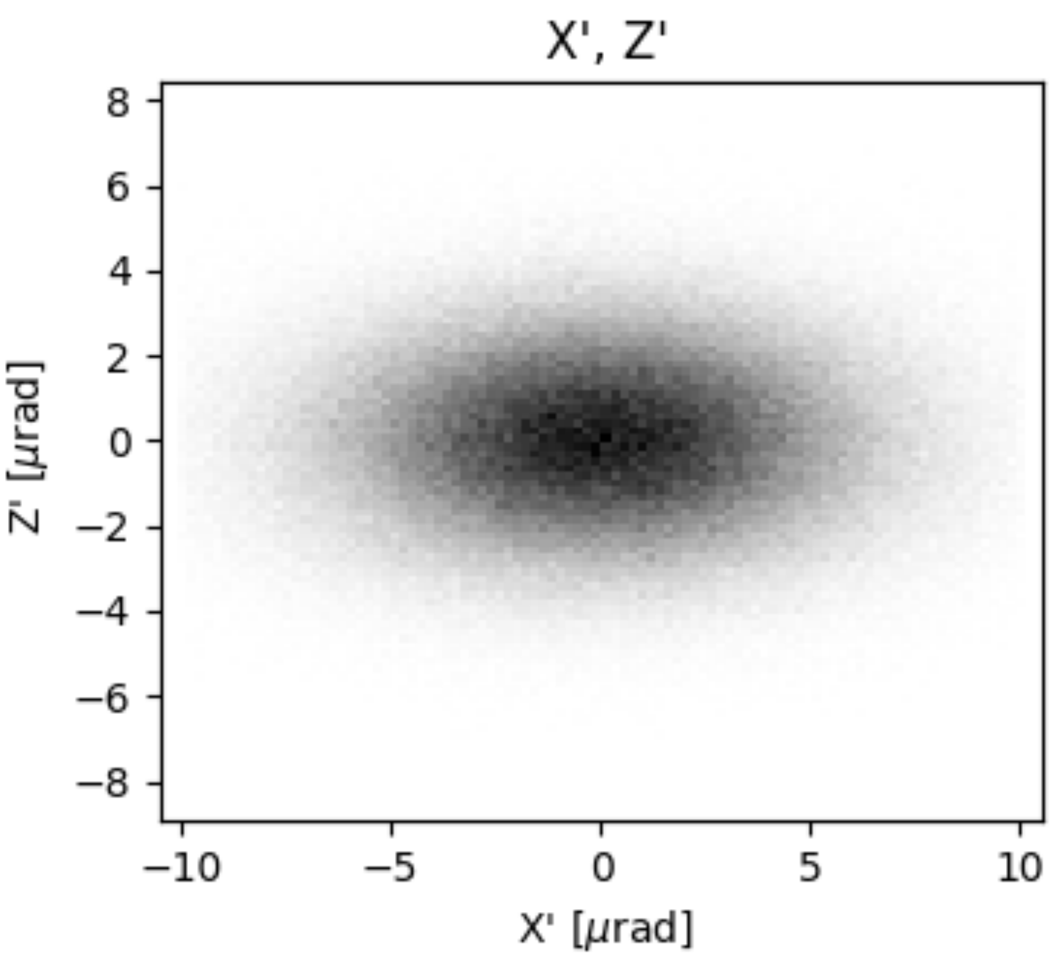
FWHM (X)=105 μm FWHM(Z)=3 μm

Angular dimensions:

$$\sigma_x' = 3.8\mu rad \qquad \sigma_z' = 1.82\mu rad$$

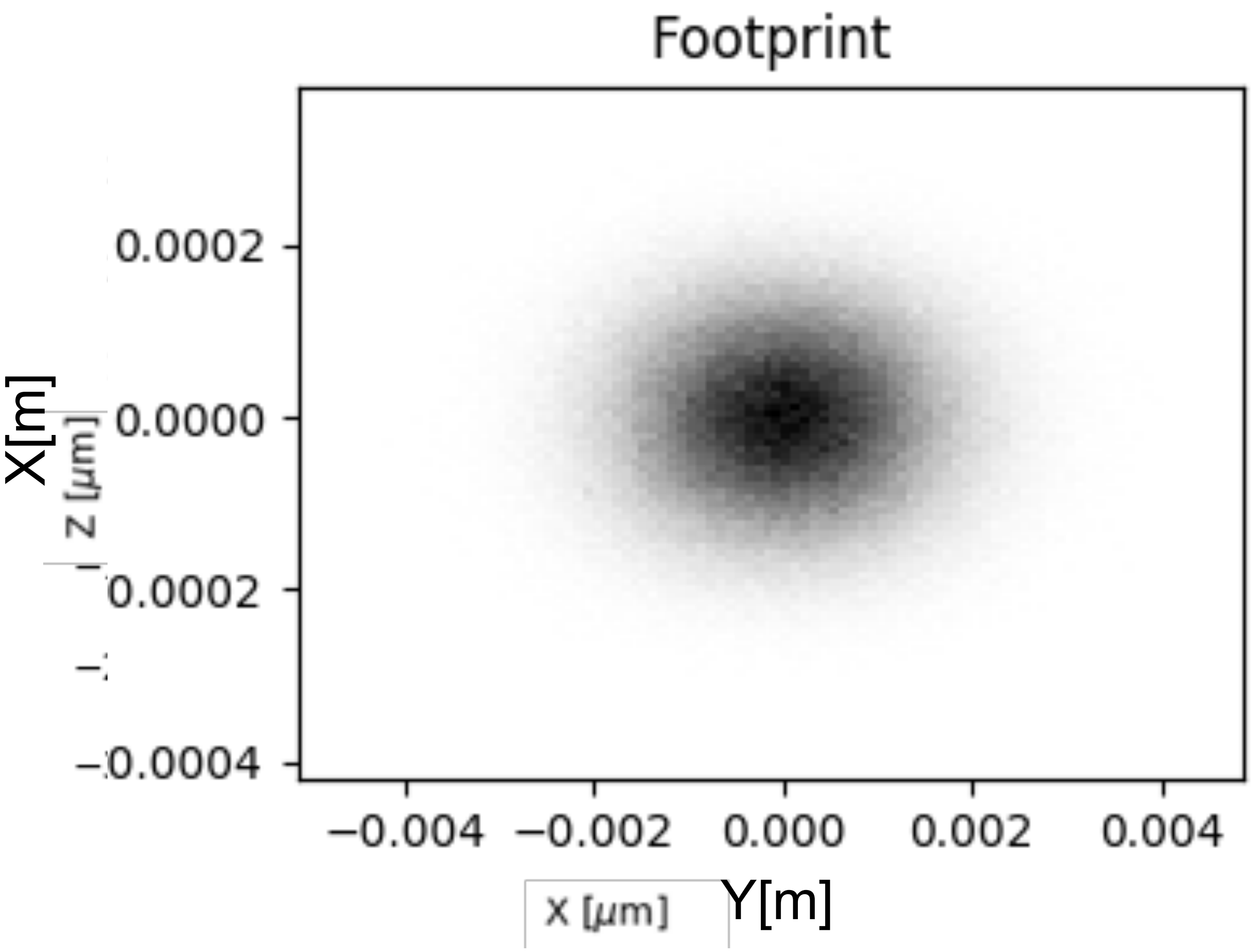
FWHM (X')=8.6 μrad FWHM(Z')=4.2 μrad





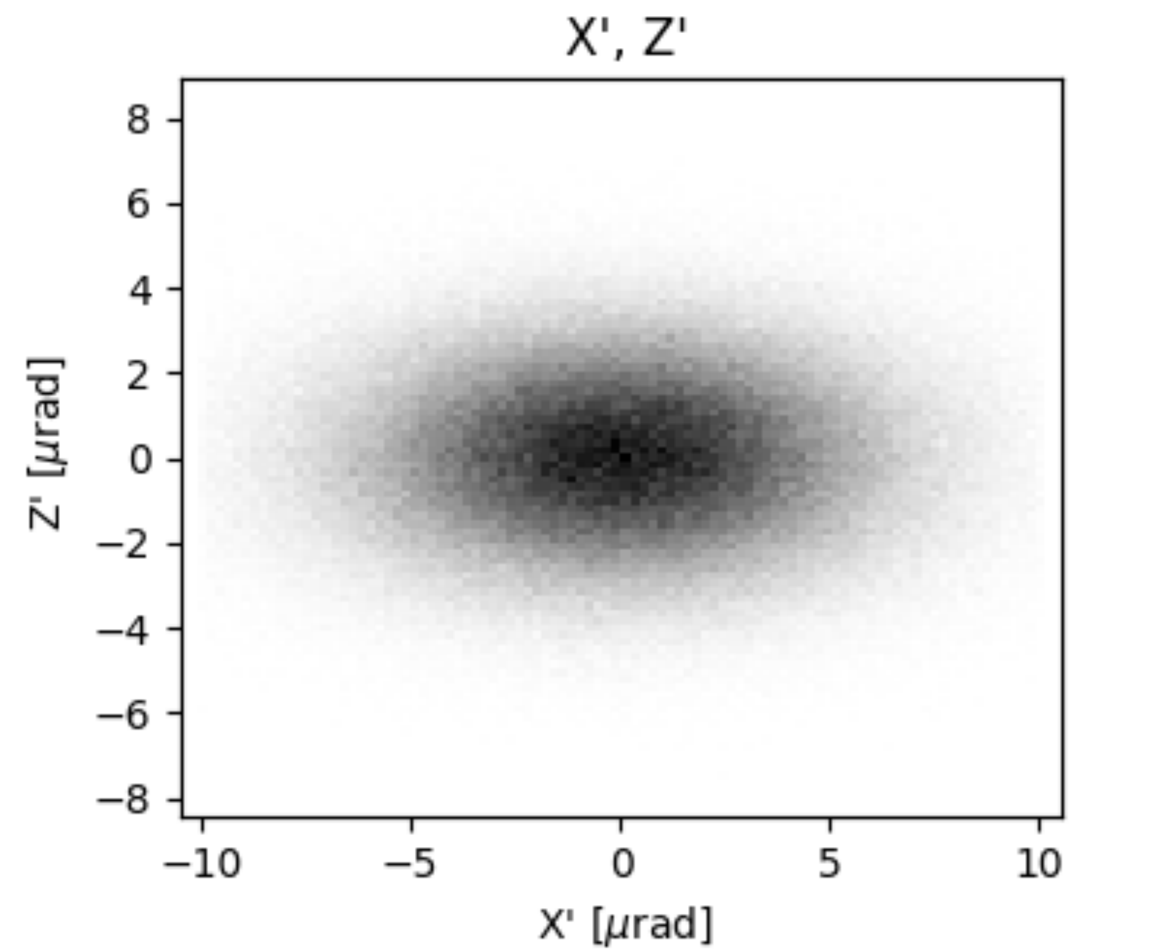
Plane mirror, r = 20 m, r’ =20 m, $\theta = 88°$

Spatial Dimensions:



FWHM(X)=250 µm FWHM(Z)=150 µm

Angular dimensions:



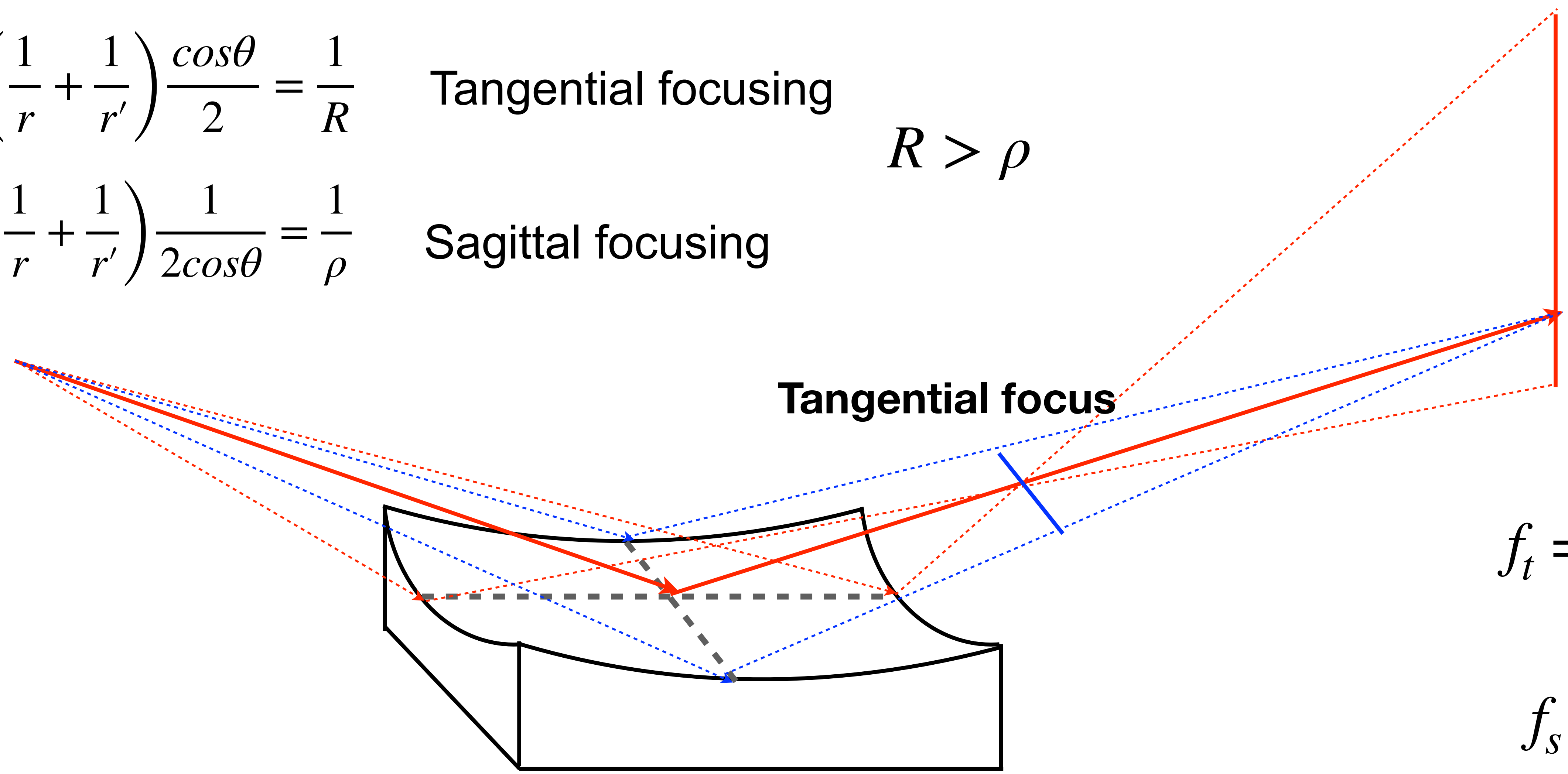
FWHM (X’)=8.6 µrad FWHM(Z’)=4.2 µrad

Toroidal mirror: focussing properties

$$\left(\frac{1}{r}+\frac{1}{r'}\right)\frac{cos\theta}{2}=\frac{1}{R}$$ Tangential focusing

$$\left(\frac{1}{r}+\frac{1}{r'}\right)\frac{1}{2cos\theta}=\frac{1}{\rho}$$ Sagittal focusing

$$R > \rho$$



$$f_t=\frac{R\cdot cos\theta}{2}$$

$$f_s=\frac{\rho}{2cos\theta}$$

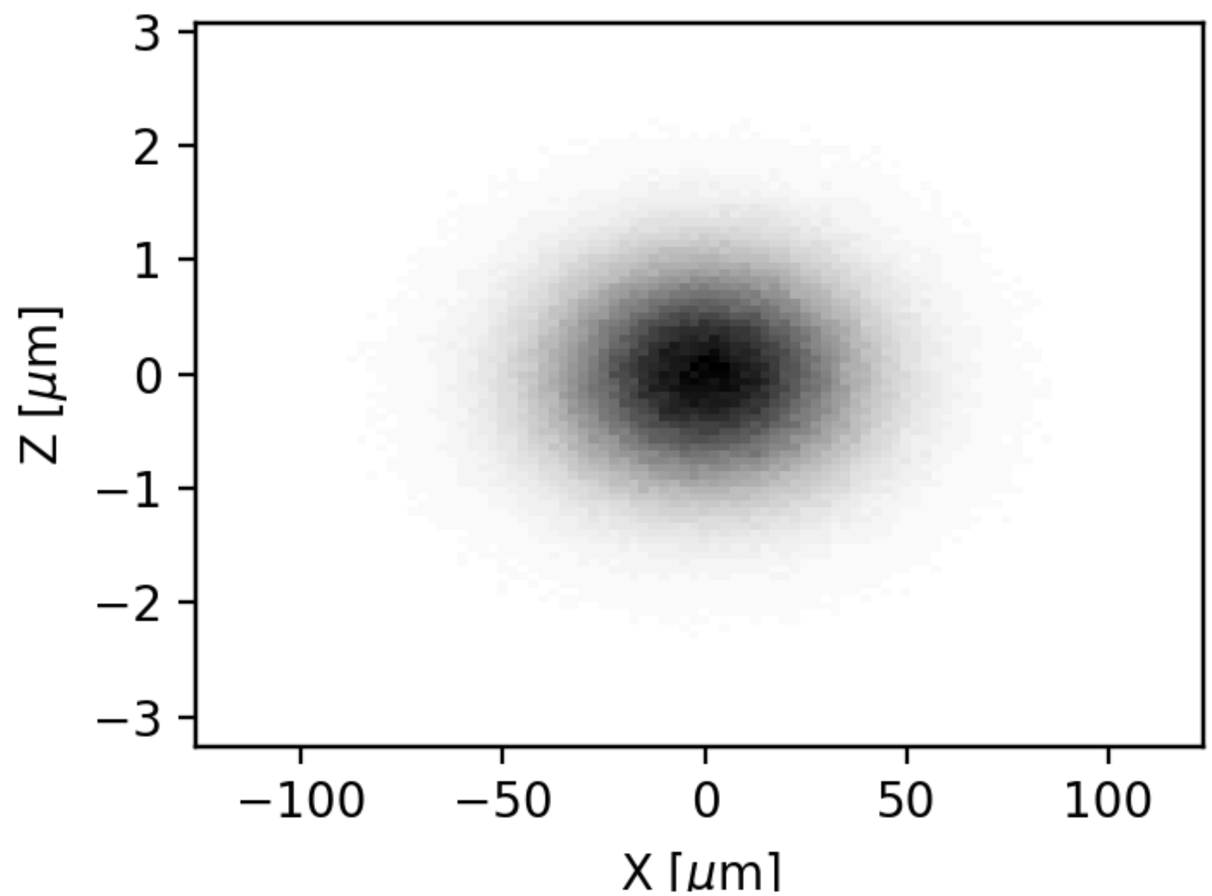
Condition for a stigmatic image of a point source:

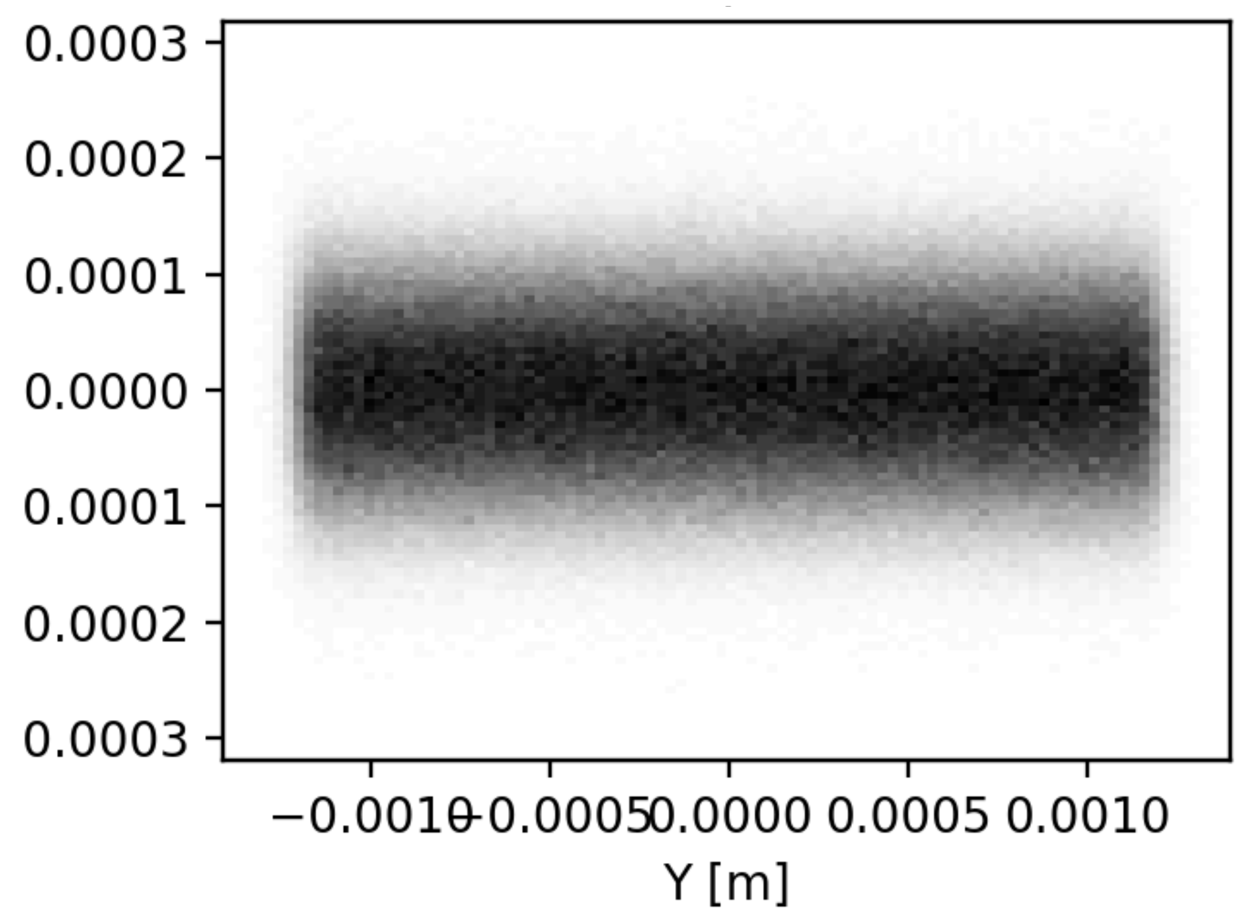
$$\frac{\rho}{R}=cos^2\theta$$

Toroidal mirror, r = 20 m, r' =10 m, $\theta = 88°$

$$R = \left(\left(\frac{1}{r} + \frac{1}{r'} \right) \frac{cos\theta}{2} \right)^{-1} = 382 \text{ m} \qquad \rho = \left(\left(\frac{1}{r} + \frac{1}{r'} \right) \frac{1}{2cos\theta} \right)^{-1} = 0.46 \text{ m}$$

$$f_t = \frac{R \cdot cos\theta}{2} = 6.6 \text{ m} \qquad f_s = \frac{\rho}{2cos\theta} = 6.6 \text{ m}$$





FWHM (X)=55 μm FWHM(Z)=1.5μm

FWHM (Y)=2.4mm FWHM(X)=0.2 mm

Spherical mirrors

Same as toroidal mirrors with:

$$R = \rho$$

$$\left(\frac{1}{r}+\frac{1}{r'}\right)\frac{cos\theta}{2}=\frac{1}{R} \qquad \left(\frac{1}{r}+\frac{1}{r'}\right)\frac{1}{2cos\theta}=\frac{1}{R}$$

$$f_t = \frac{R\cdot cos\theta}{2}$$

$$f_s = \frac{R}{2cos\theta}$$

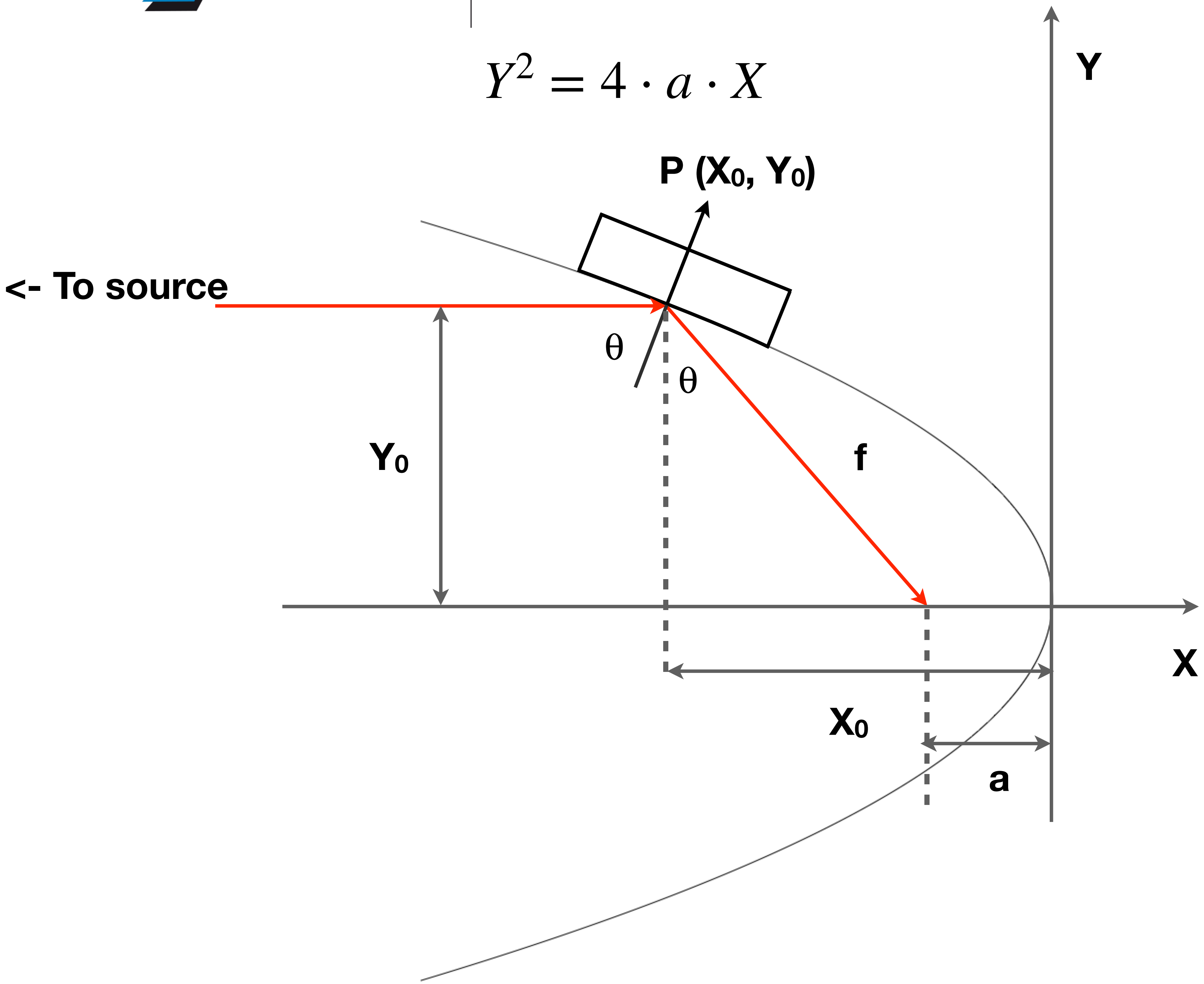
A stigmatic image is only possible if:

$$\frac{\rho}{R} = cos^2\theta = 1$$

i.e. this is possible only for normal incidence!

Paraboloidal mirror

$$Y^2 = 4 \cdot a \cdot X$$



P (X0, Y0):

$$X_0 = a \cdot tan^2\theta$$

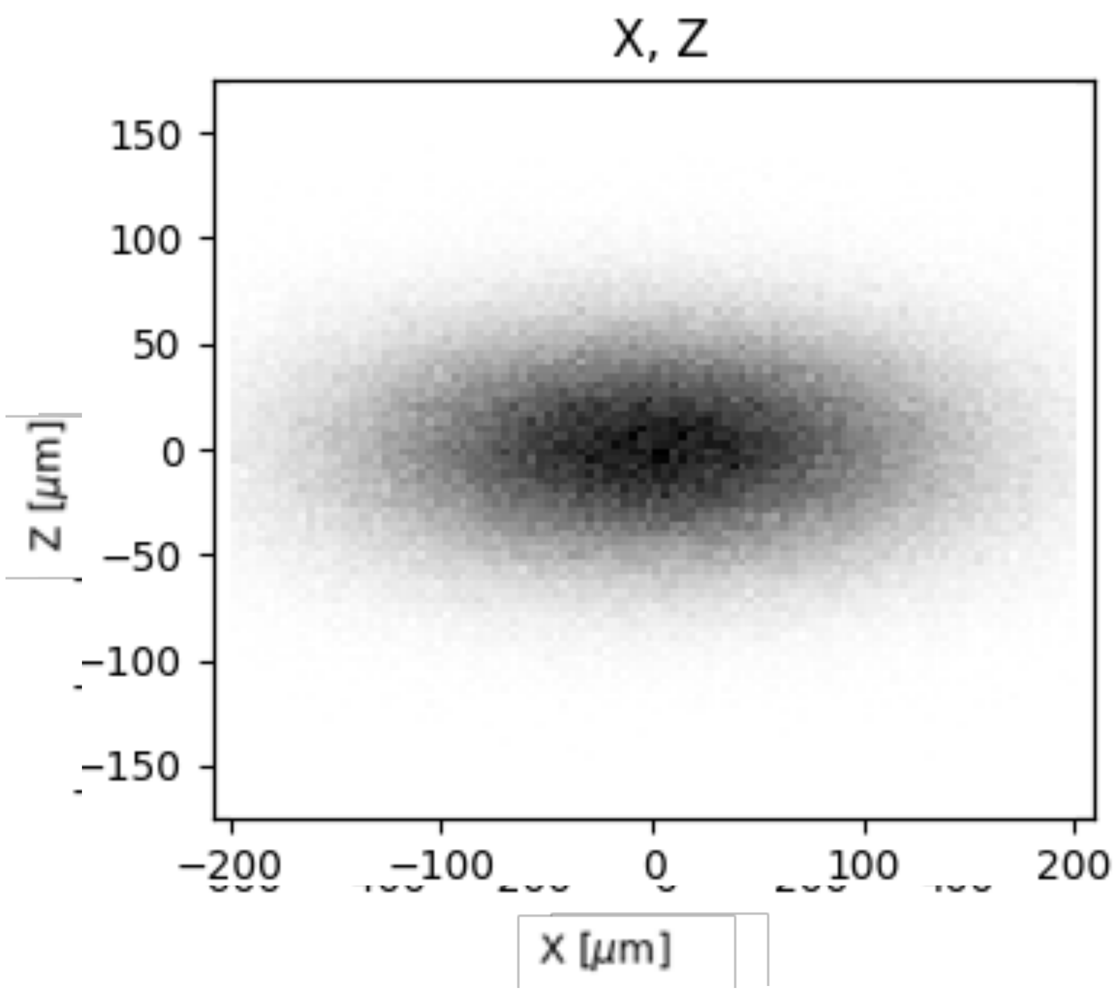
$$Y_0 = 2a \cdot tan\theta$$

$$f = \frac{a}{cos^2\theta}$$

Paraboloidal mirror, r = 20 m, r' =20 m, $\theta = 88°$

Parabola parameter $a = f\cos^2\theta$ = 0.02435m

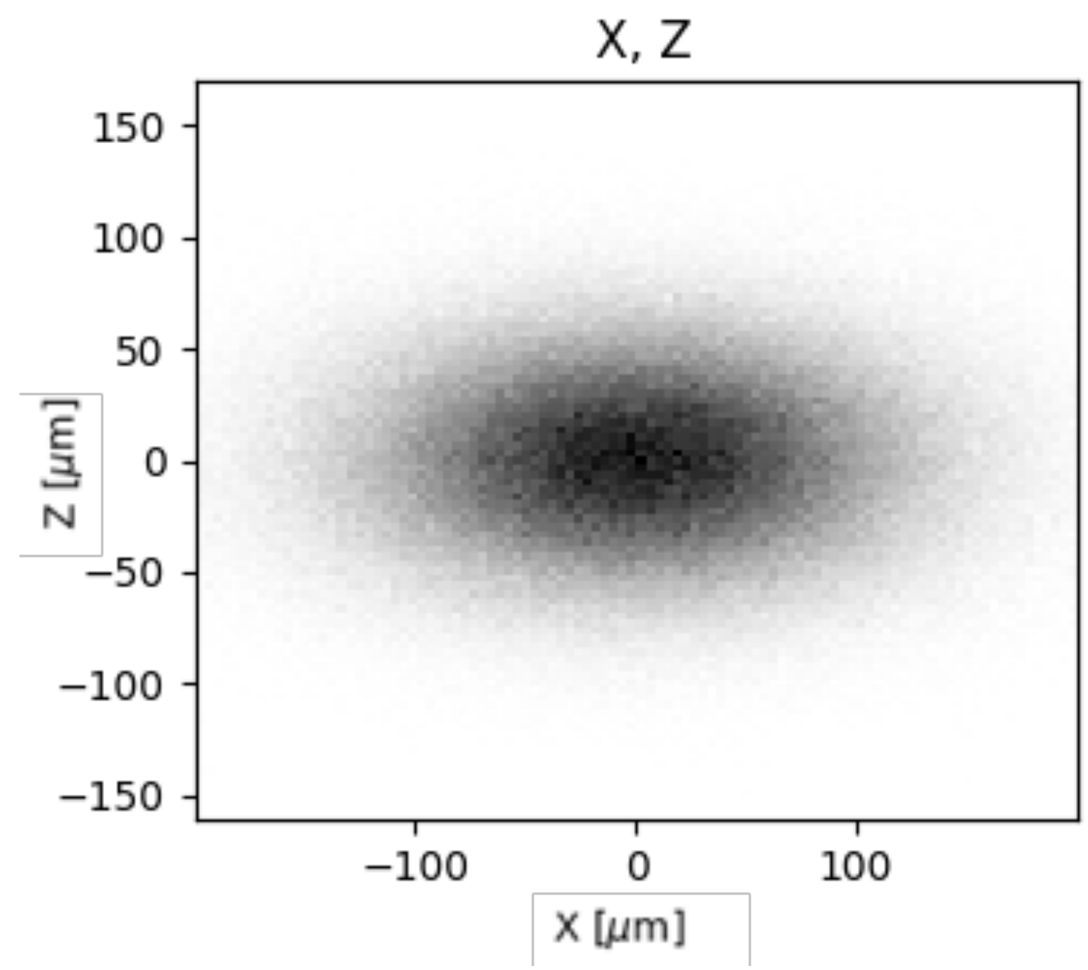
Source image @ 20 mt



FWHM (X)=201 µm FWHM(Z)=85 µm

FWHM (X')=8.6 µrad FWHM(Z')=4.2 µrad

Paraboloidal Mirror image



FWHM (X)=172 µm FWHM(Z)=83 µm

FWHM (X')=5.2µrad FWHM(Z')=0.1µrad

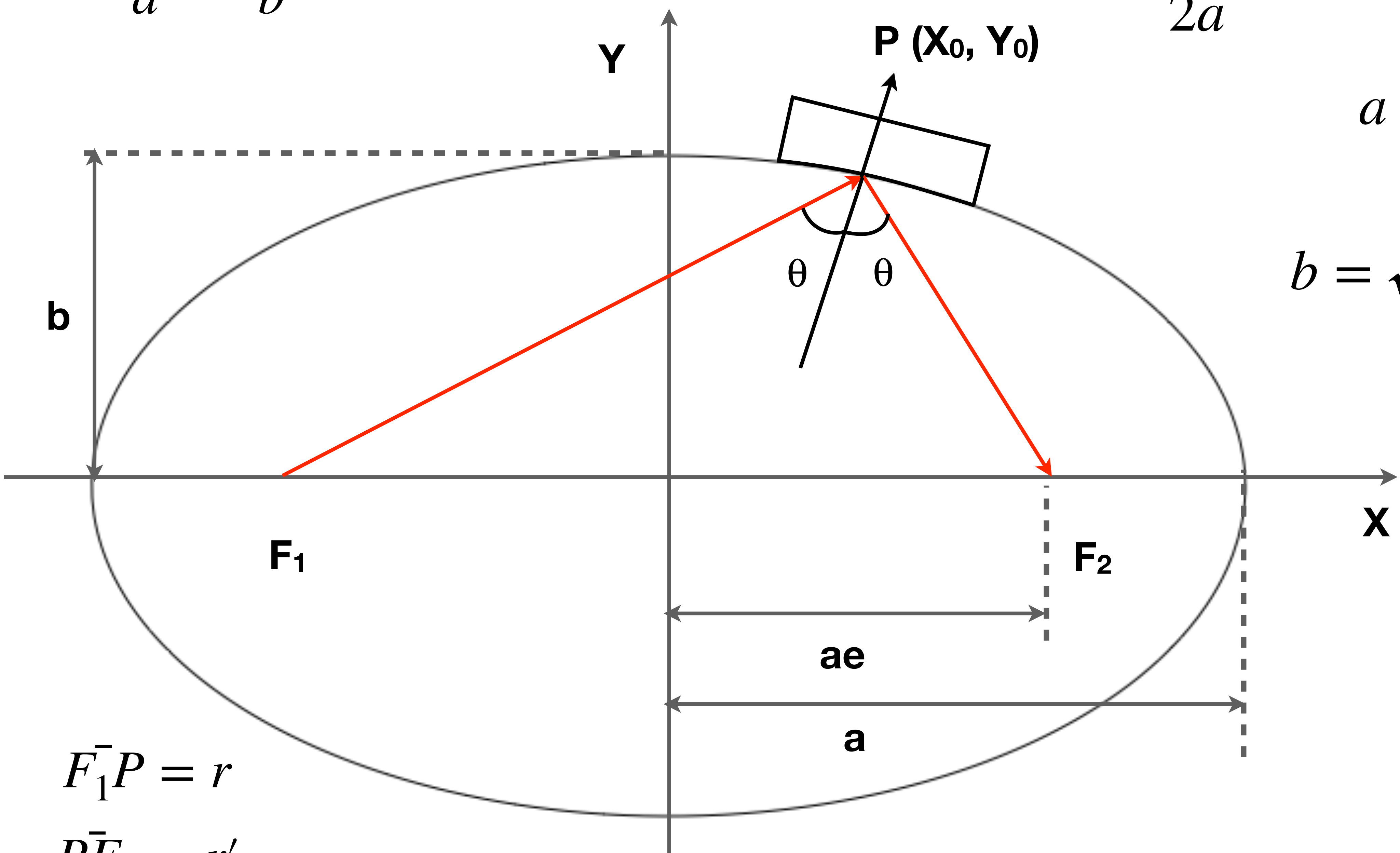
Ellipsoidal mirror

$$\frac{X^2}{a^2} + \frac{Y^2}{b^2} = 1$$

$$e = \frac{1}{2a}\sqrt{r^2 + r'^2 - 2rr'cos2\theta}$$

$$a = \frac{(r + r')}{2}$$

$$b = \sqrt{a^2\left(1 - e^2\right)}$$



$$\overline{F_1P} = r$$

$$\overline{PF_2} = r'$$

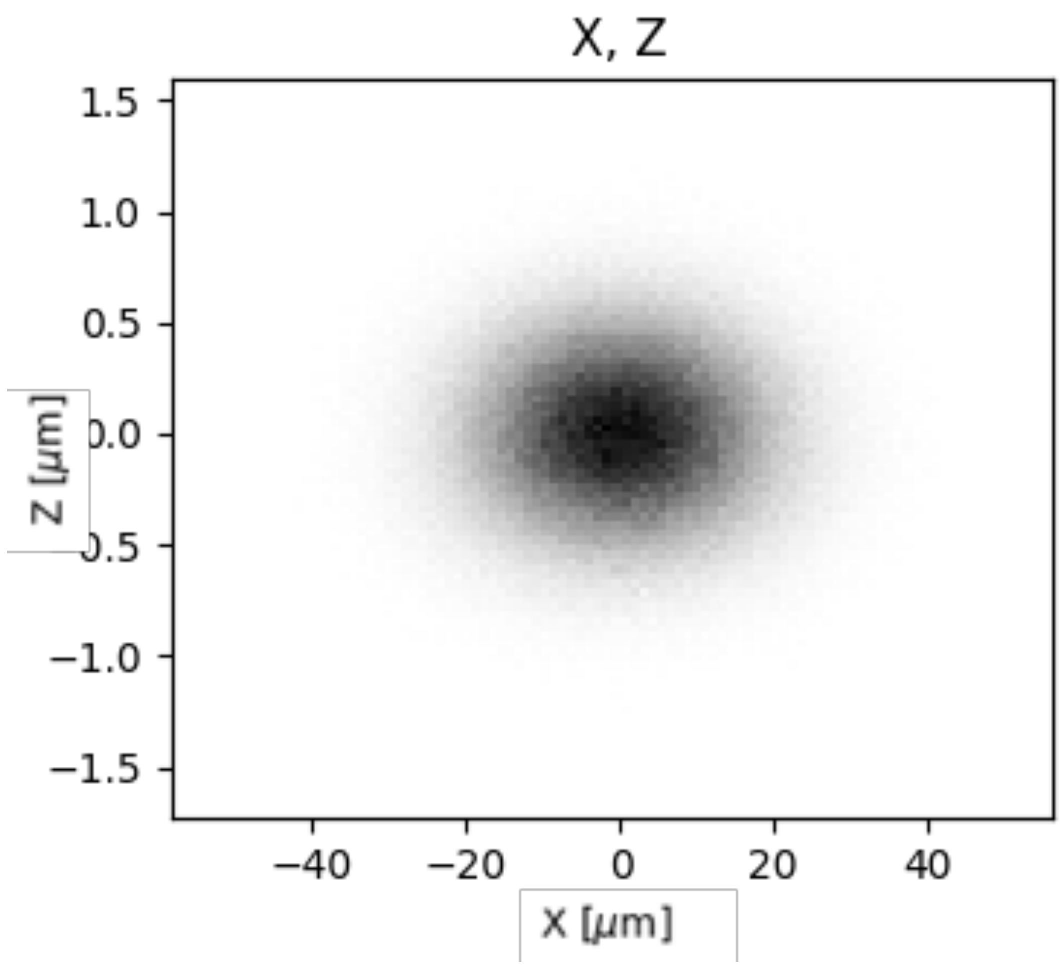
Ellipsoidal mirror, r = 20 m, r' =5 m, $\theta = 88°$

a = 12.5 m, b = 0.349 m, e=0.999610

Our source dimensions are: FWHM (X)=105 μm FWHM(Z)=3 μm

$$M = \frac{r'}{r} = 0.25$$

i.e. we expect a focus of ~ 26 x 0.75 μm (FWHM)

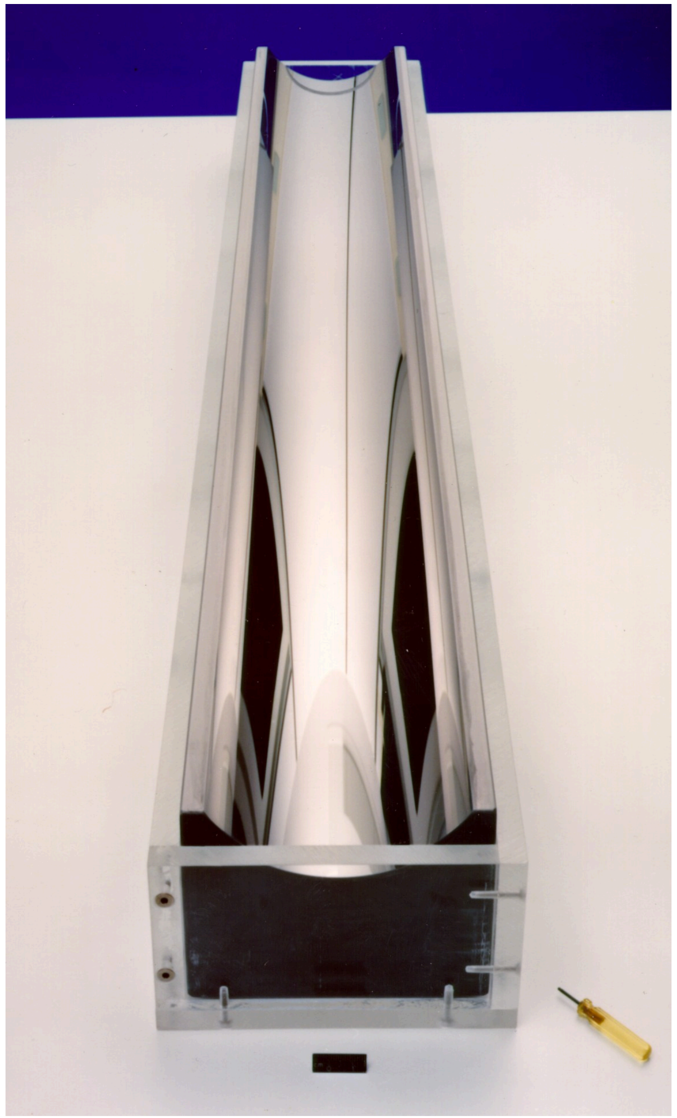


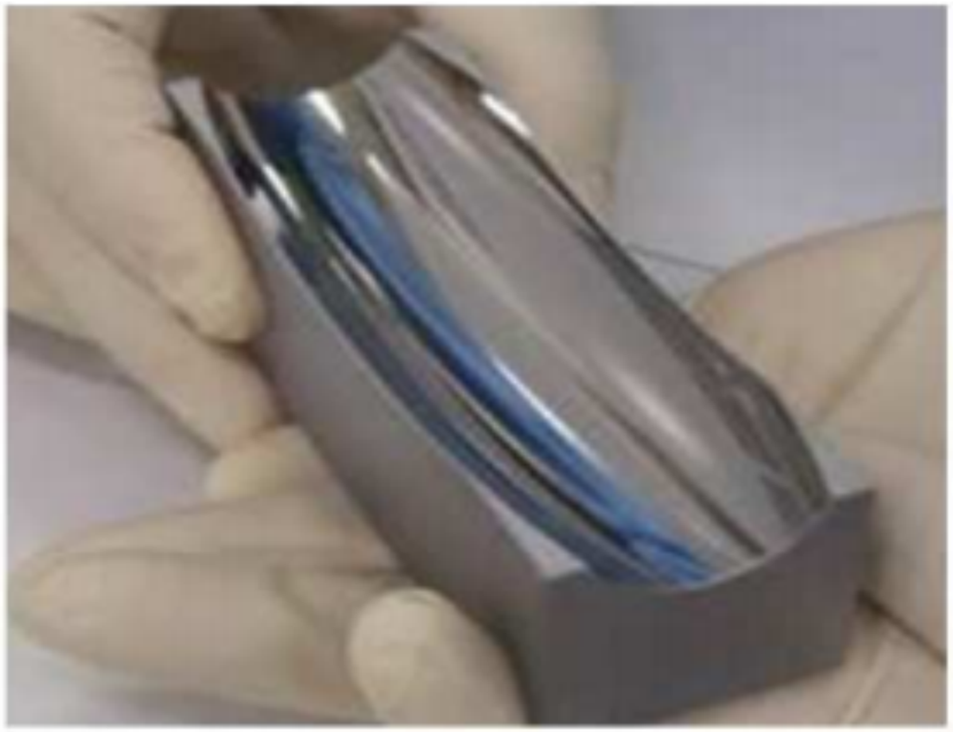
FWHM (X)=26 μm FWHM(Z)=0.7 μm

WARNING!

All the simulations above are for educational purposes!

- Reflectivity set to 1, and independent of energy
- Ideal source
- No mirror errors (roughness, figure errors, etc)





http://www.esrf.eu/home/UsersAndScience/Experiments/CBS/ID09/OpticsHutch/mirror.html

http://www.crystal-scientific.com/mirror_plano.html

R. Radhakirshnan et al,
DOI 10.1149/07711.1255ecst

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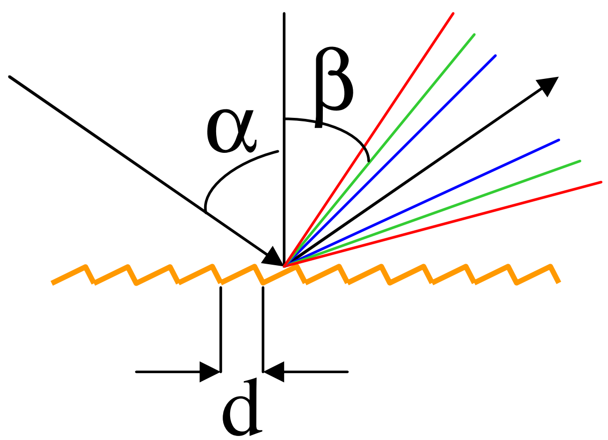
Diffracting elements

Gratings
Crystals
Multilayers
Zone Plates

Monochromatization
Focussing

Usage: Overwhelmingly for monochromatization

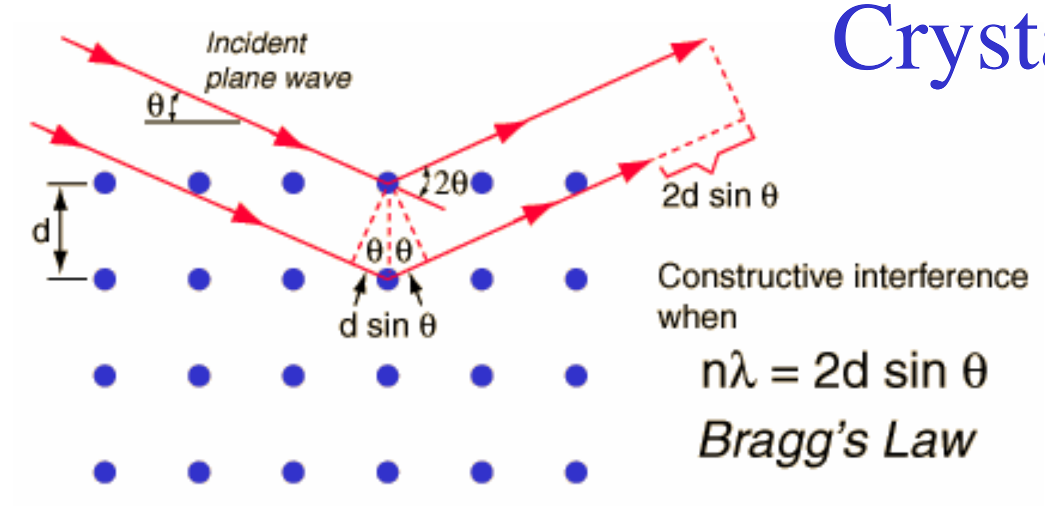
Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray



Grating

Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Crystal



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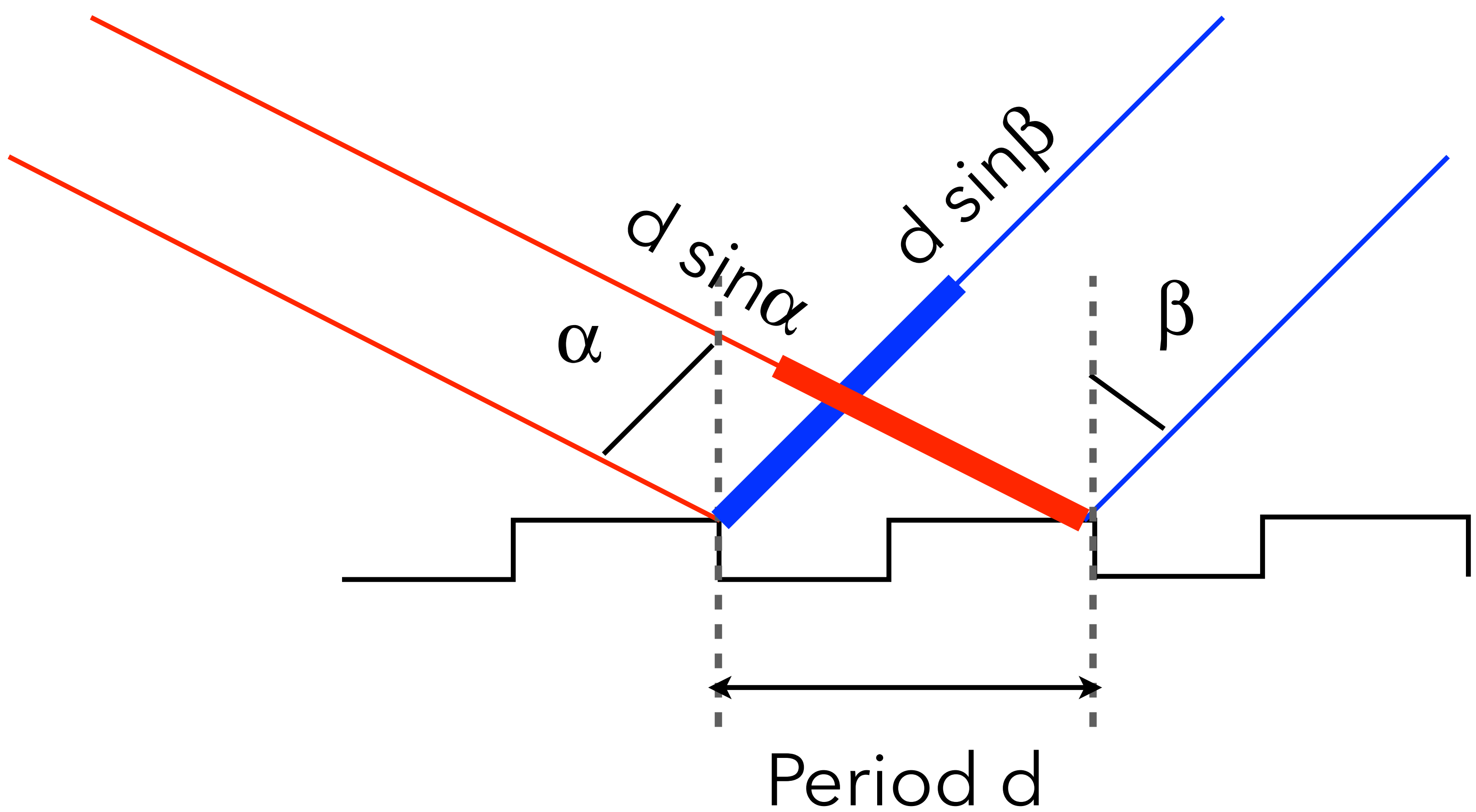
Diffraction gratings

Artificial periodic structure, with a precisely defined period d.



Grating equation

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

m is the diffraction order

α and β have opposite signs if on opposite side of the surface normal

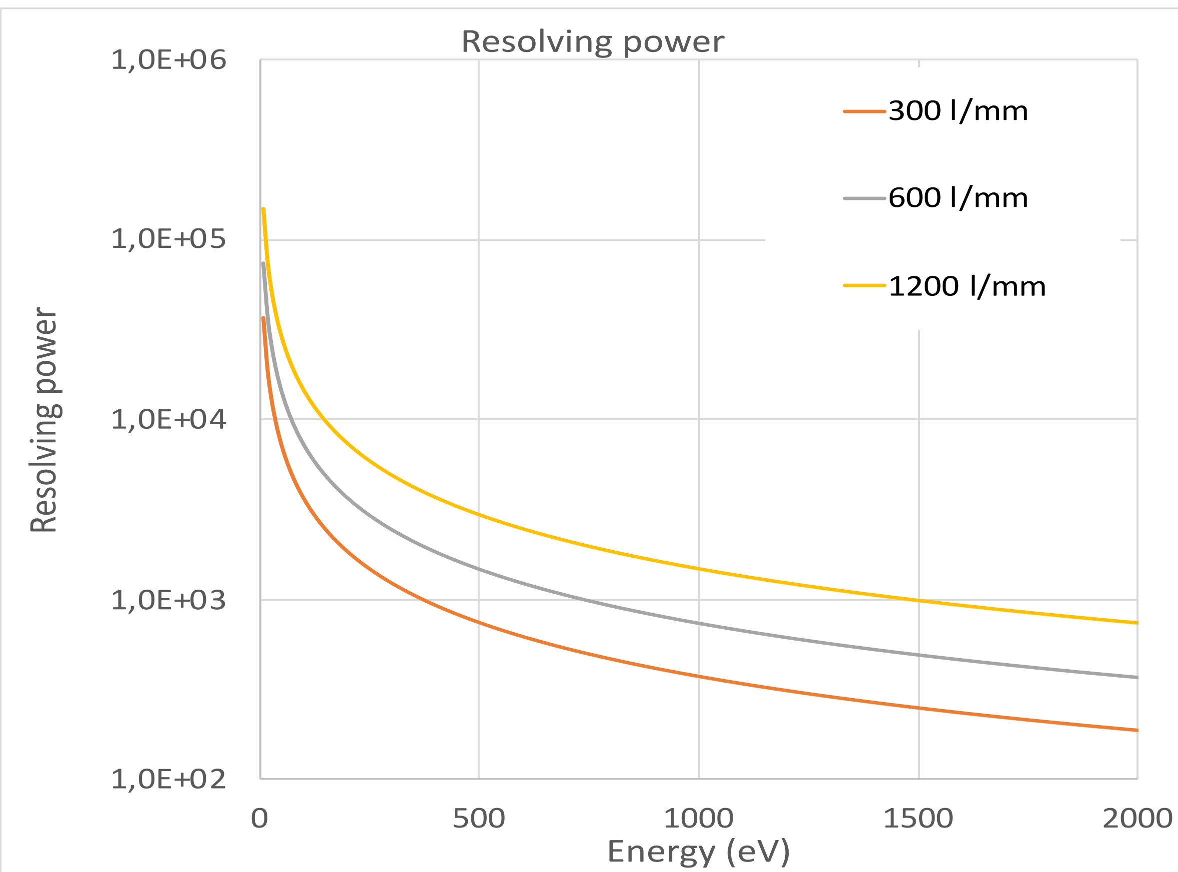
Line density

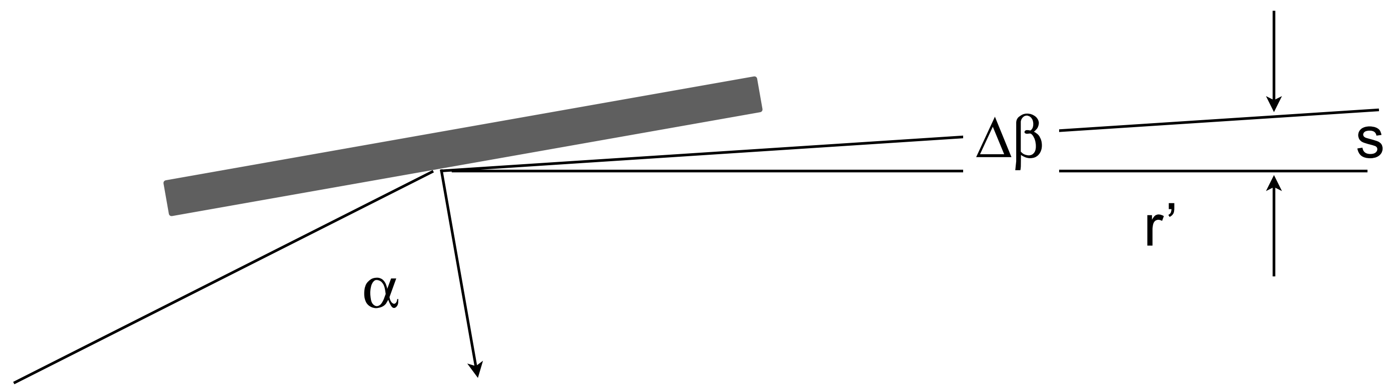
$$L = \frac{1}{d}$$

Grating resolving power

Angular dispersion of a grating with line density L: $\Delta\lambda = \frac{s' \cos\beta}{Lmr'}$

Resolving power R: $R = \frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda} = \frac{\lambda L m r'}{s' \cos\beta}$



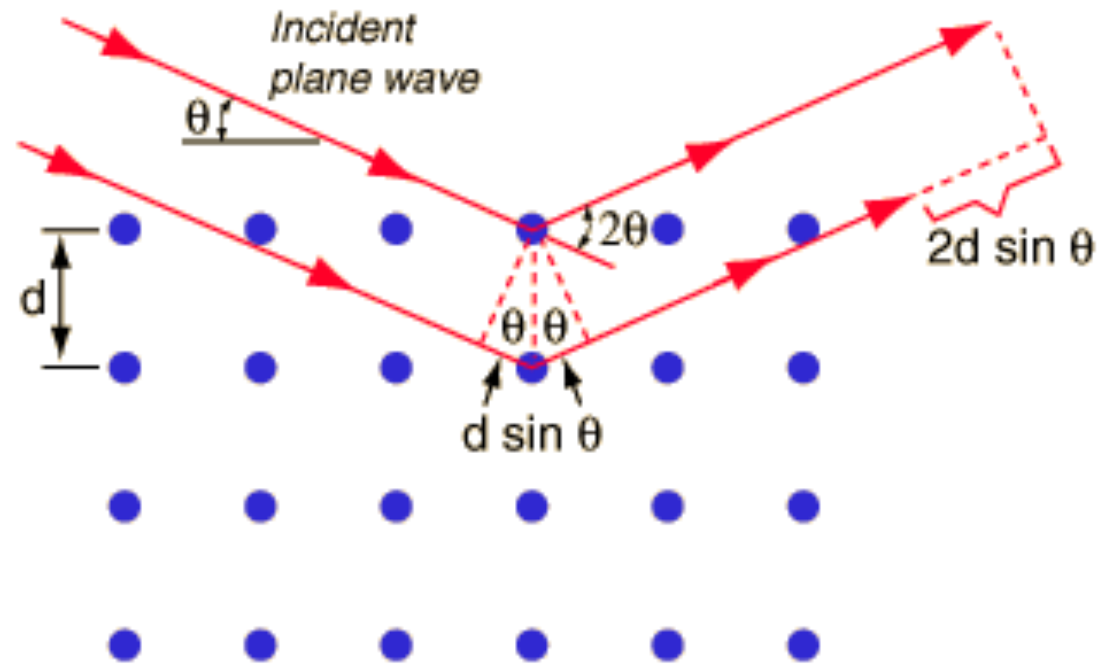


If R=1000, @ 100eV:

$\Delta E = 100 meV$

Crystals

Based on Bragg's law: $2d\sin\theta = m\lambda$



Since $\sin\theta \leq 1$, $\lambda \leq \lambda_{MAX}$ $(E \geq E_{MIN})$ =2d

Si(111): d=3.13 Å (E_{MIN}~2keV)

Si(311): d=1.64 Å (E_{MIN}~3.8keV)

InSb(111): d=3.74 Å (E_{MIN}~1.7keV)

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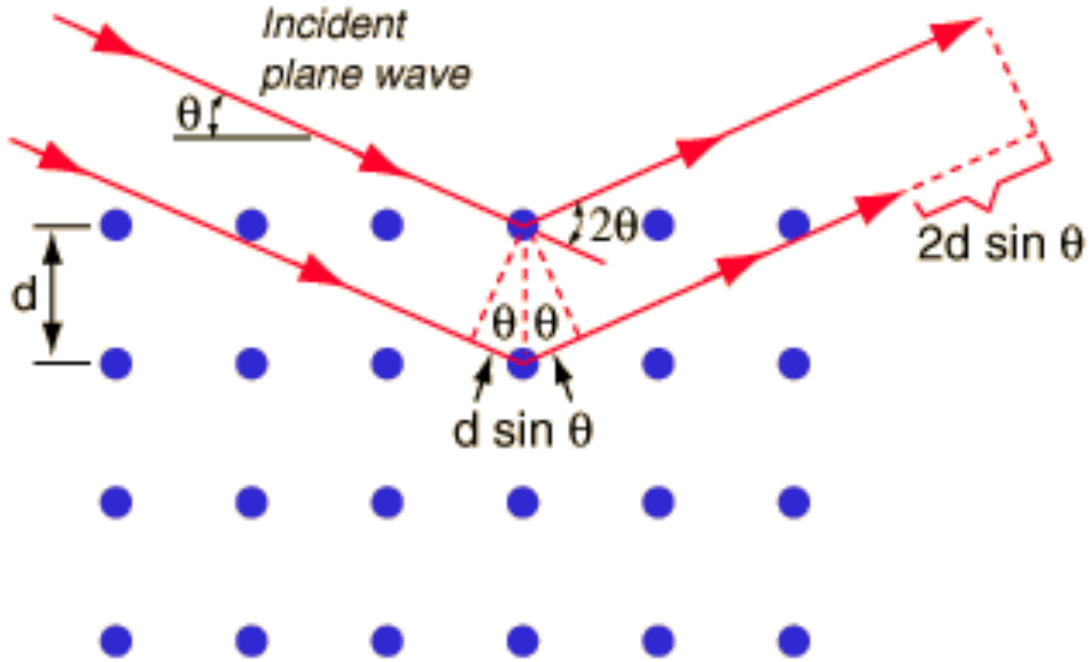
Crystals' resolving power



$$\frac{\Delta E}{E} = \frac{\Delta \lambda}{\lambda} = \Delta \theta \frac{\cos\theta}{\sin\theta}$$

Angular spread of the beam

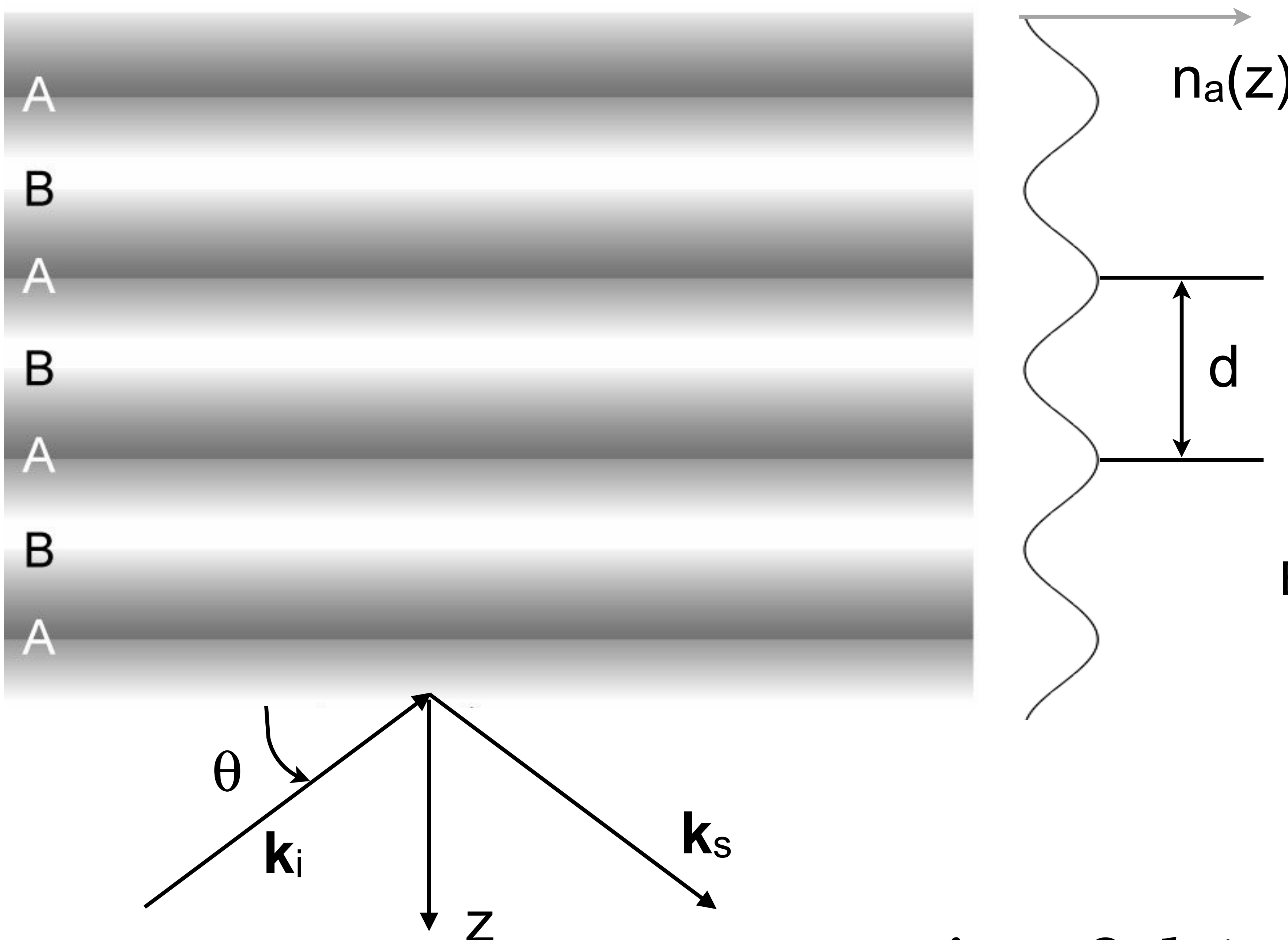
Where does $\Delta\theta$ come from?

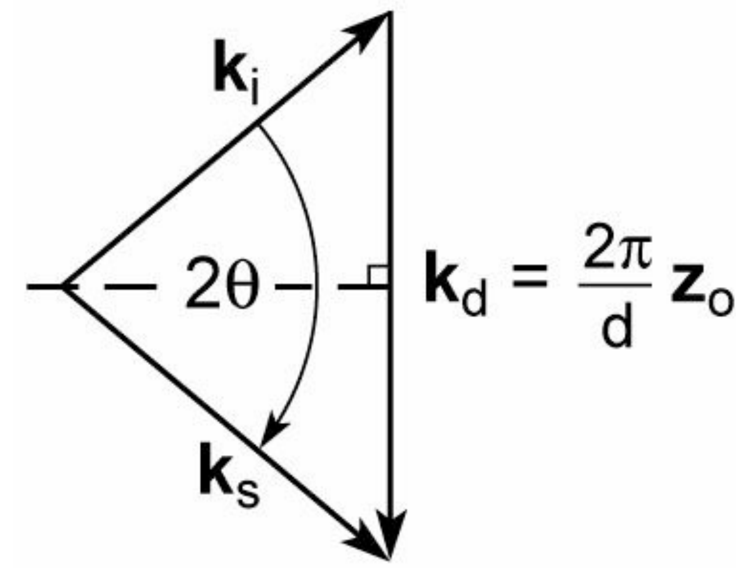
$\Delta\theta_{beam}$ Angular divergence of the incoming beam *

$\omega_{crystal}$ Intrinsinc width of Bragg reflection, the Darwin curve

* more on this later…

Multi-layer mirrors





$$\omega_s = \omega_i + \omega_d$$

$$\mathbf{k}_s = \mathbf{k}_i + \mathbf{k}_d$$

But $\omega_d = 0$, therefore:

$$|\mathbf{k}_s| = |\mathbf{k}_i| = 2\pi/\lambda$$

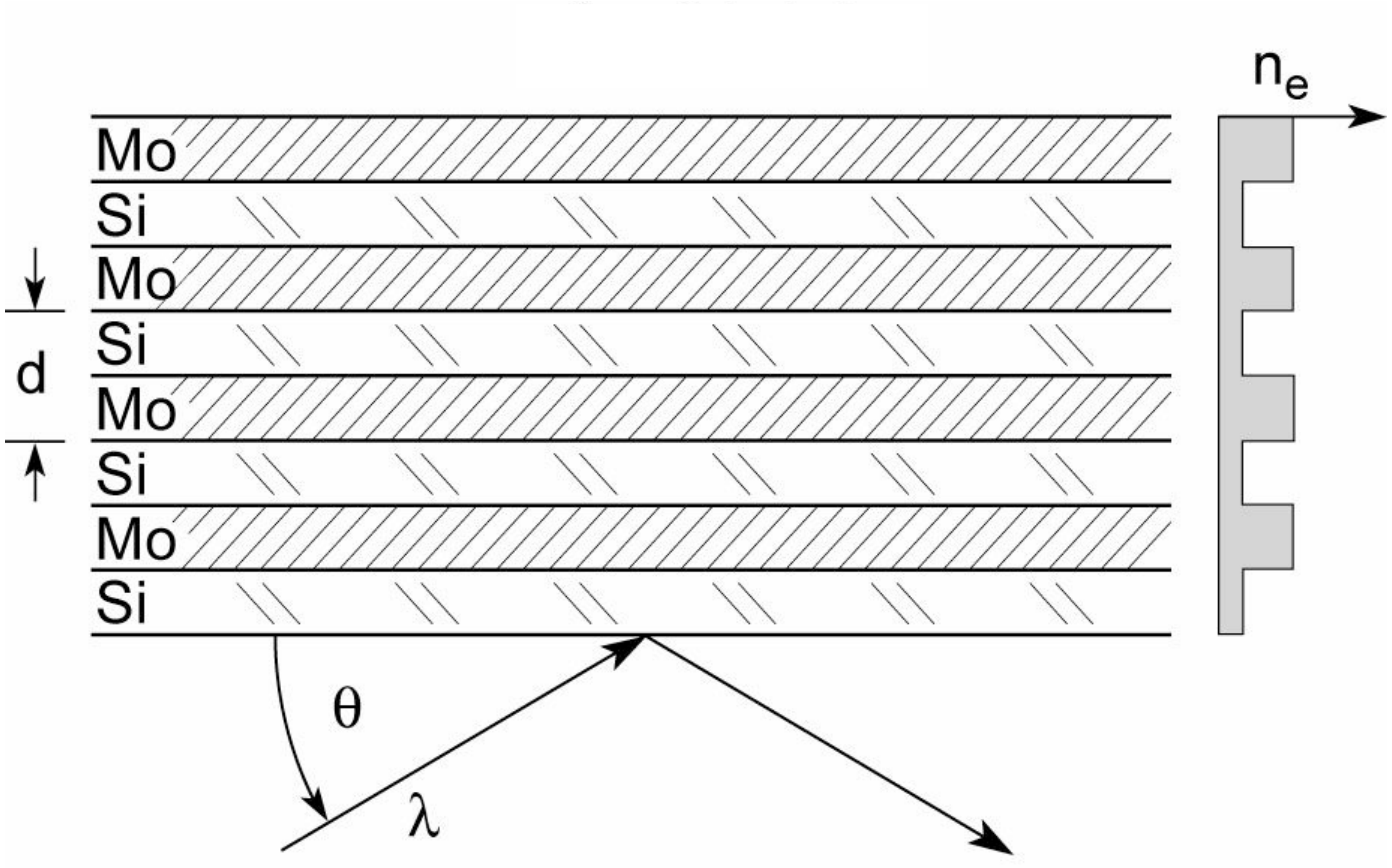
$$sin\theta = \frac{k_d/2}{k_i}$$

$$\lambda = 2dsin\theta$$

D. Attwood, *X-Rays and Extreme Ultraviolet Radiation*,Cambridge University Press, 2017

Multi-layer mirrors

What if $n_a(z)$ is still periodic, but not a simple sinusoid?



$$m\lambda = 2d\sin\theta$$

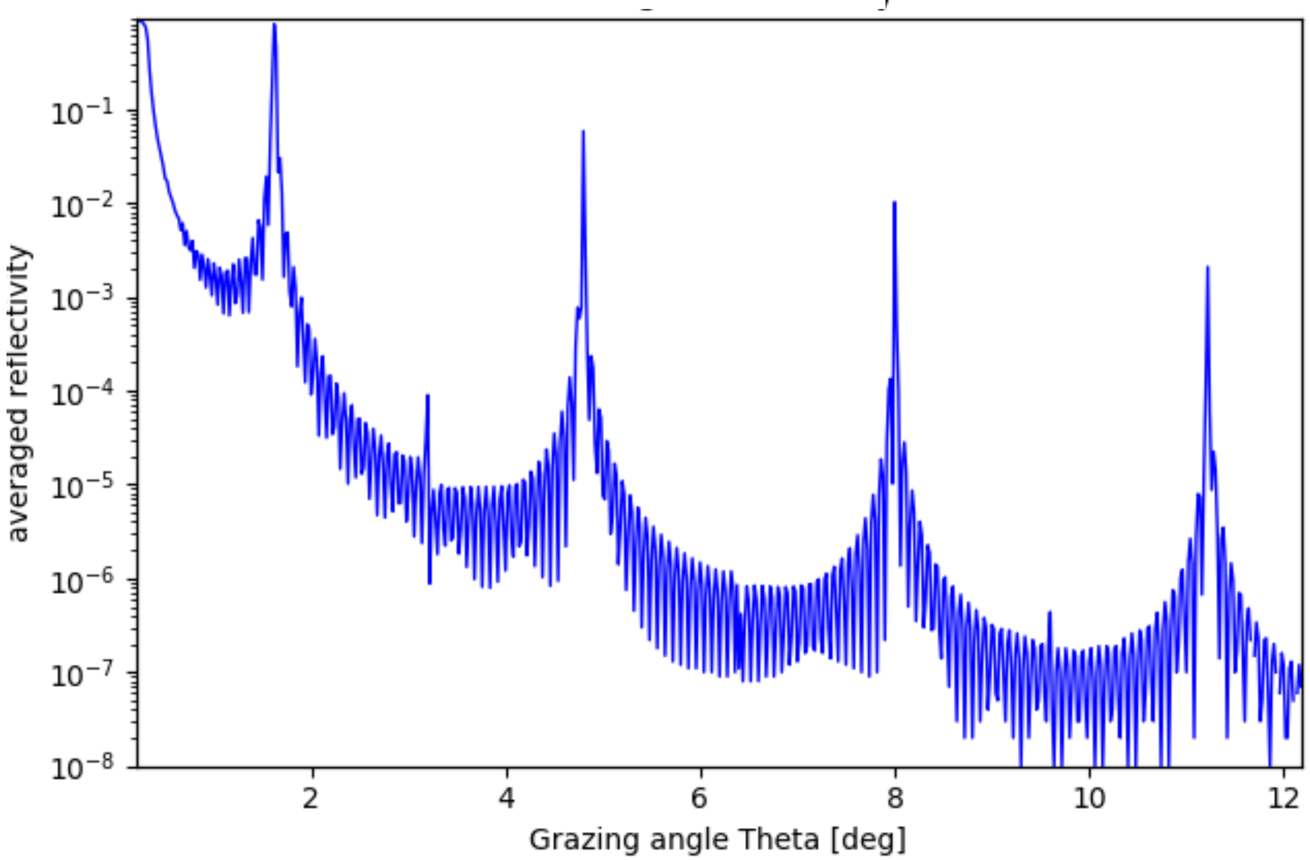
If $\theta = \pi/2$, and m=1:

$$\lambda = 2d$$

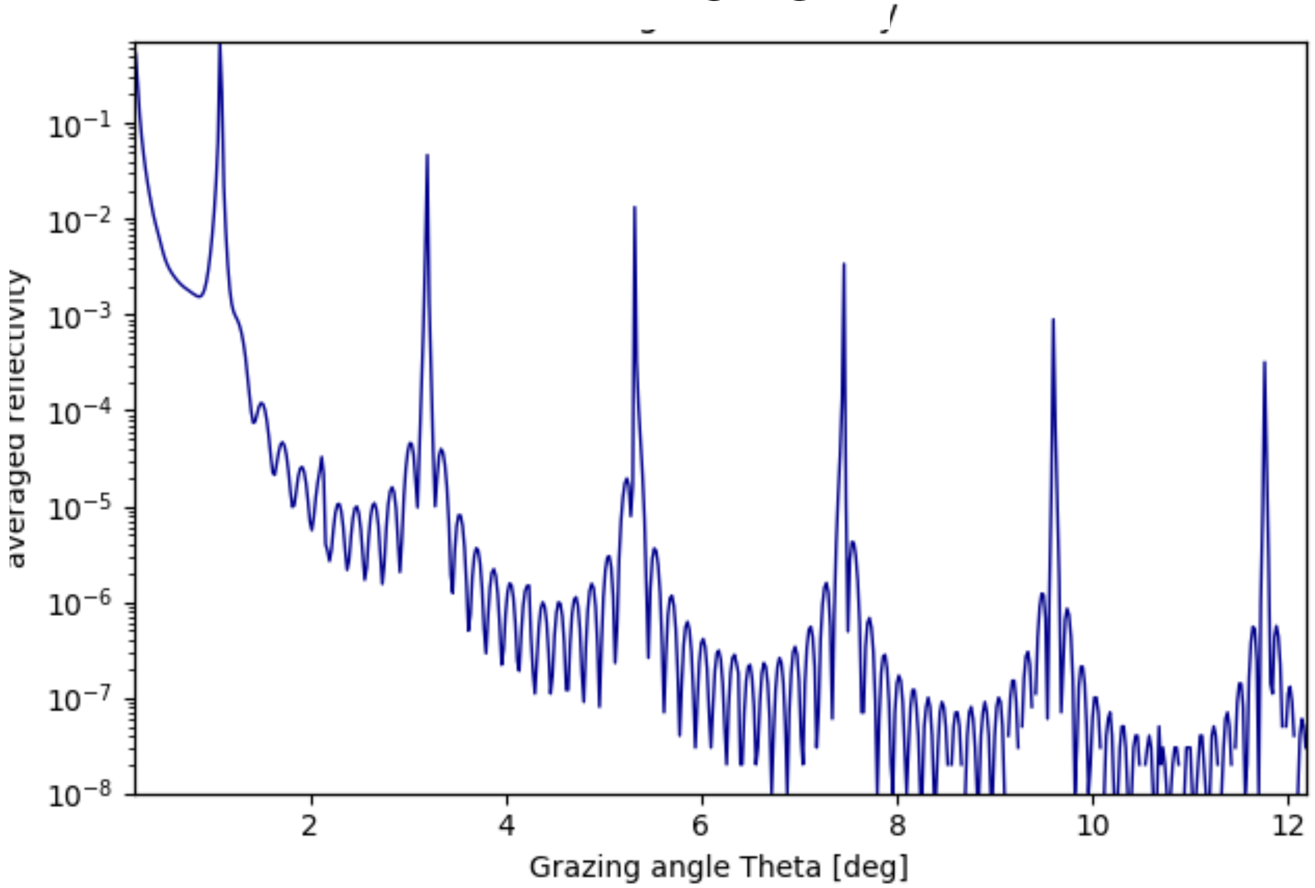
Multi-layer mirrors

W/C, d=22.3 Å, Γ=0.5, N= 100

E=10keV



E=15keV



Monochromator

The need for collimated illumination

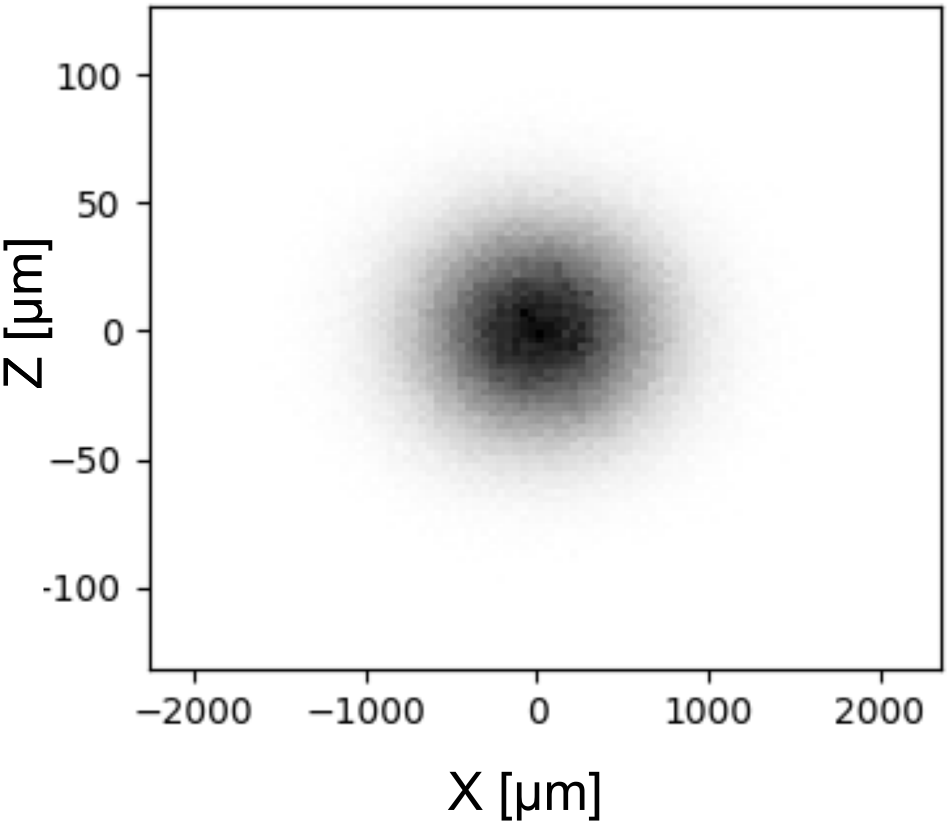
Crystals Energy resolution:

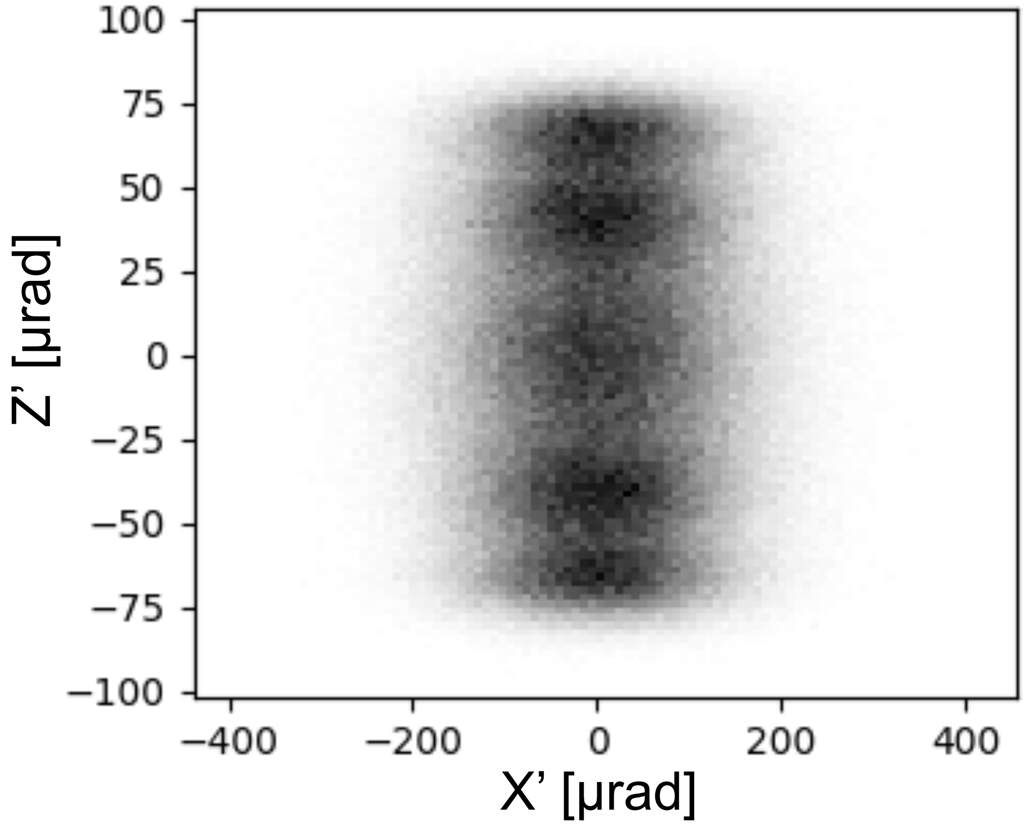
$$\frac{\Delta E}{E} = \frac{\Delta\lambda}{\lambda} = \Delta\theta \frac{\cos\theta}{\sin\theta}$$

Same for multilayers

Gratings

$$\frac{\Delta E}{E} = \frac{\Delta\lambda}{\lambda} = \frac{\cos\beta}{\lambda L m r'} \Delta\beta$$





Undulator

5th Harmonic (~1 keV)
ΔE=500eV

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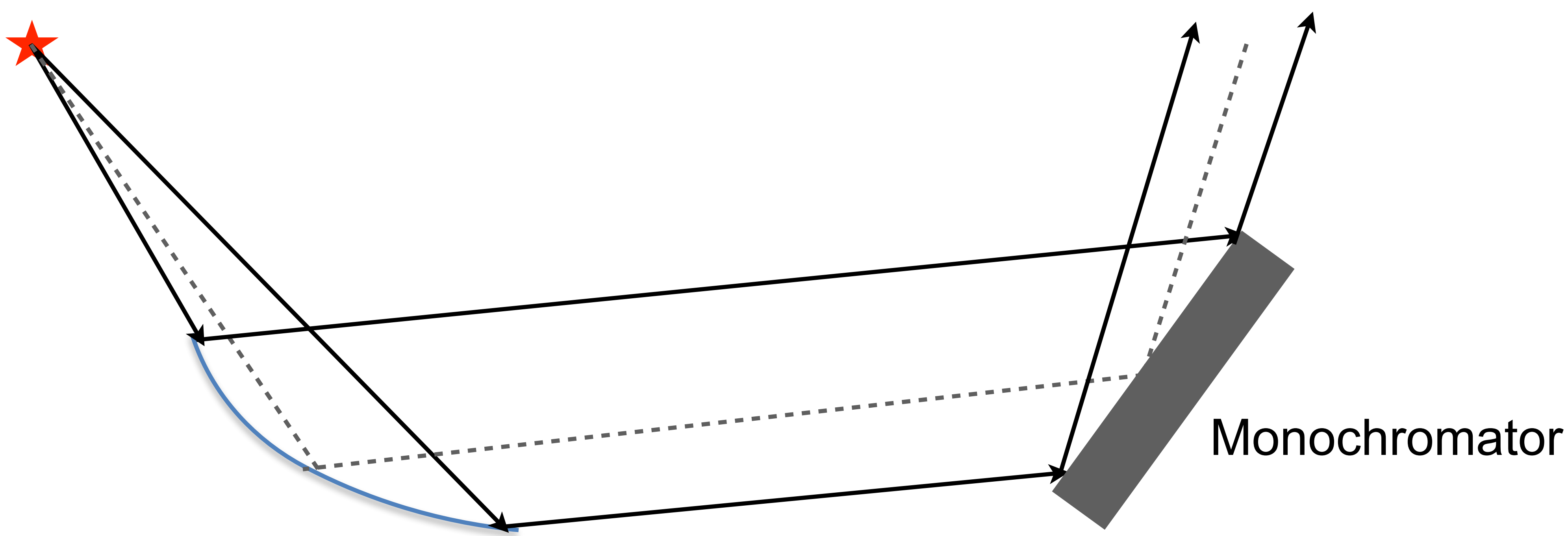
The need for collimated illumination

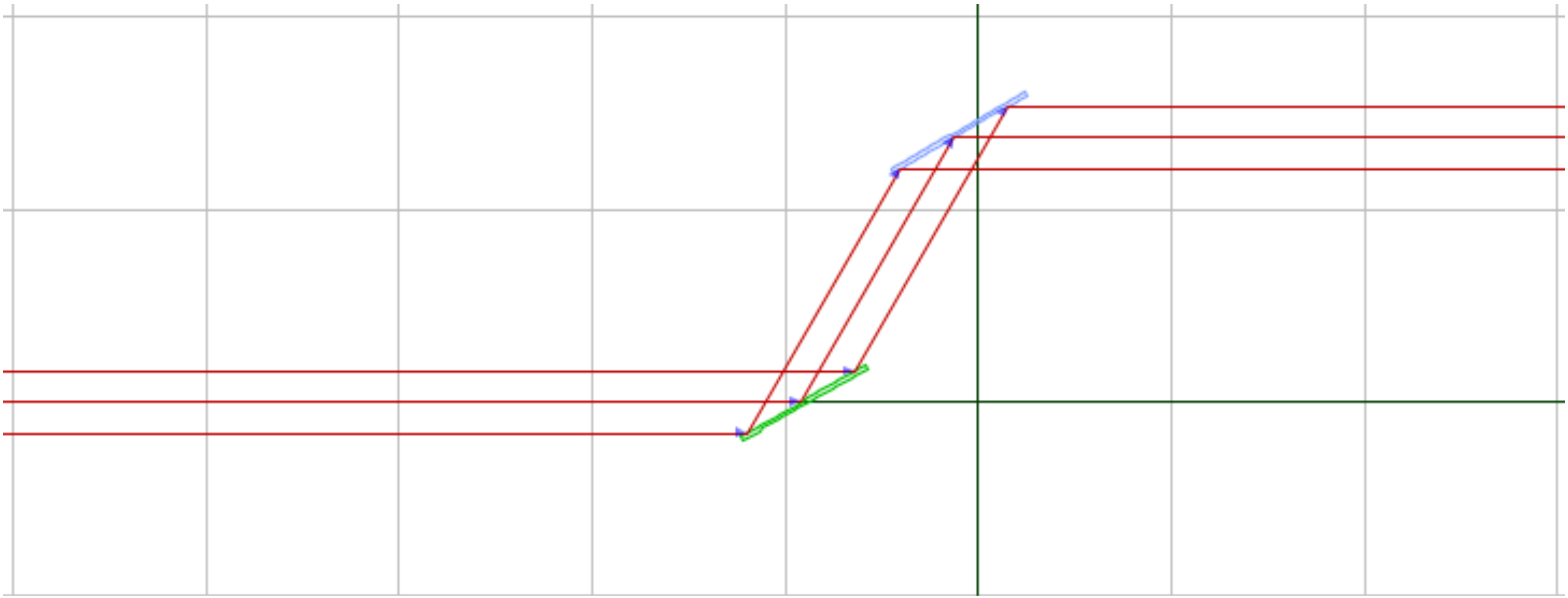
Collimating mirror before monochromator



Mirror calculated setting virtual source distance (r) very far (~100s m) *

* more on this later…

DCM in parallel configuration



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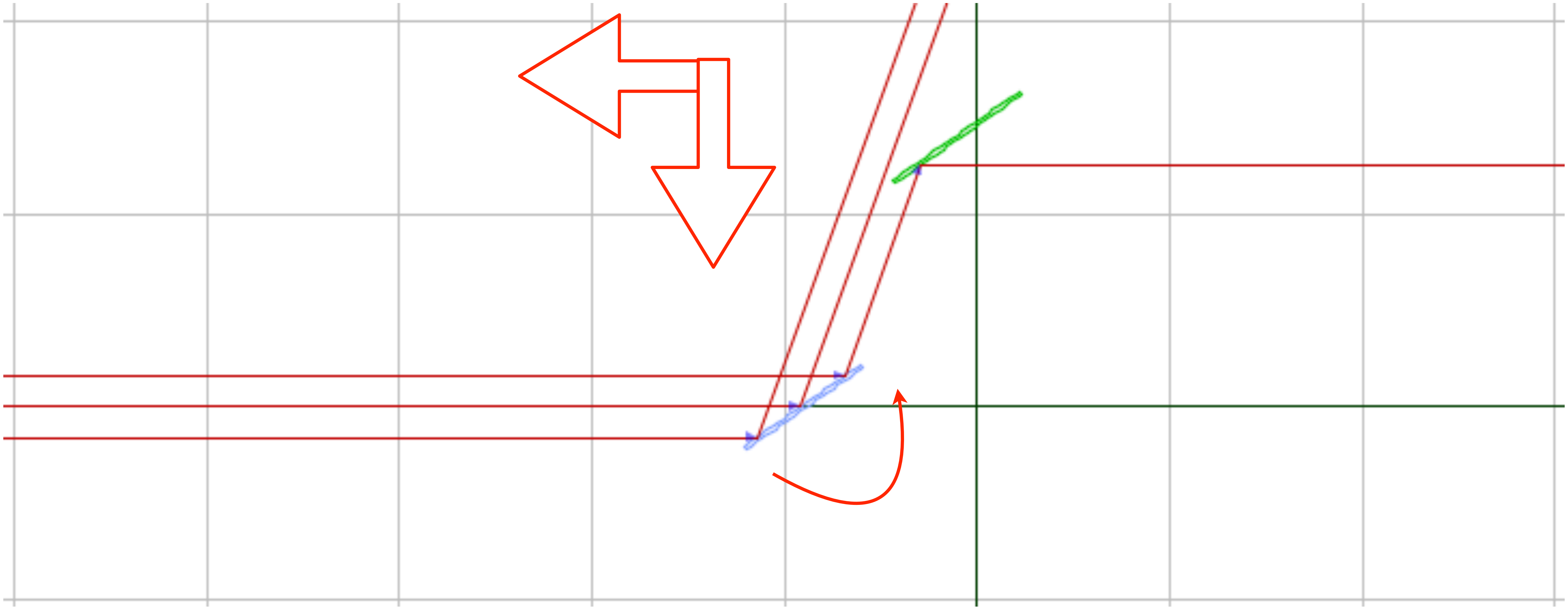
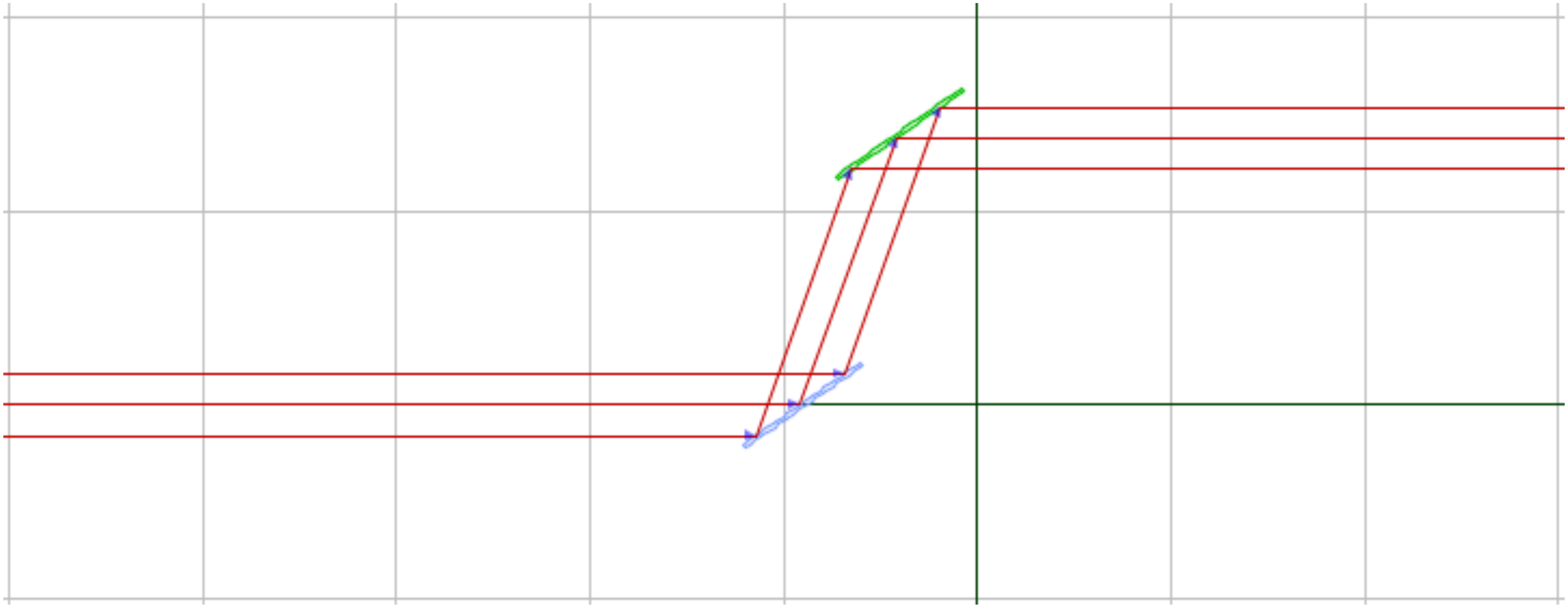
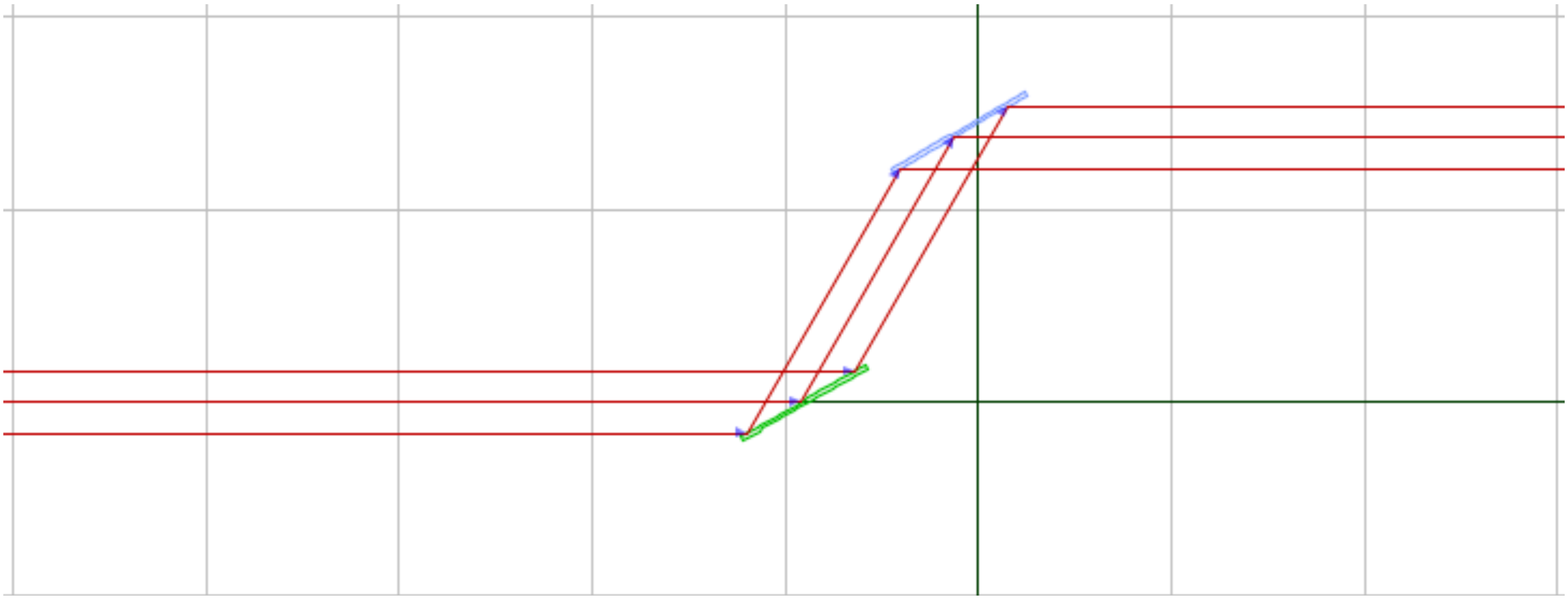
DCM in parallel configuration



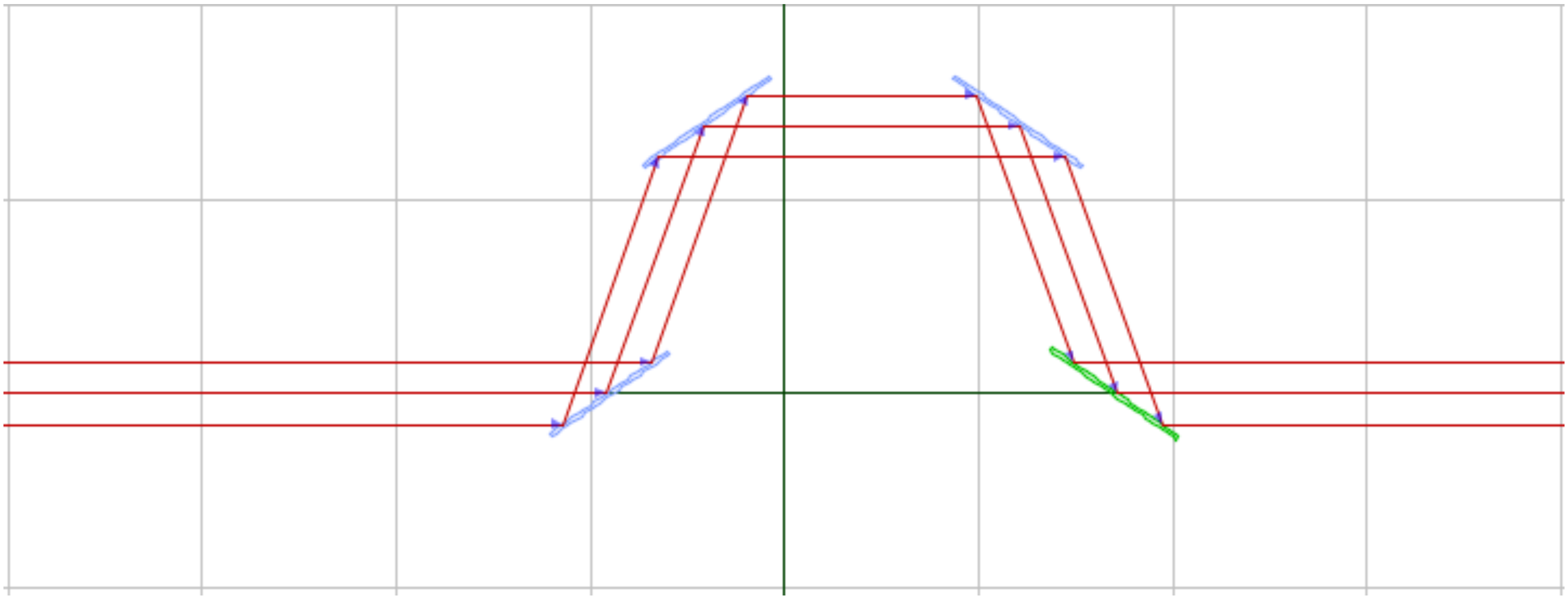
DCM in parallel configuration



DCM in parallel configuration



2 X DCM in parallel configuration

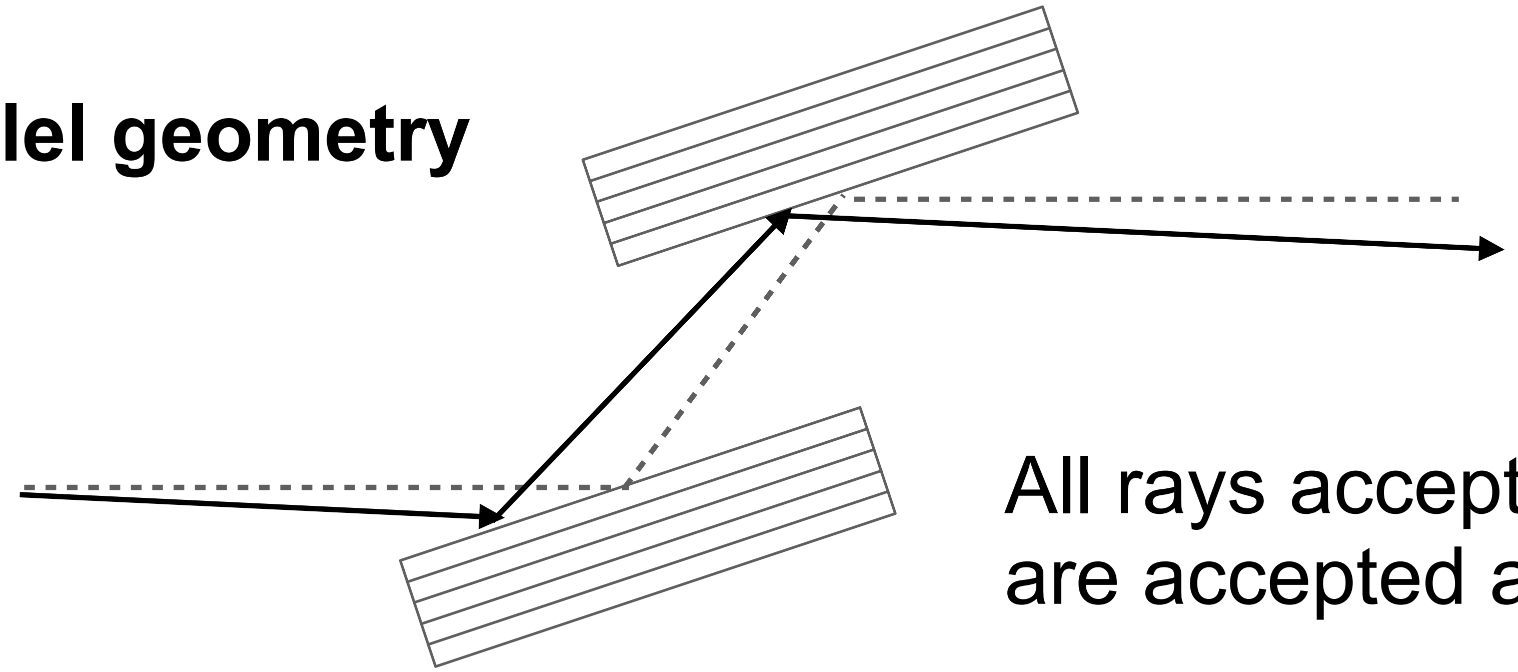


Double Crystal monochromator

$$2d\sin\theta = m\lambda$$

$$\frac{\Delta E}{E} = \frac{\Delta\lambda}{\lambda} = \Delta\theta\frac{\cos\theta}{\sin\theta}$$

Parallel geometry

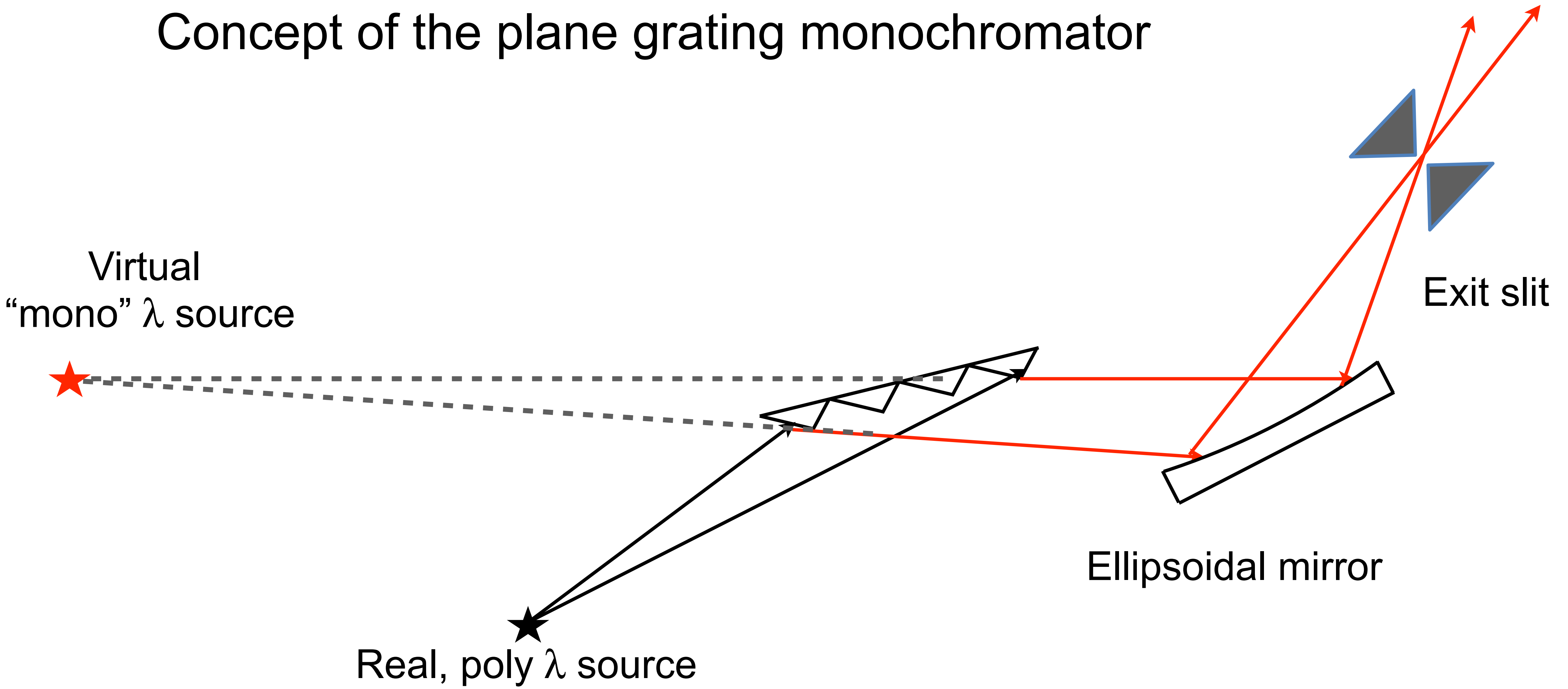


All rays accepted by first crystal are accepted also by the second

Second crystal acts merely as a mirror

Plane grating monochromator

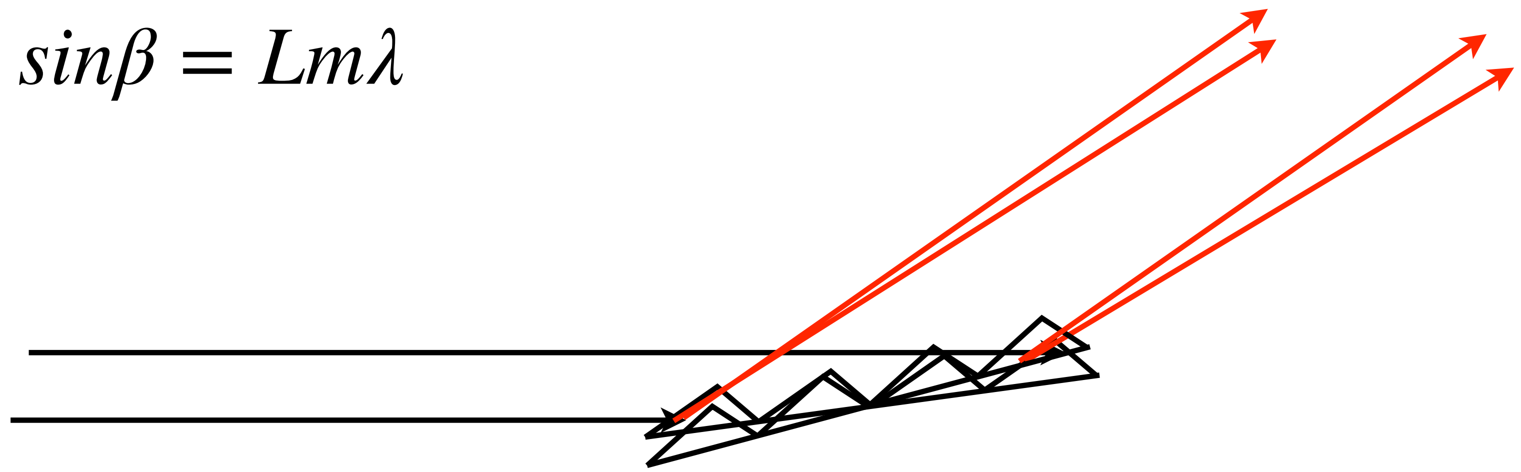
Concept of the plane grating monochromator

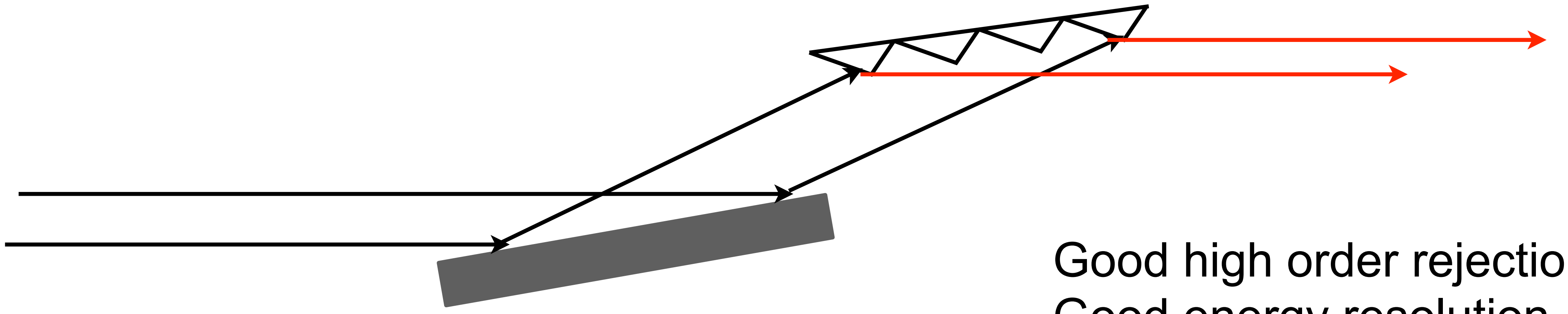


H. Petersen. O. Communication, vol. 40, no. 6. 1982, pp. 402–406.

Plane grating monochromator

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

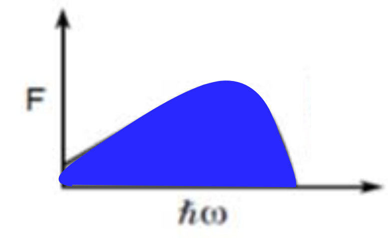
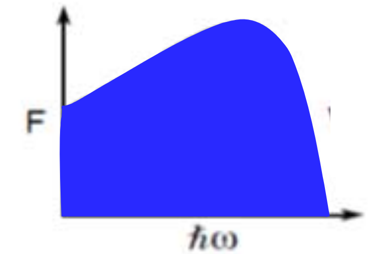
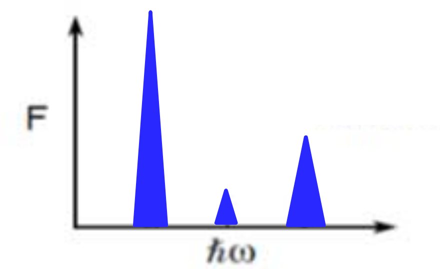




Plane pre-mirror

Good high order rejection
Good energy resolution
Fixed exit slit

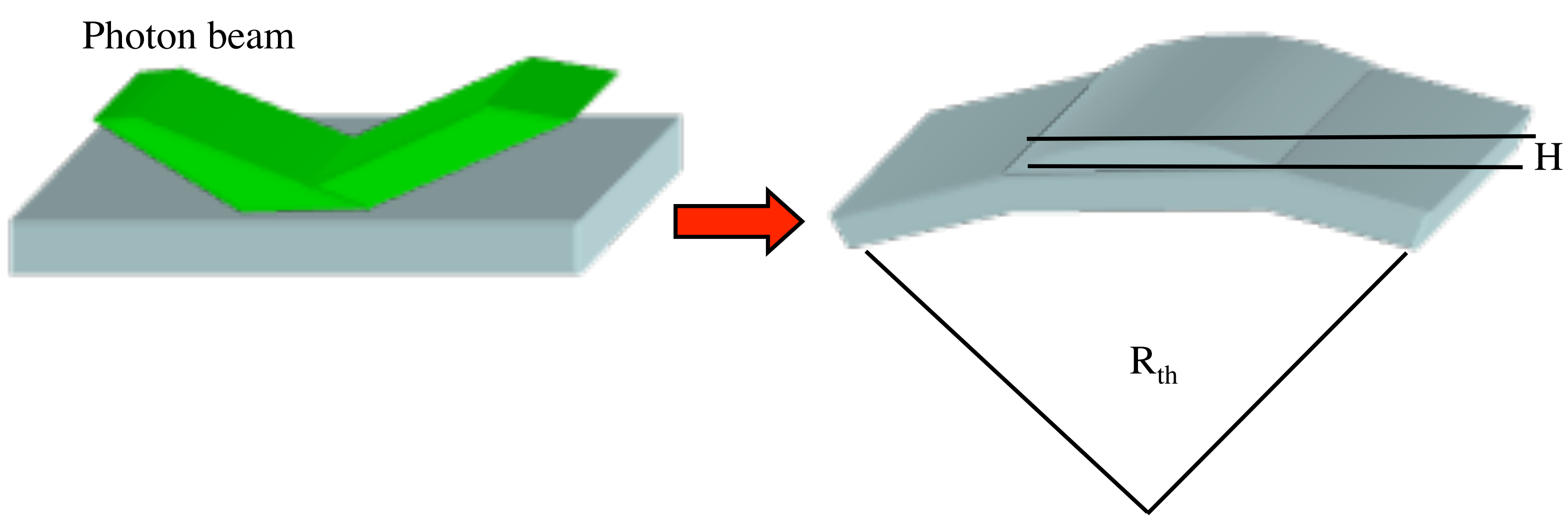
Something to keep in mind: thermal loads!

Source	Spectrum	Typical (total) power emitted
Bending magnet		~ 100's W
Wiggler		~ few kW
Undulator		~ 0.1 - 1 kW

From first mono element standpoint: kW in, NOTHING out!

Thermal load issues (besides melting)

Q is the incoming power, D the mirror/crystal thickness



$$R_{Th} = \frac{k}{\alpha Q}$$

$$H = \alpha\left(\frac{QD^2}{2k} + \frac{QD}{h}\right)$$

For H_2O - cooled Si:

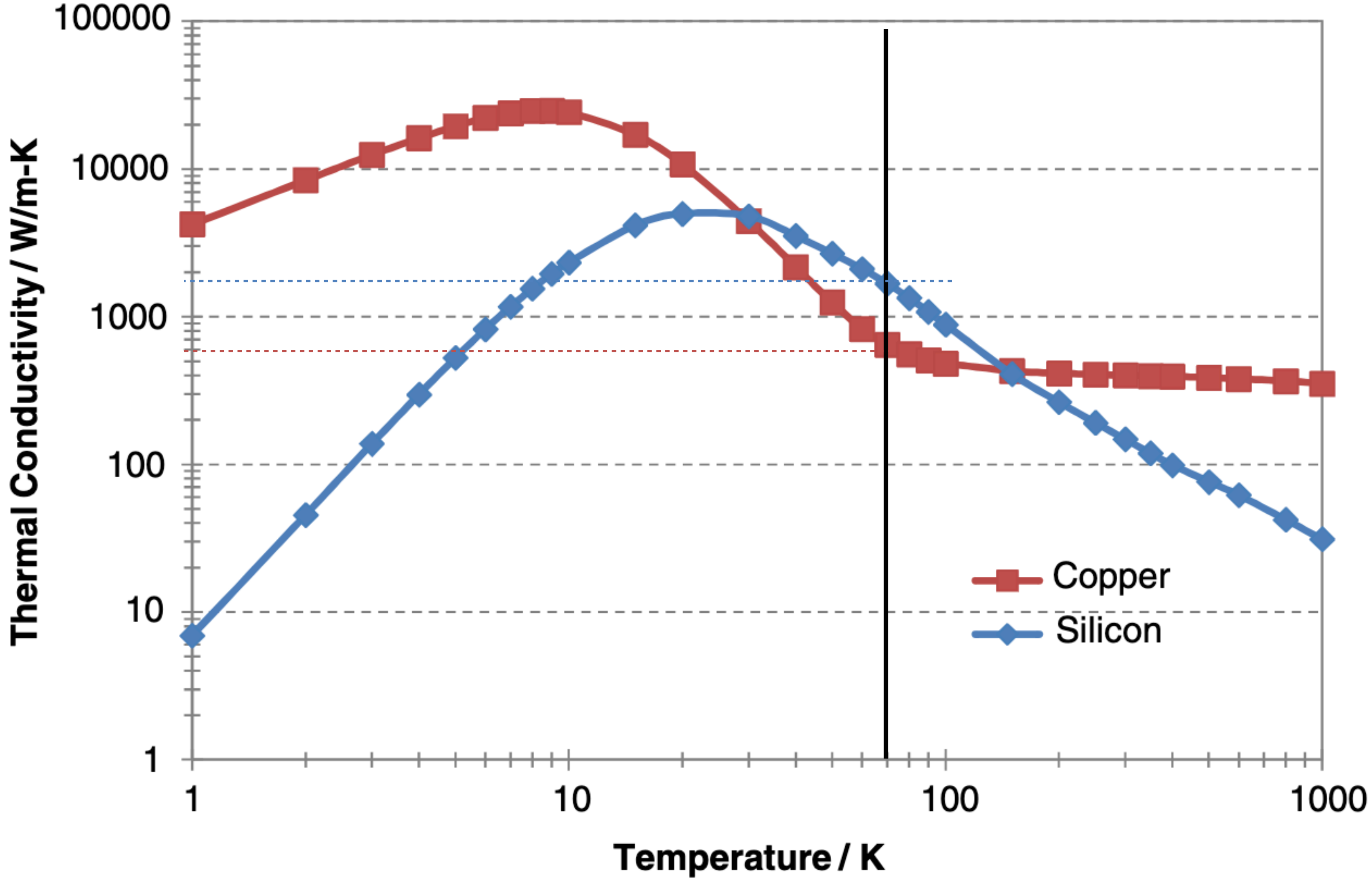
α =4.2 10^{-6} °C^{-1}

k = 1.2 W/cm °C

h = 1 W/cm^2

Smither, Nucl. Instr. Meth. in Phys. Res. **A291** (1990)

Silicon vs Copper Thermal conductivity



M White *et al* 2014 *Metrologia* **51** S245

Elettra Sincrotrone Trieste

… finally a couple of examples

Elettra Sincrotrone Trieste

TwinMic Beamline @ Elettra

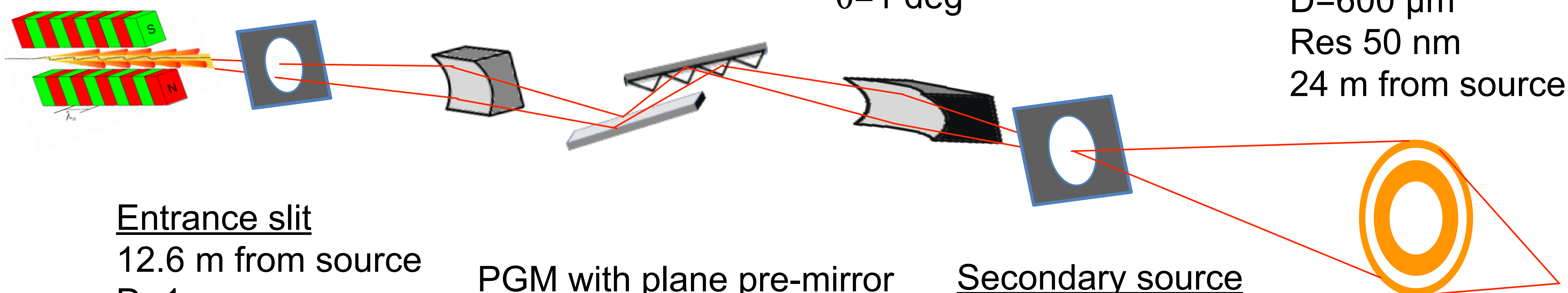
Photon energy: 400eV to 2 keV
X-ray microscopy and microFluorescence

<u>Undulator source</u>
N=17
Period=56mm
Min gap: 25 mm

<u>Cylindrical mirror</u>
16 m from source
Au coated
ρ=0.56m
θ=1 deg

<u>Toroidal mirror</u>
20 m from source
Au Coated
R=211m
ρ=0.07m
θ=1 deg

<u>Zone Plate</u>
D=600 μm
Res 50 nm
24 m from source



<u>Entrance slit</u>
12.6 m from source
D=1mm

<u>PGM with plane pre-mirror</u>
18 m from source
Blazed grating, θ_b=1.1 deg
Au coated
L= 600 l/mm

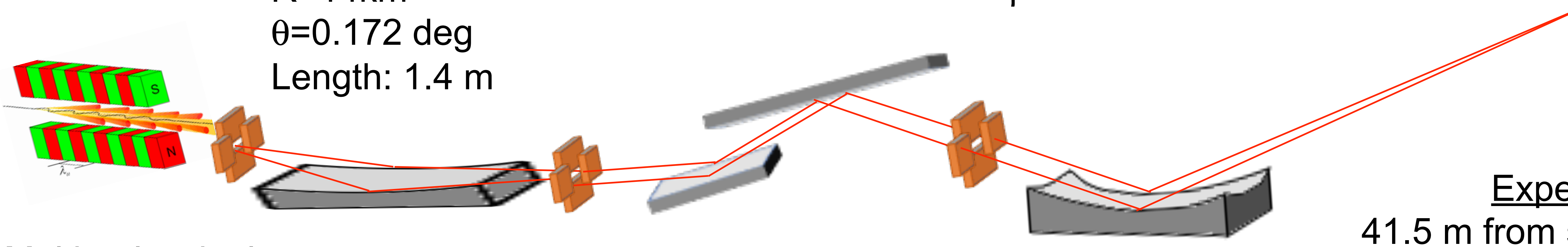
<u>Secondary source</u>
22 m from source
5-100μm diameter

<u>Experiment</u>
~ 24.5 m from source
Focal spot dia:
100 nm to 1.5 μm

Elettra Sincrotrone Trieste

Diffraction Beamline @ Elettra

Photon energy: 4 to 21 keV



Multi-pole wiggler
N=54, 1.5T mag field
Period=140mm
Critical Energy: 5.8keV @ 2.4GeV
5kW total power @ 140 mA

Cylindrical mirror for vertical collimation
22 m from source
Pt Coated
R=14km
θ=0.172 deg
Length: 1.4 m

Double crystal mono
24 m from source
Si(111), ω_s=25 μrad @ 8keV

Toroidal focussing mirror
28 m from source
Sagittally cylindrical, bendable
R=9km (5km to ∞)
ρ=0.055 m

Experiment
41.5 m from source
Focal spot:
0.7 x 0.2 mm^2
$\Delta E/E$~4000

Thank you!