The Abdus Salam International Centre for Theoretical Physics
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Beamline design and instrumentation

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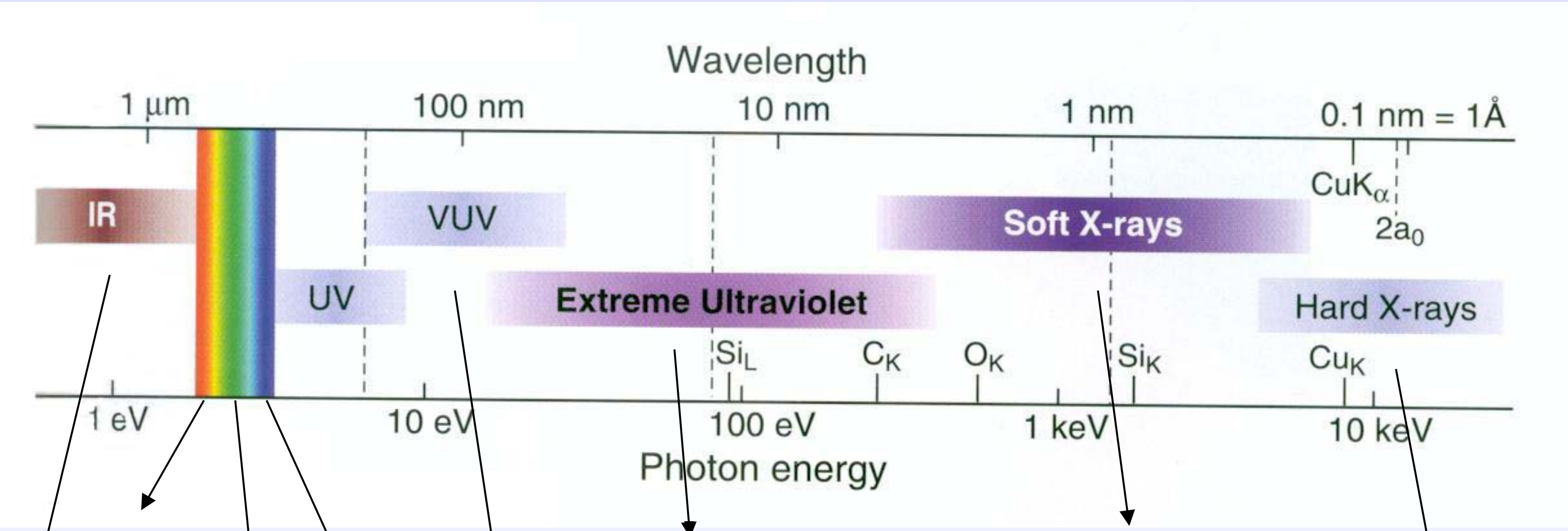
Main properties of Synchrotron Radiation

- Broad energy spectrum

Spectral range

$$E(eV) = \frac{1240}{\lambda(nm)}$$



Red:650nm
Green:530nm
Blue:470nm

1meV-1.2eV
1mm-1μm

4-30eV
300-40nm

30-250eV
40-5nm

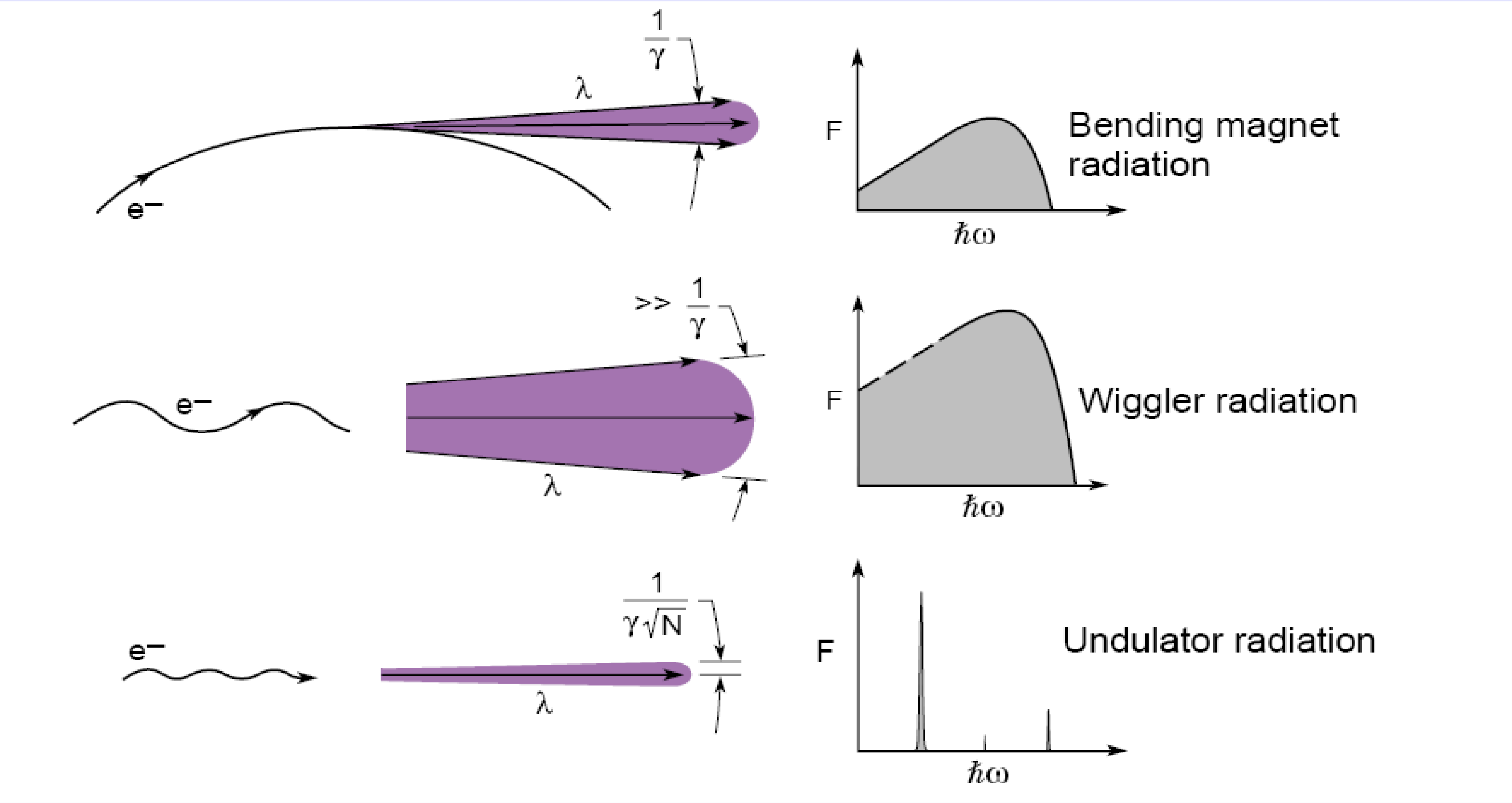
250eV-several keV

2-several tens of keV

D.Attwood, "Soft x-rays and extreme ultraviolet radiation", Cambridge University Press, 1999

Three Synchrotron Light sources

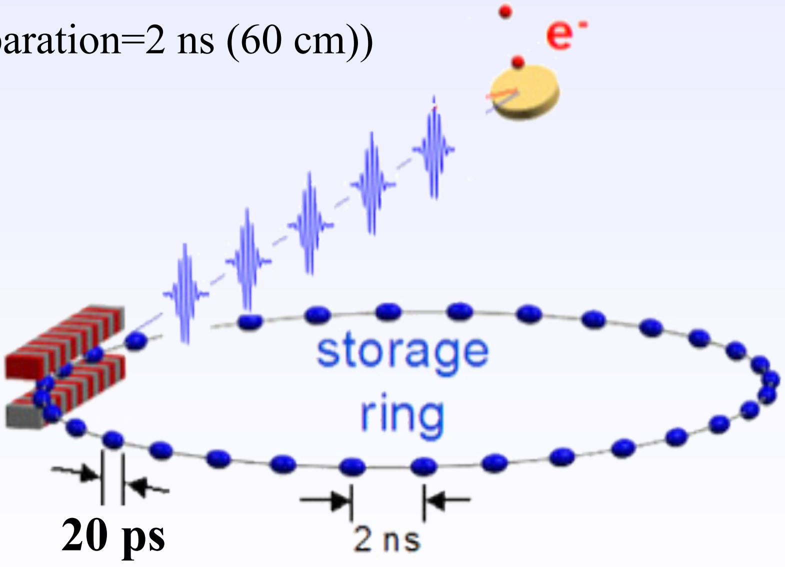
the spectrum is continuus only for bending magnets and wigglers!



D.Attwood, “Soft x-rays and extreme ultraviolet radiation”, Cambridge University Press, 1999

Main properties of Synchrotron Radiation

- Broad energy spectrum
- High intensity
- Small divergence, small source size
  (Elettra Undulator @400eV: 560μm×50μm; 110μrad×85μrad FWHM)
- Pulse time structure
  (Elettra 432 electron bunches: duration=20 ps, separation=2 ns (60 cm))



Main properties of Synchrotron Radiation

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  (Elettra Undulator @400eV: 560μm×50μm; 110μrad×85μrad FWHM)

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- High degree of polarization

Spectral brightness

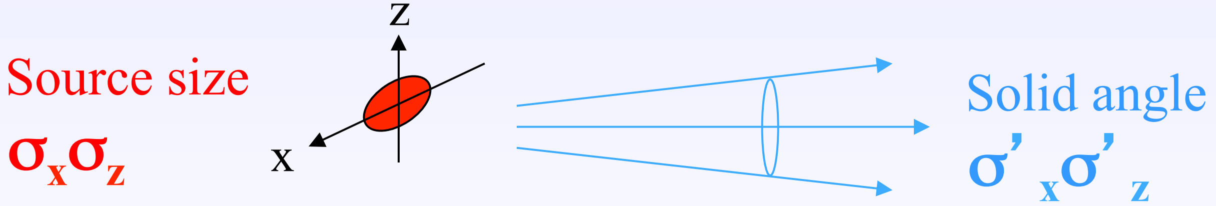
$$Spectral\ Brightness = \frac{photon\ \ flux}{I}\frac{1}{\sigma_x\sigma_z\sigma'_x\sigma'_z BW}$$

I = electron current in the storage ring, usually 100mA

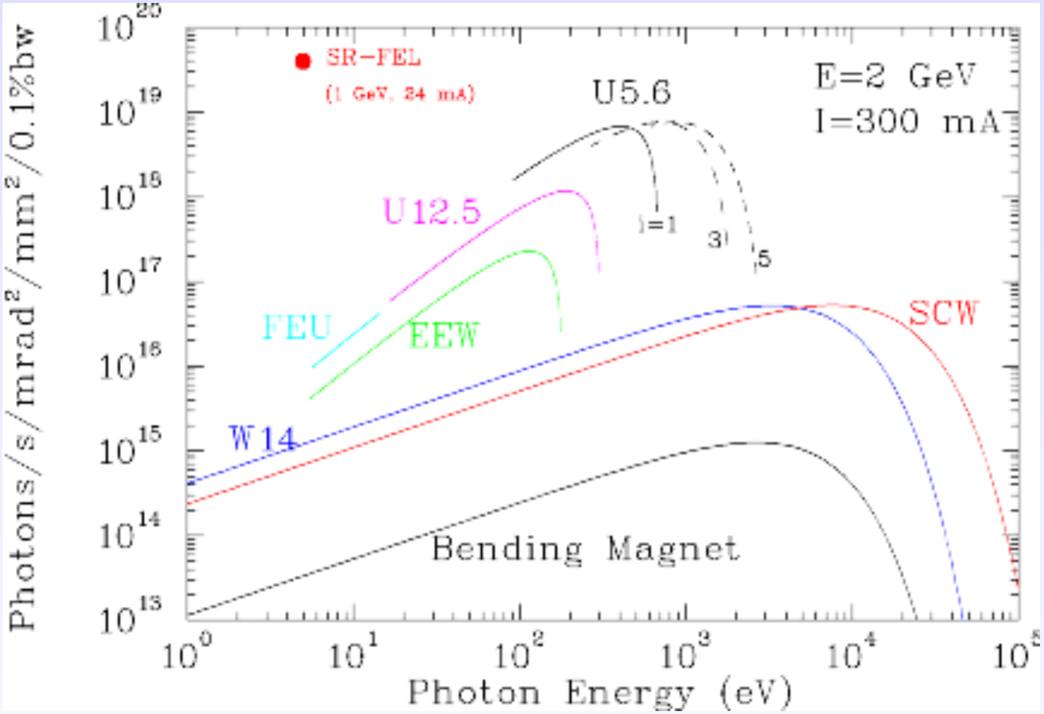
$\sigma_x\sigma_z$ = transverse area from which SR is emitted

$\sigma'_x\sigma'_z$ = solid angle into which SR is emitted

BW = spectral bandwidth, usually: $\frac{\Delta E}{E} = 0.1\%$



SR spectral brightness at ELETTRA



$$Spectral\ Brightness = \frac{photon\ flux}{I}\frac{1}{\sigma_x\sigma_z\sigma'_x\sigma'_z BW}$$

Why is brightness important? (1)

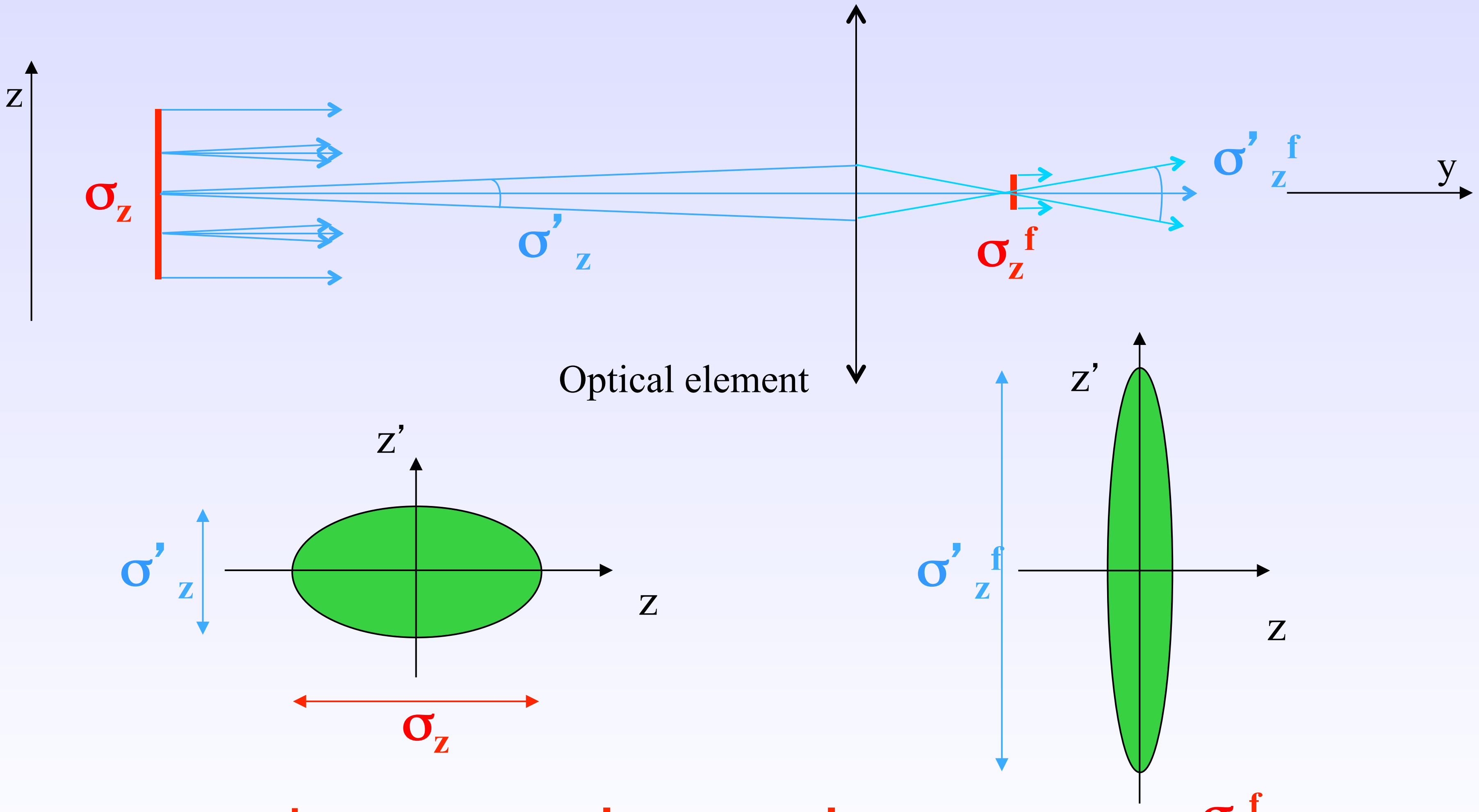
$$Spectral\ Brightness = \frac{photon\ flux}{I}\frac{1}{\sigma_x\sigma_z\sigma'_x\sigma'_z BW}$$

More flux → more signal at the experiment

But why combining the flux with geometrical factors?

Liouville's theorem: for an optical system the occupied phase space volume cannot be decreased along the optical path (without loosing photons) → **$(\sigma\sigma')_{final} \geq (\sigma\sigma')_{initial}$**

Example: a focusing beam



Liouville's theorem: $(\sigma\sigma')_{final} \geq (\sigma\sigma')_{initial}$

Why is brightness important? (2)

To focus the beam in a small spot (which is needed for achieving energy and/or spatial resolution) one must accept an increase in the beam divergence.

Not bright source: $(\sigma\sigma')_{initial}$ large	+	Liouville's theorem: $(\sigma\sigma')_{final} \geq (\sigma\sigma')_{initial}$

→ high beam divergence

High beam divergence along the beamline:

→ high optical aberrations
→ large optical devices
→ high costs and low optical qualities

With a not bright source the spot size can be made small only reducing the photon flux.

The high spectral brightness of the radiation source allows the development of monochromators with high energy resolution and high throughput and gives also the possibility to image a beam down to a very small spot on the sample with high intensity.

The beamline (1)

The researcher needs at his experiment a certain number of photons/second into a phase volume of some particular characteristics. Moreover, these photons have to be monochromatized.

The beamline:

- *de-magnifies, monochromatizes and refocuses the source onto a sample*
- *must preserve the excellent qualities of the radiation source*

Conserving brightness

Brightness decreases because of:

• micro-roughness and slope errors on optical surfaces

• thermal deformations of optical elements due to heat load produced by the high power radiation

• aberrations of optical elements

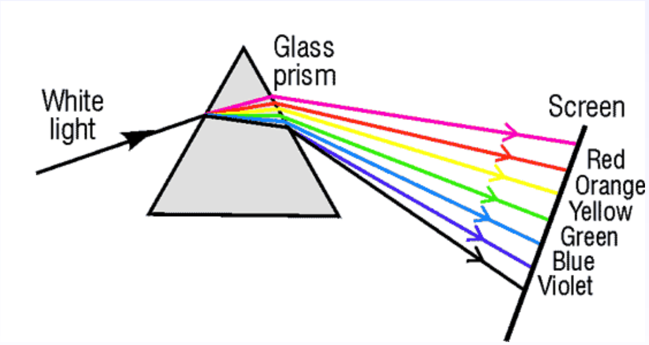
The beamline (2)

Not a simple pipe!

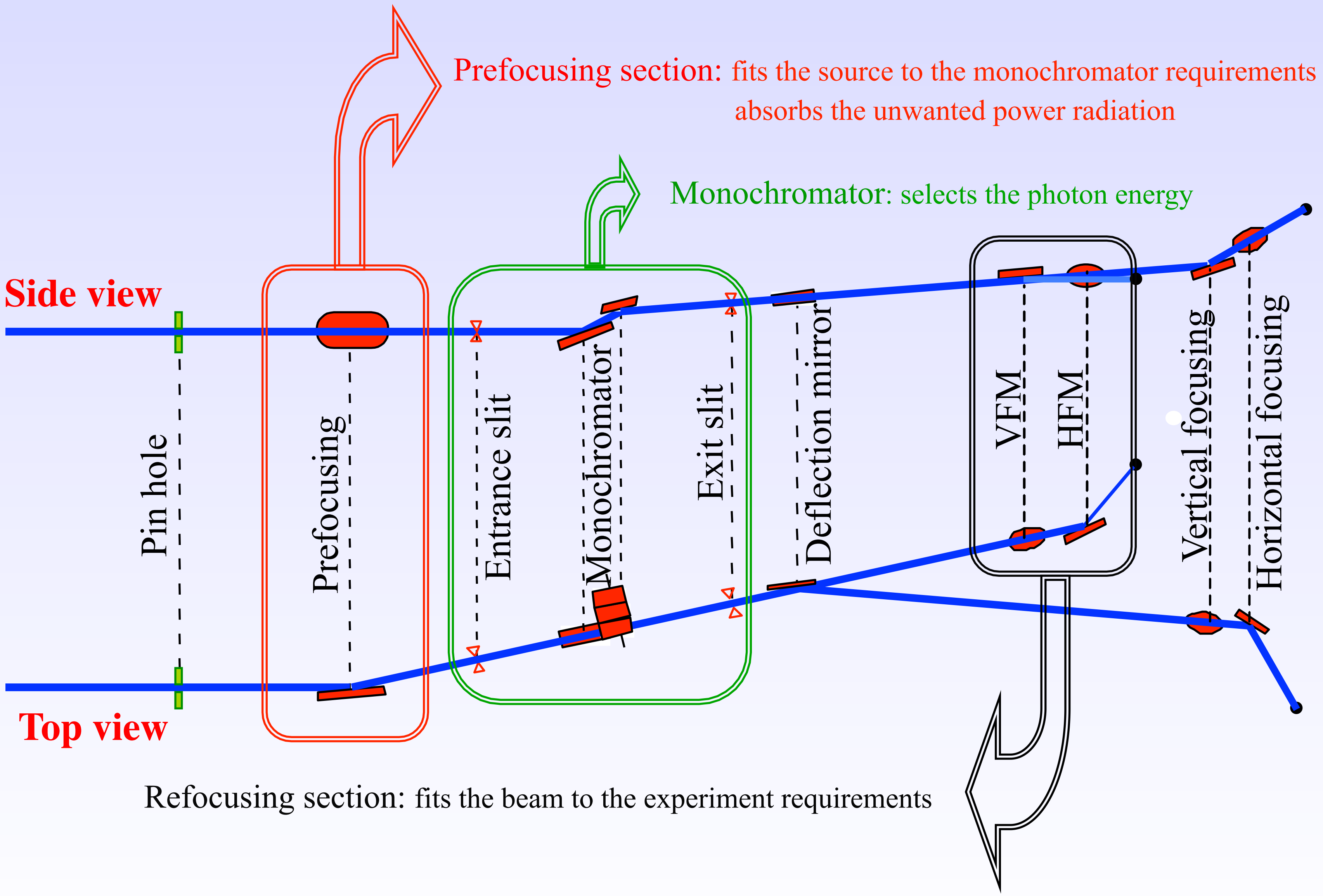
Basic optical elements:

• mirrors, to deflect, focus and filter the radiation

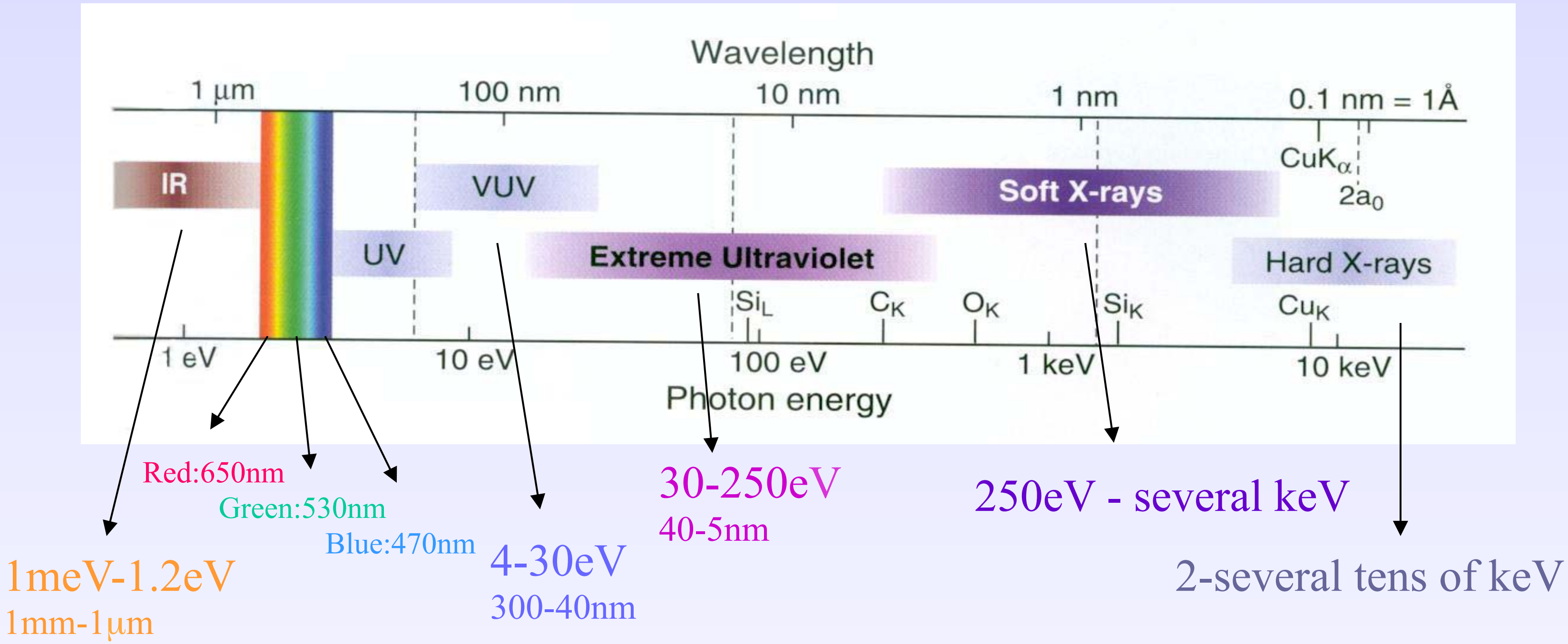
• monochromators (gratings and crystals), to select photon energy



Beamline structure: example



VUV, EUV and soft x-rays



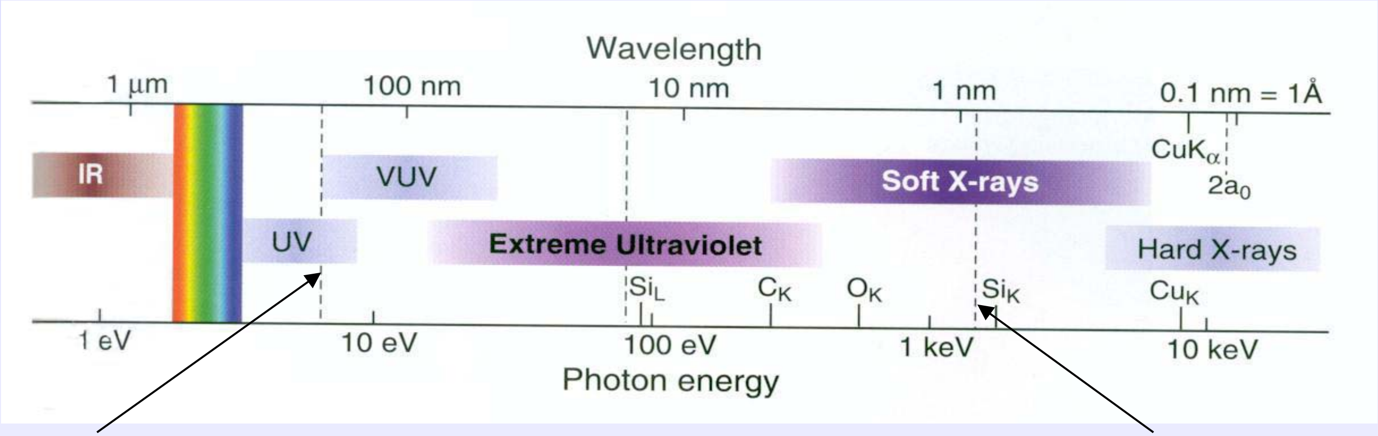
These regions are very interesting because are characterized by the presence of the absorption edges of most low and intermediate Z elements

→ photons with these energies are **a very sensitive tool** for elemental and chemical identification

But… these regions are difficult to access.

Ultra-high vacuum

VUV, EUV and soft x-rays have a high degree of absorption in all materials:



Transmission limit of common fused silica window: ~8eV Absorption limit of 8μm Be foil: ~1.5keV

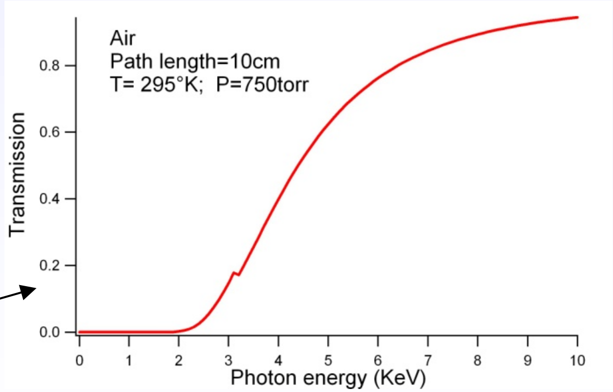
→ No windows

→ The entire optical system must be kept under UH Vacuum

Ultrahigh vacuum conditions (P=10^{-9} mbar) are required:

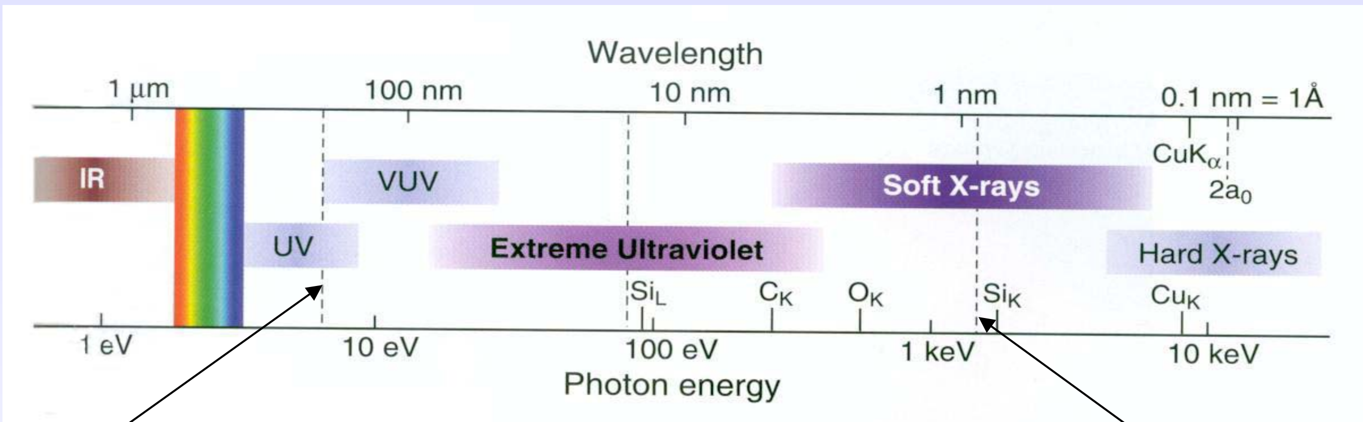
- Not to disturb the storage ring and the experiment
- To avoid photon absorption in air
- To protect optical surfaces from contamination (especially from carbon)

In the hard x-ray region, it is not necessary to use UHV:



No refractive optics

VUV, EUV and soft x-rays have a high degree of absorption in all materials:



Transmission limit of common fused silica window: ~8eV   Absorption limit of 8µm Be foil: ~1.5keV

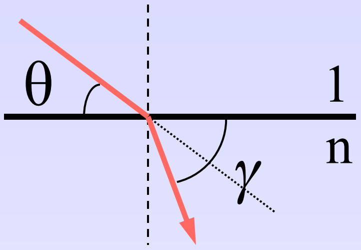
→ The only optical elements which can work in the VUV, EUV and soft x-rays regions are mirrors and diffraction gratings, used in total external reflection at grazing incidence angles

Exceptions: multilayer coated mirrors, zone plates

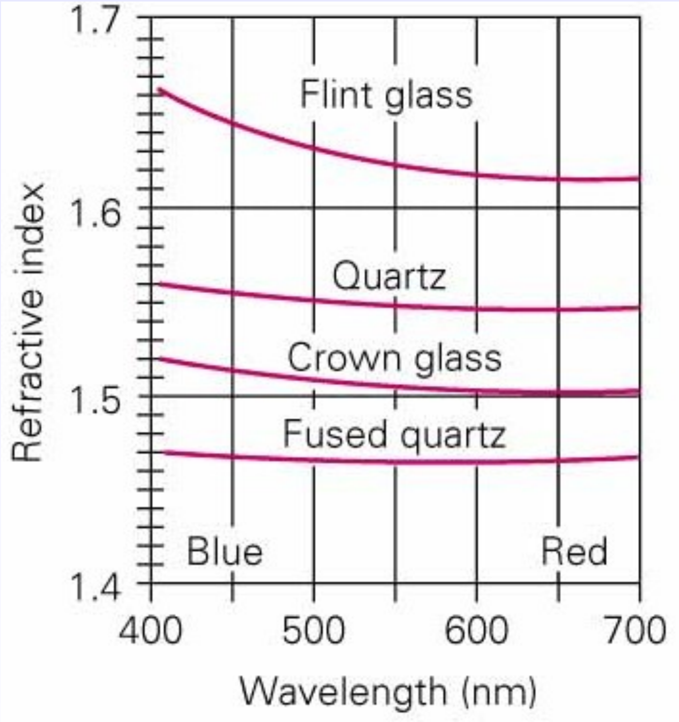
Snell's law, visible light

$n_1 \cos\theta = n_2 \cos\gamma$

→ $\mathbf{\cos\theta = n \cos\gamma}$ with $n = n_2/n_1$



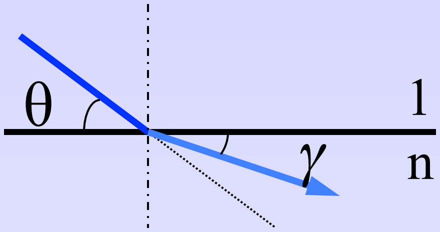
n > 1 → γ > θ



Visible light, when entering a medium of greater refractive index, is bent towards the surface normal.

This is the case for visible light impinging from air on a glass

Snell's law, X-rays



$n_1 \cos\theta = n_2 \cos\gamma$

→ $\mathbf{\cos\theta = n \cos\gamma}$ with $n = n_2/n_1$

$n < 1$ → $\gamma < \theta$

Complex refractive index, with real component slightly less than unity:

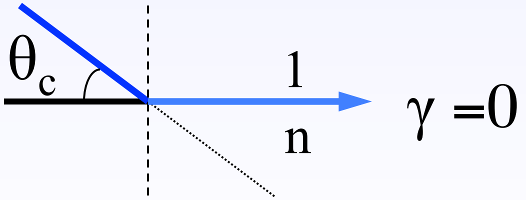
$n = 1 - \delta$ where: $0 < \delta << 1$

Typical values:
$\delta \approx 10^{-2}$ for 250 eV (5 nm)
$\delta \approx 10^{-4}$ for 2.5 keV (0.5 nm)

→ X-ray radiation is refracted in a direction slightly further from the surface normal

→ the refraction angle γ can equal 0, indicating that the refracted wave doesn't penetrate into the material but rather propagates along the interface.
The limiting condition occurs at the critical angle of incidence θ_c: $\cos\theta_c = n$

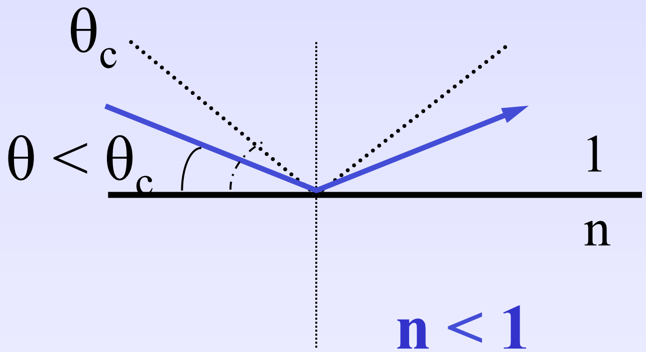
$$1 - \frac{\vartheta_c^2}{2} = 1 - \delta \quad \rightarrow \quad \boxed{\theta_c = \sqrt{2\delta}}$$



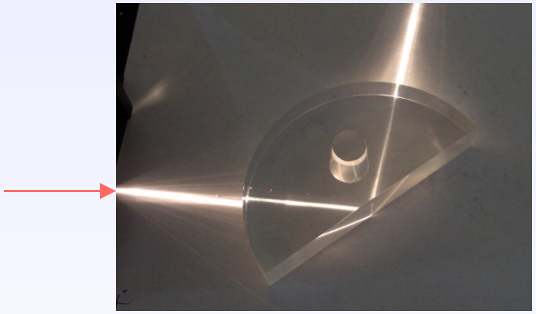
$n < 1$

Total external reflection

If radiation impinges at a grazing angle **$\theta < \theta c$,** it is **totally external reflected**.



It is the counterpart of total internal reflection of visible light. Visible light is totally reflected at the glass/air boundary if $\theta < \theta_{c.}$=48.2°

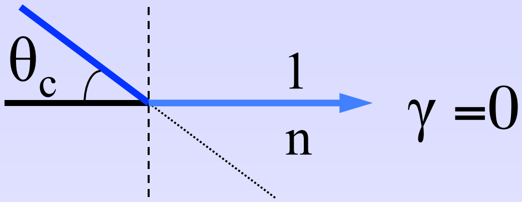


$n * \cos \theta c = 1 \rightarrow \theta c = \arccos(1/n) = 48.2°$

n =1.5 refraction index of glass

Critical angle

$$\theta_c = \sqrt{2\delta}$$



n < 1

$$\delta = \frac{n_a r_e \lambda^2 f_1^0(\lambda)}{2\pi}$$

n_a atomic density, slowly varying with Z,
f_1^0 real component of the atomic scattering factor, $f_1^0 \sim Z$

$$\theta_c \,\alpha\, \lambda \sqrt{Z}$$

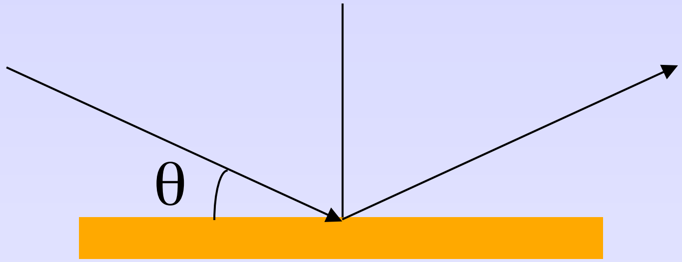
θ_c increases working at lower photon energy and using a material of higher atomic number Z.

Gold (Z=79):
600 eV → θc ≈ 7.4°
1200 eV → θc ≈ 3.7°
5 keV → θc ≈ 0.9°

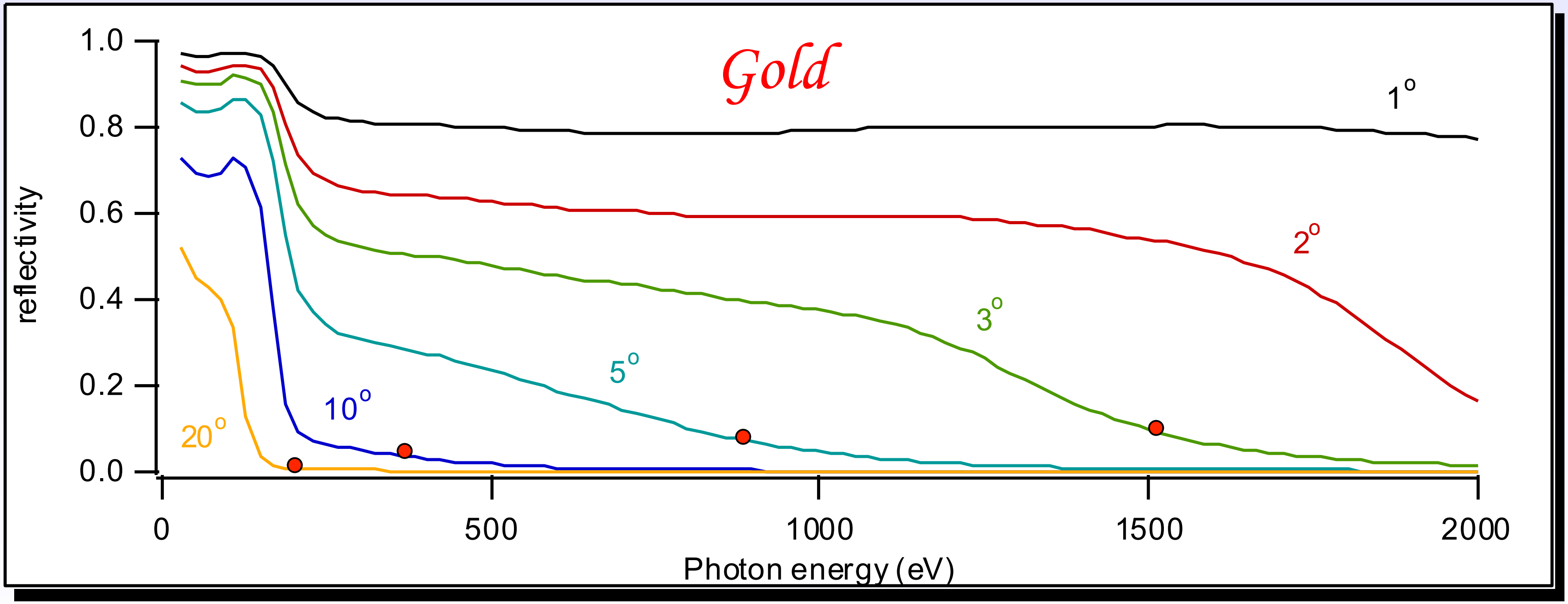
Nickel (Z=28):
6 keV → θc ≈ 10 mrad (0.57°)

Carbon (Z=6):
100 eV → θc ≈ 250 mrad (14°)

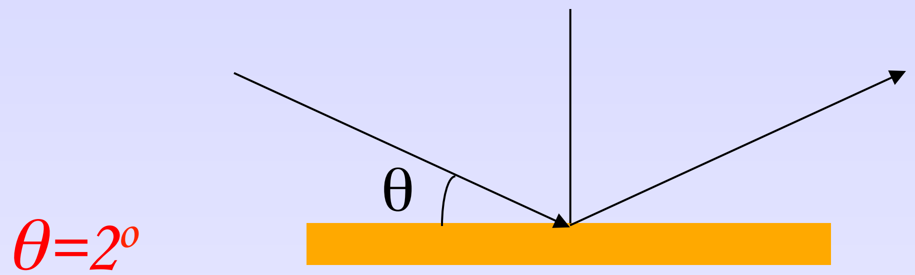
Mirror reflectivity (1)

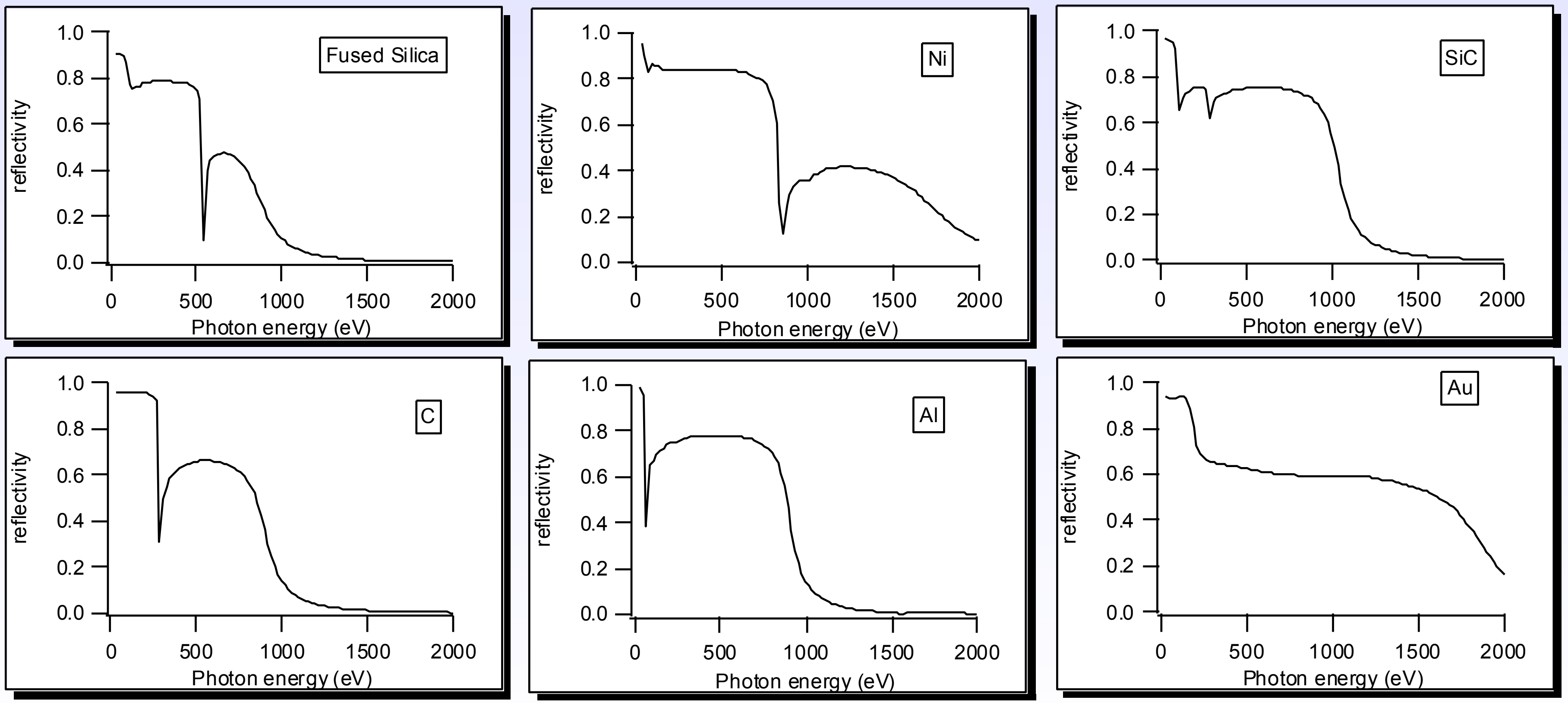


Reflectivity drops down fast with the increasing of the grazing incidence angle
→ only reflective optics at grazing incidence angles
(typically 1°-2° for soft x-rays, few mrad for hard x-rays, 1 mrad= 0.057°)



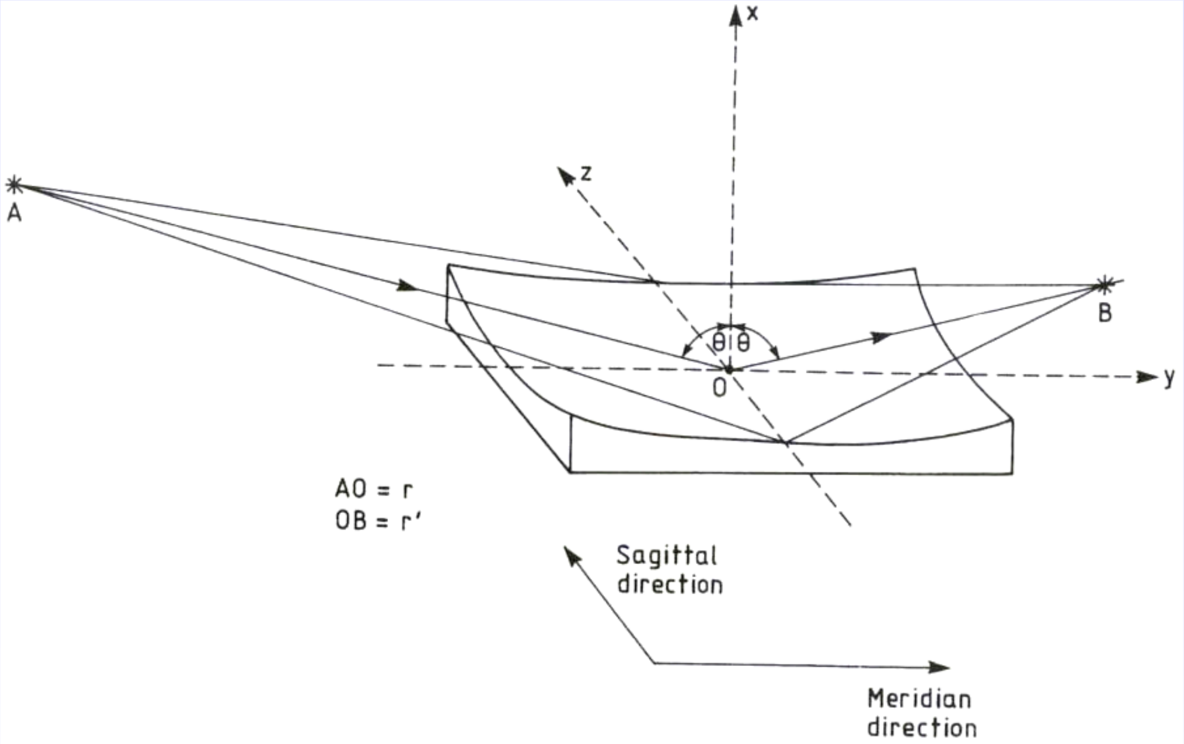
Mirror reflectivity (2)





Focusing properties of mirrors

X-rays mirrors can have different geometrical shapes, their optical surface can be a plane, a sphere, a paraboloid, an ellipsoid and a toroid.

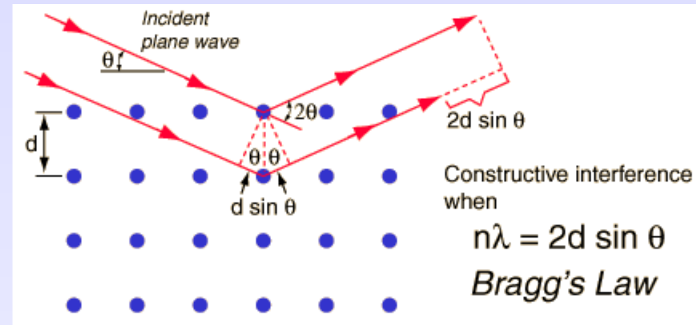


The meridional or tangential plane contains the central incident ray and the normal to the surface. The sagittal plane is the plane perpendicular to the tangential plane and containing the normal to the surface.

Monochromators

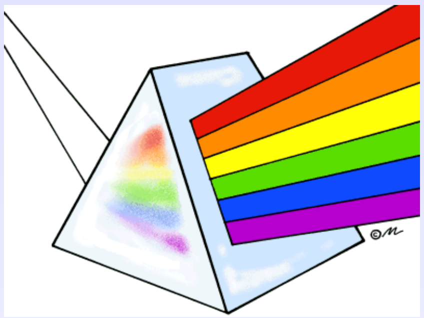
Microwave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Crystal

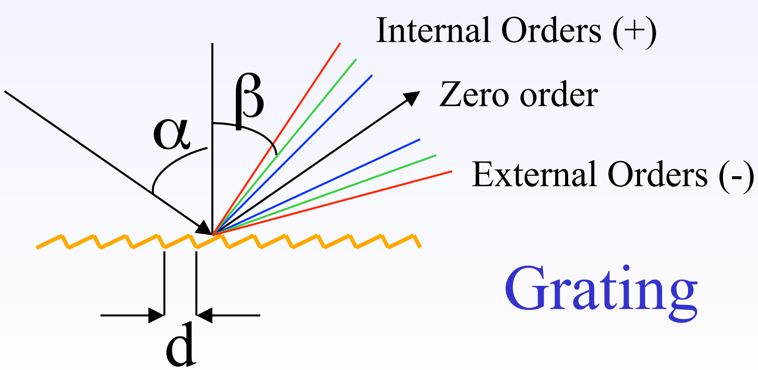


Microwave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

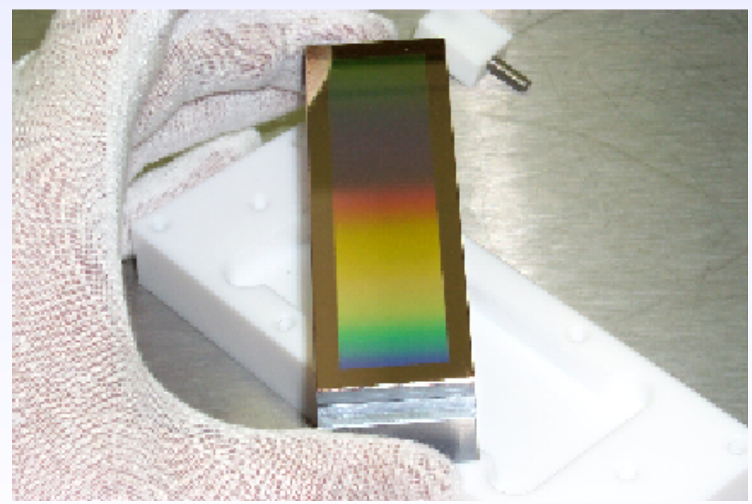
Prism



Microwave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray



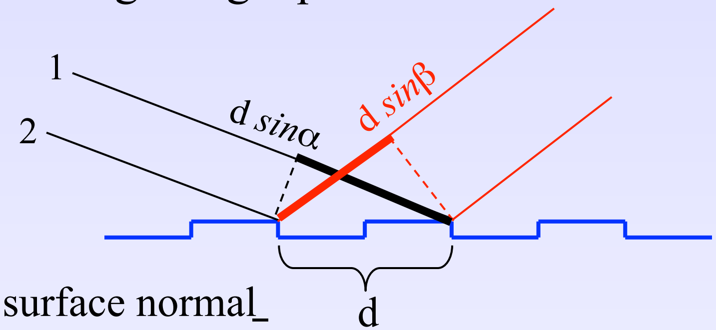
Grating



Gratings

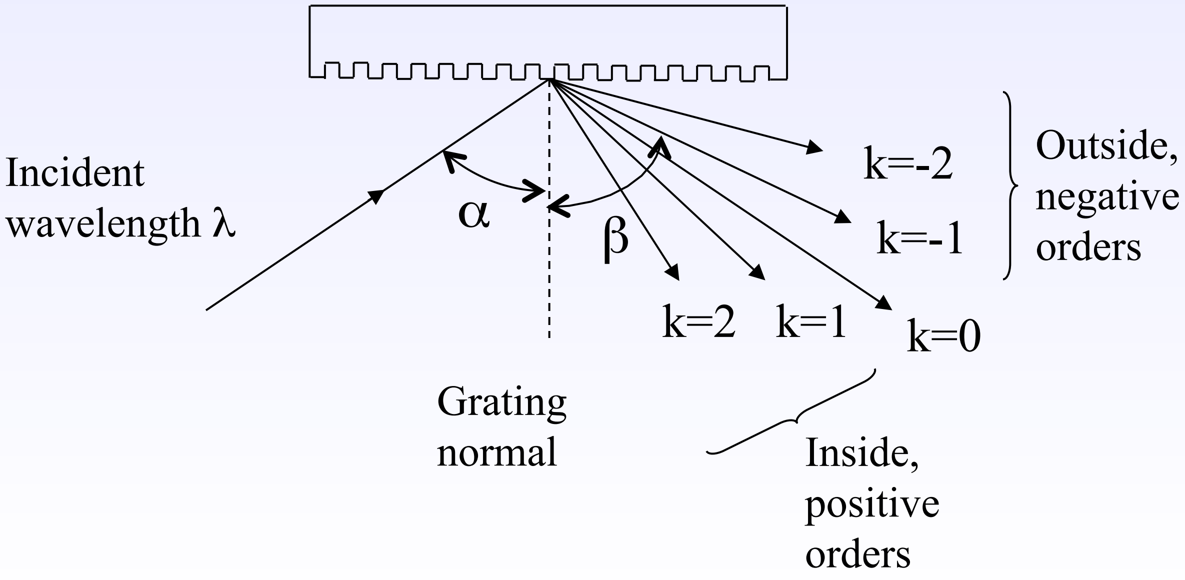
The diffraction grating is an artificial periodic structure with a well defined period d. The diffraction conditions are given by the well-known grating equation:

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

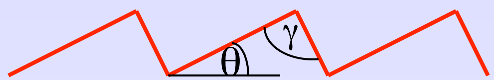


α and β are of opposite sign if on opposite sides of the surface normal

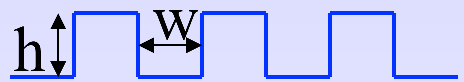
N=1/d is the groove density, k is the order of diffraction (±1,±2,...)



Gratings profiles (1)

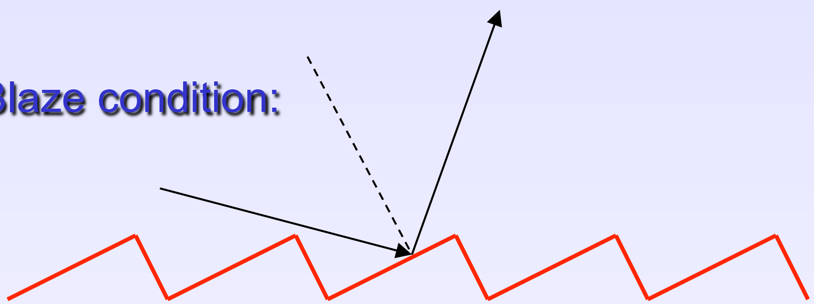


Blaze profile

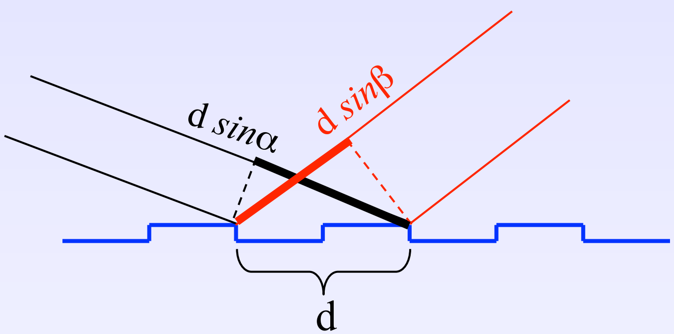


Laminar profile

Blaze condition:



Blaze angle=(α+β)/2



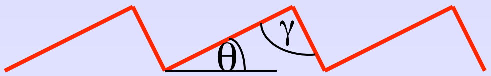
The angle θ is chosen such that for a given wavelength the diffraction direction coincides with the direction of specular reflection from the individual facets

$$1\lambda$$
$$k\lambda = d(\sin\alpha + \sin\beta)$$
$$2\frac{\lambda}{2}$$

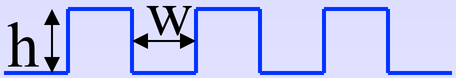
Blaze gratings: higher efficiency

Laminar gratings: higher spectral purity

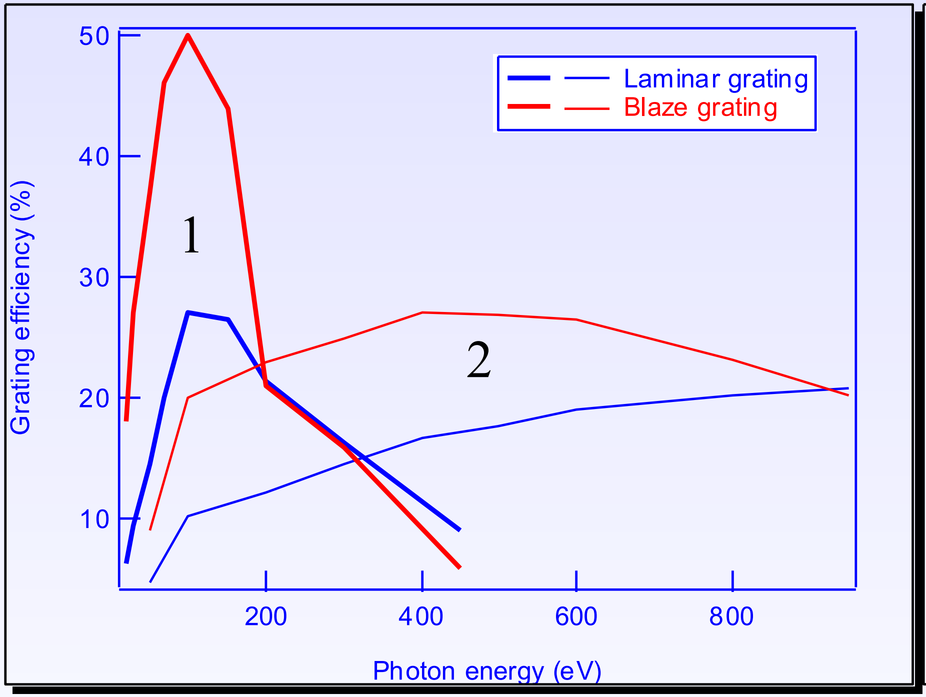
Gratings profiles (2)

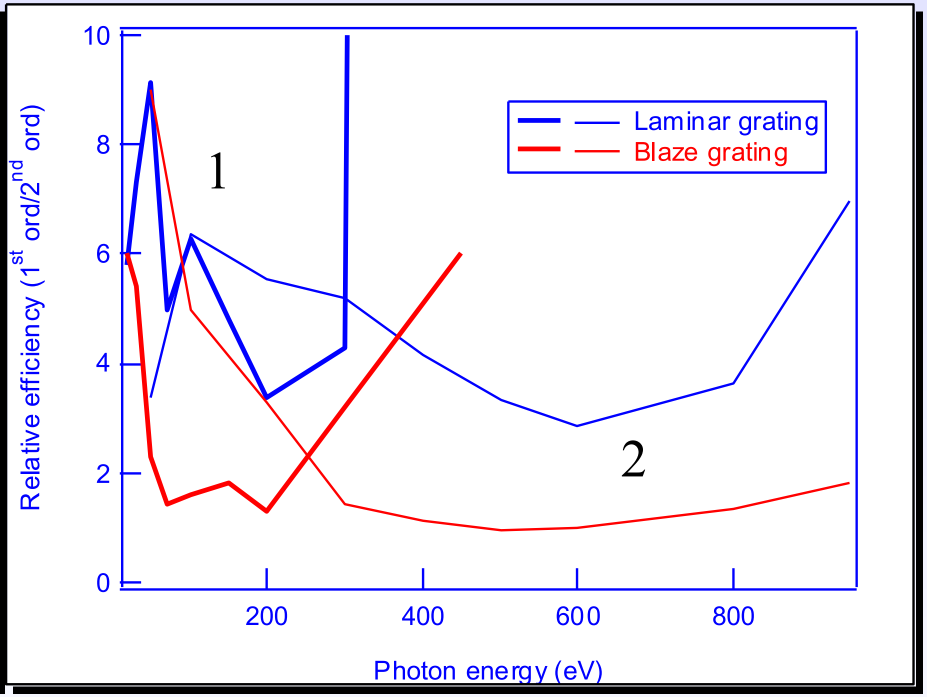


Blaze profile



Laminar profile

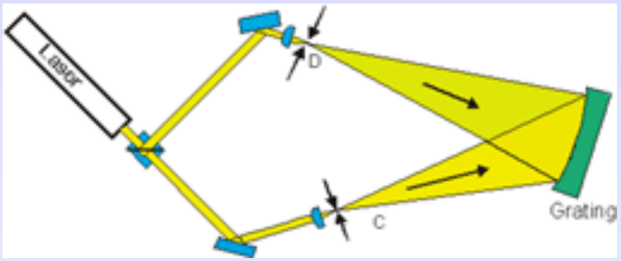


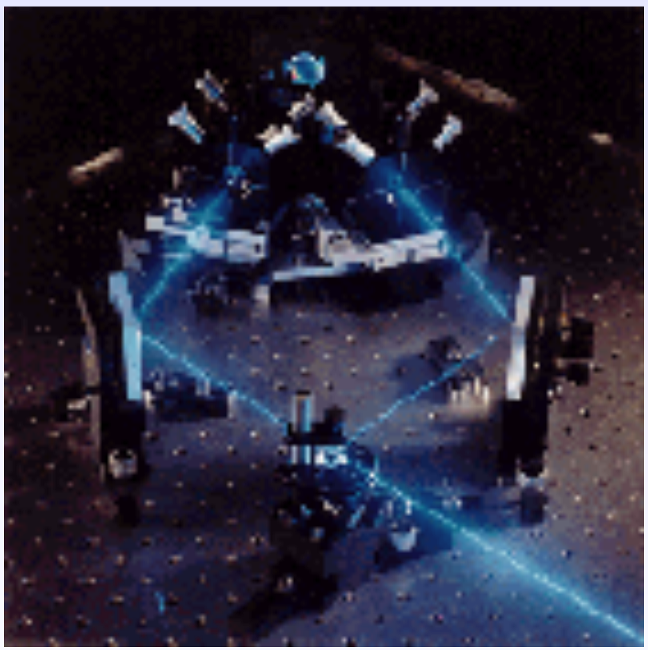


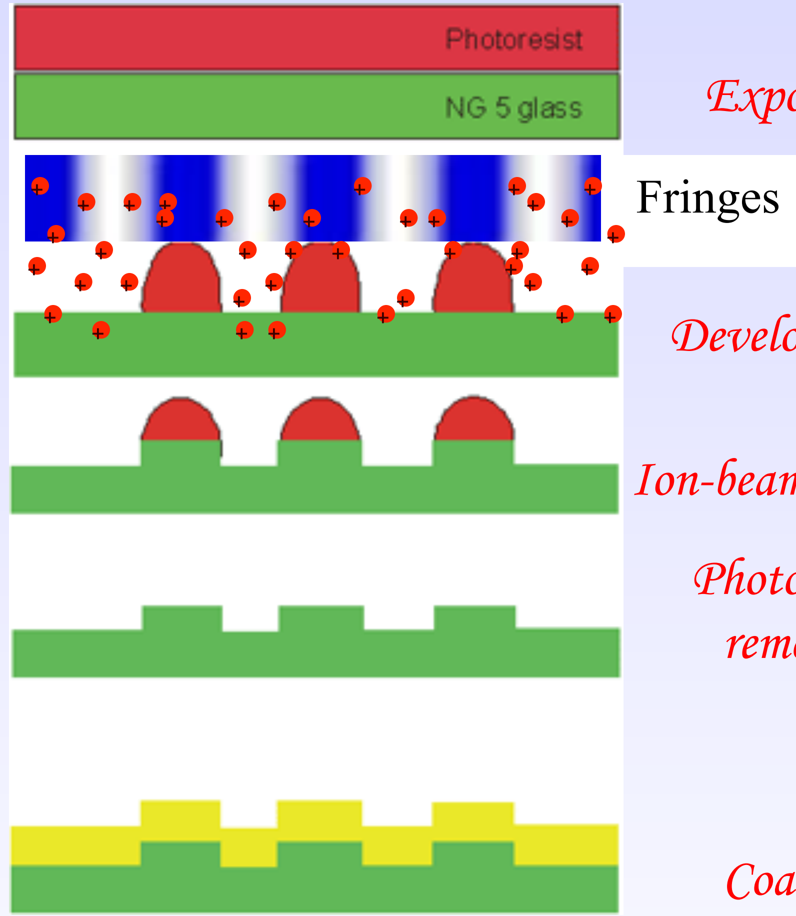
$$d(\sin\alpha + \sin\beta) = k\lambda$$

Grating 1: N=200 g/mm (d=5 μm)
Grating 2: N=400 g/mm (d=2.5 μm)

Holographically recorded grating







Exposure

Development

Ion-beam etching

Photoresist removal

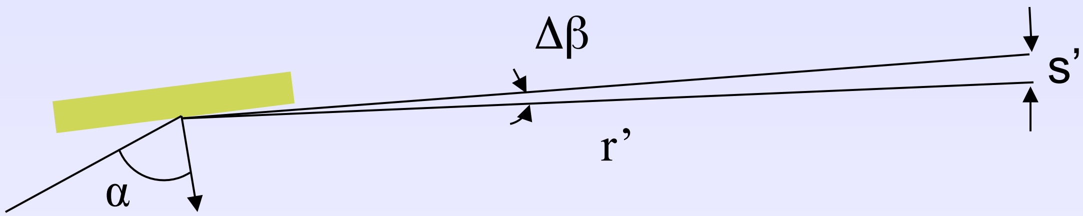
Coating

Grating resolving power (1)

Differentiating the grating equation: $\sin\alpha + \sin\beta = Nk\lambda$
the **angular dispersion** of the grating is obtained:

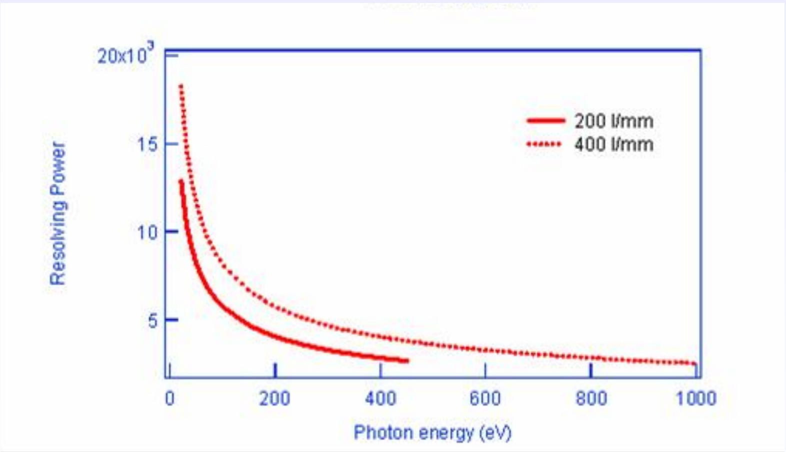
(higher groove density → higher angular dispersion)

$$\Delta\lambda = \frac{\cos\beta}{Nk}\Delta\beta$$



The **resolving power** is defined as:

$$R = \frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda}$$



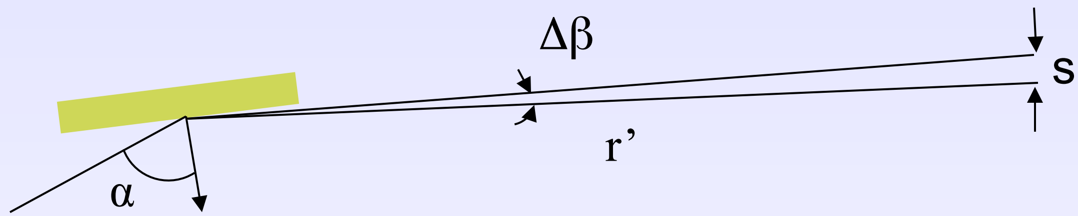
R=10000 @100 eV → ΔE=100 eV/10000=10 meV

Grating resolving power (2)

Angular dispersion : $\Delta\lambda = \dfrac{\cos\beta}{Nk}\Delta\beta$ Resolving power: $R = \dfrac{E}{\Delta E} = \dfrac{\lambda}{\Delta\lambda}$

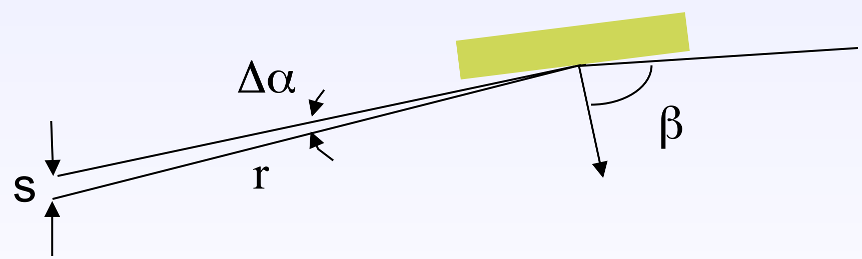
The main contribution is from the width s' of the **exit slit**:

$$\frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda} = \frac{\lambda N k r'}{(\cos\beta) s'}$$



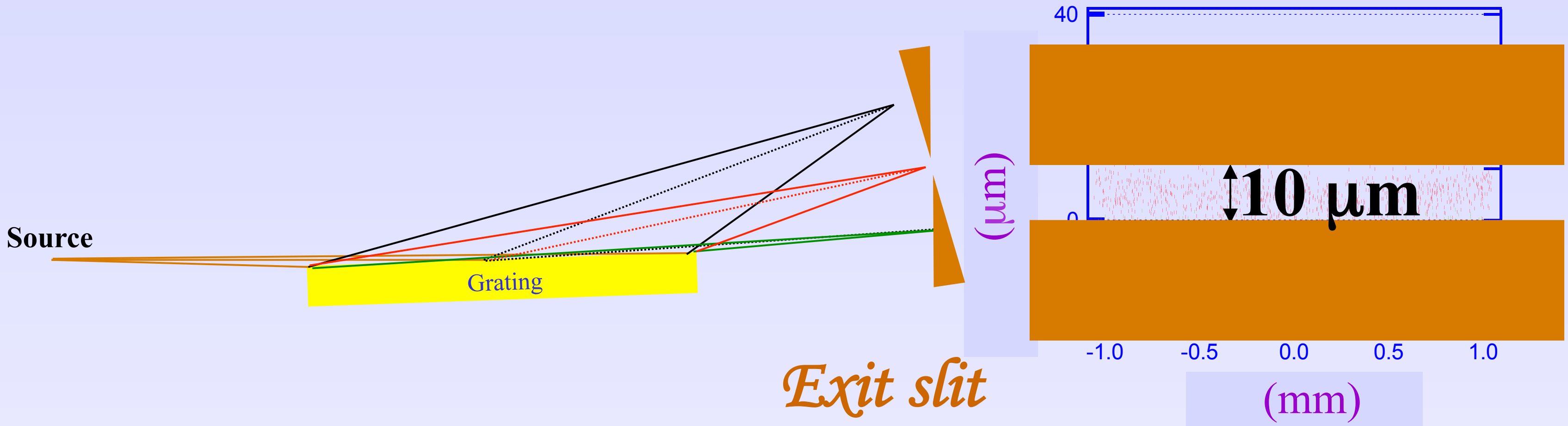
The **entrance slit** contribution is similar:

$$\frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda} = \frac{\lambda N k r}{(\cos a) s}$$



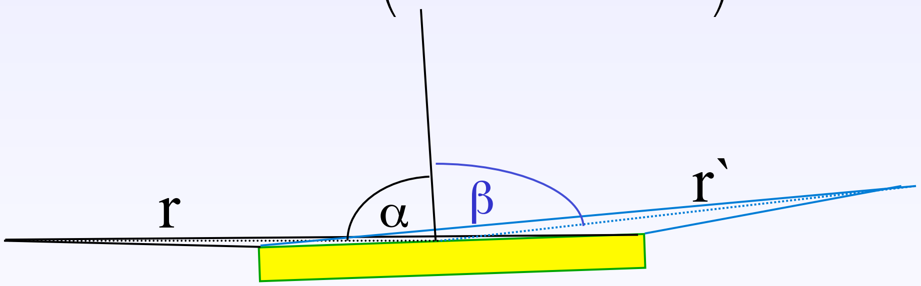
Smaller s and s' → higher resolving power

Variable included angle spherical grating monochromator (1)



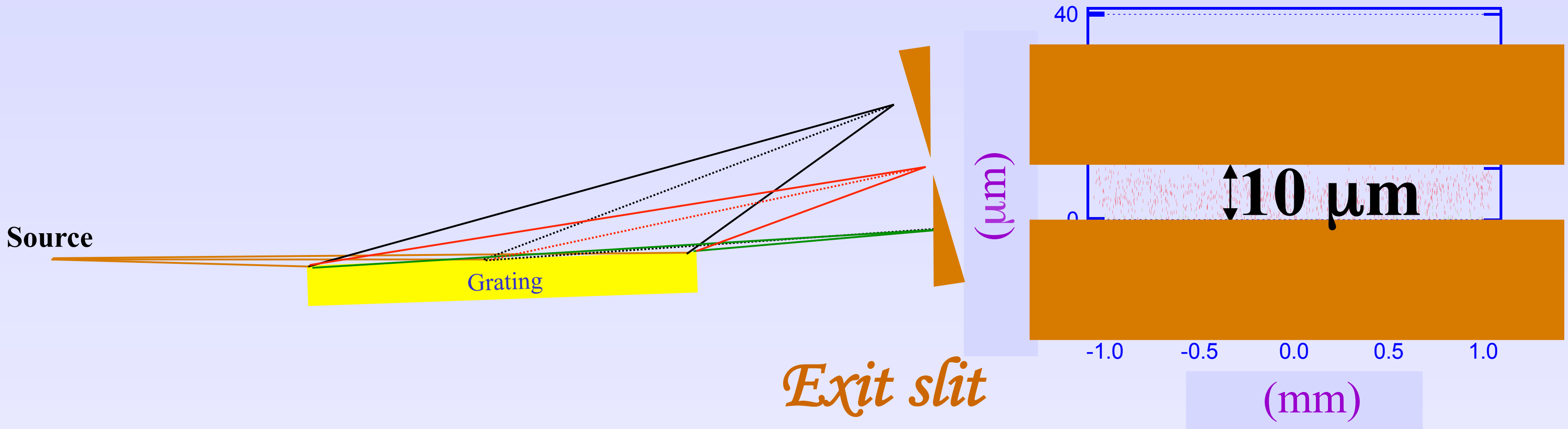
$$F_{100} = 0 \Rightarrow \sin\alpha + \sin\beta = Nk\lambda$$ grating equation

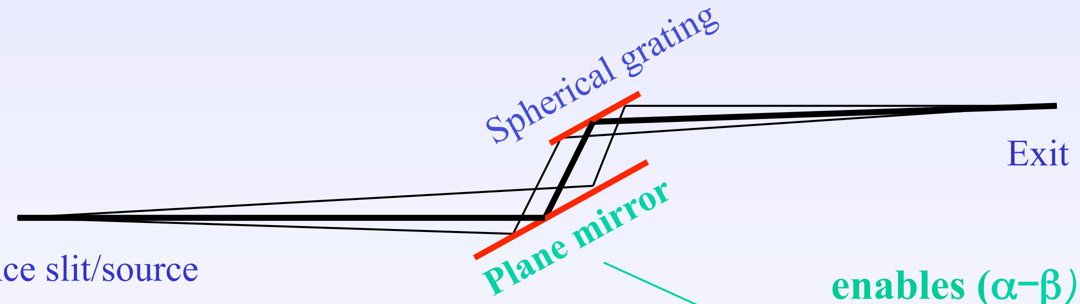
$$F_{200} = 0 \Rightarrow \left(\frac{\cos^2\alpha}{r} + \frac{\cos^2\beta}{r'}\right) - \frac{(\cos\alpha + \cos\beta)}{R} = 0$$ tangential focusing



Variable included angle=(α−β)

Variable included angle spherical grating monochromator (2)

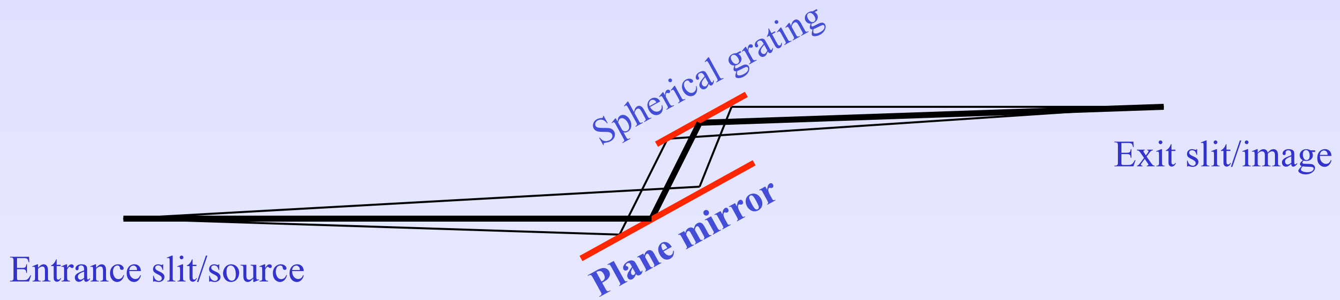




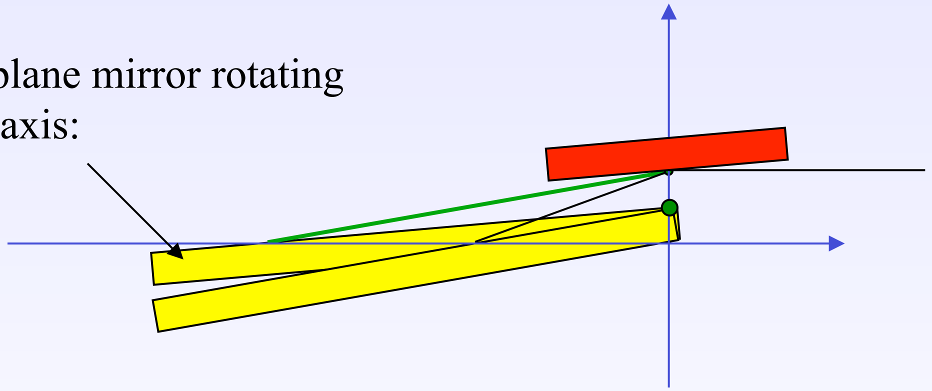
enables (α−β) to be varied keeping constant the source and the image in position and direction:

$i_{mirror} = (\alpha - \beta)/2$

Variable included angle spherical grating monochromator (3)

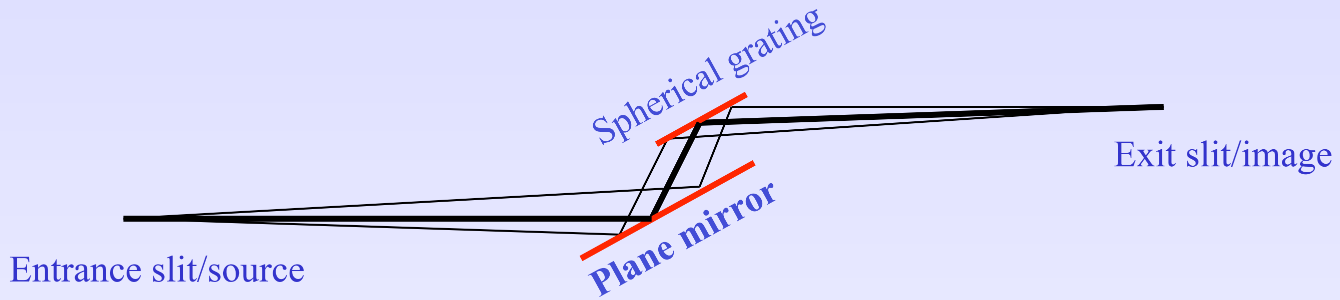


Sufficiently long plane mirror rotating about a particular axis:



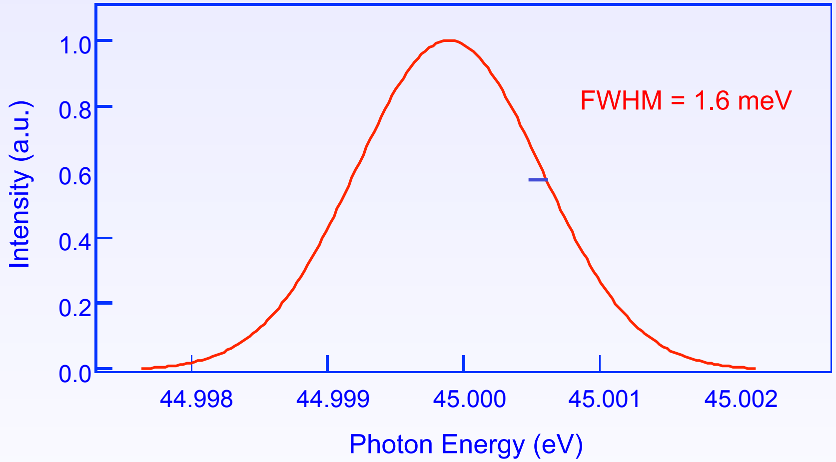
The light beam runs up and down the plane mirror as it is rotated

Variable included angle spherical grating monochromator (4)



resolving power:

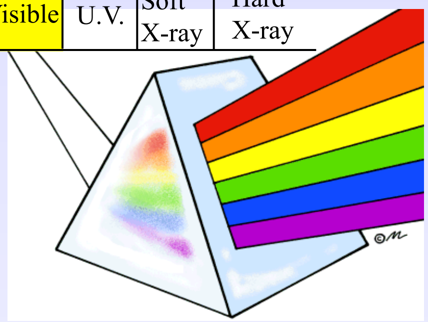
$$\frac{E}{\Delta E} = \frac{\lambda}{\Delta \lambda} = 28000$$



Monochromators

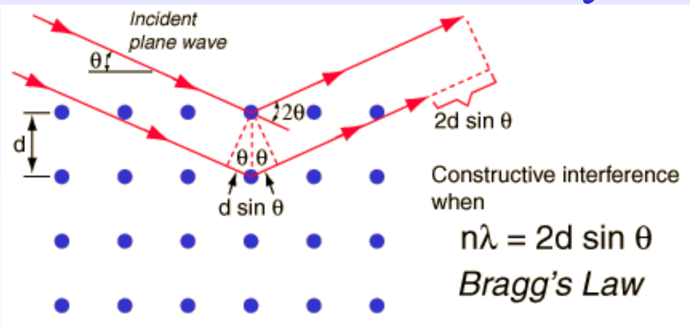
Microwave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Prism

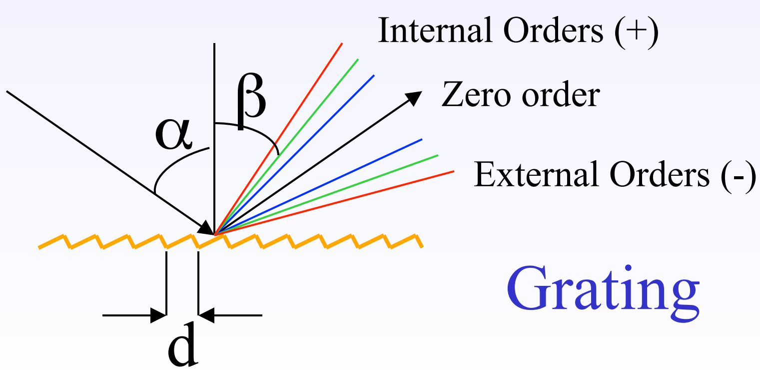


Microwave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Crystal

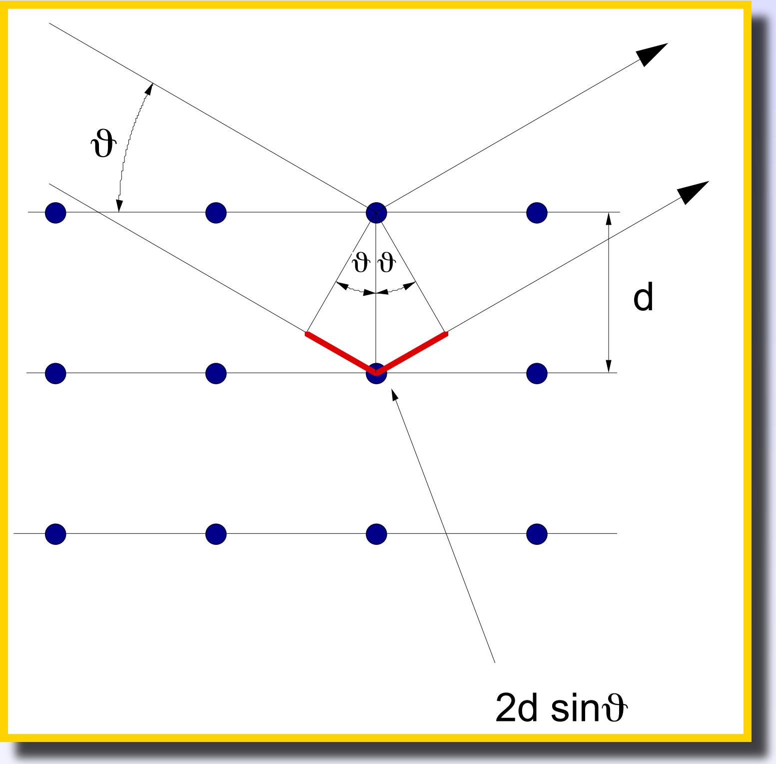


Microwave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray



Grating

Bragg's law



Radiation of wavelength λ is reflected by the lattice planes. The outgoing waves interfere. The interference is constructive when the optical path difference is a multiple of λ:

$$2d\sin\vartheta = n\lambda$$

d is the distance between crystal planes.

$$\sin\vartheta \leq 1 \Rightarrow \lambda \leq \lambda_{max} = 2d$$

The maximum reflected wavelength corresponds to the case of normal incidence: θ=90°

EXAMPLES:

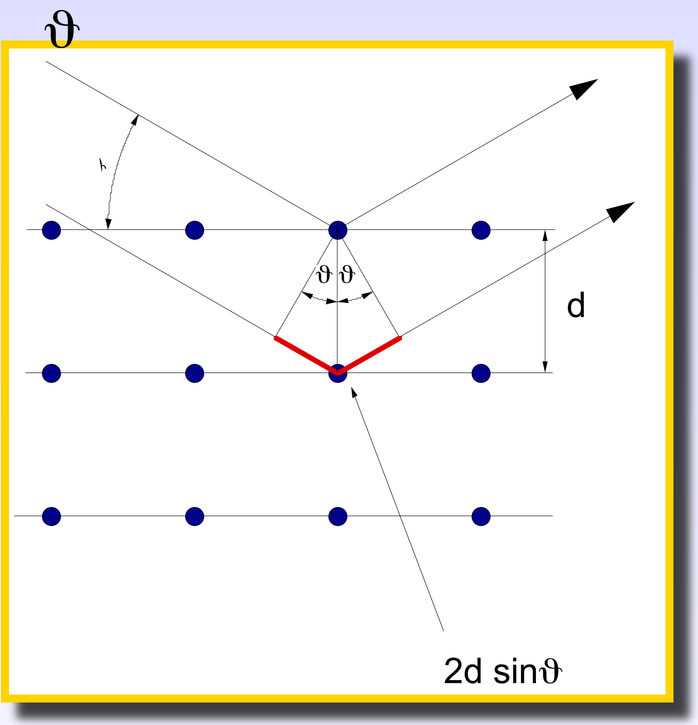
Si (111) : d=3.13Å → Emin ≈ 2 keV

Si (311) : d=1.64Å → Emin ≈ 3.8 keV

InSb (111) : d=3.74Å → Emin ≈ 1.7 keV

Be (10$\underline{1}$0) : d=7.98Å → Emin ≈ 0.8 keV

Energy resolution



$$2d\sin\vartheta = n\lambda$$

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

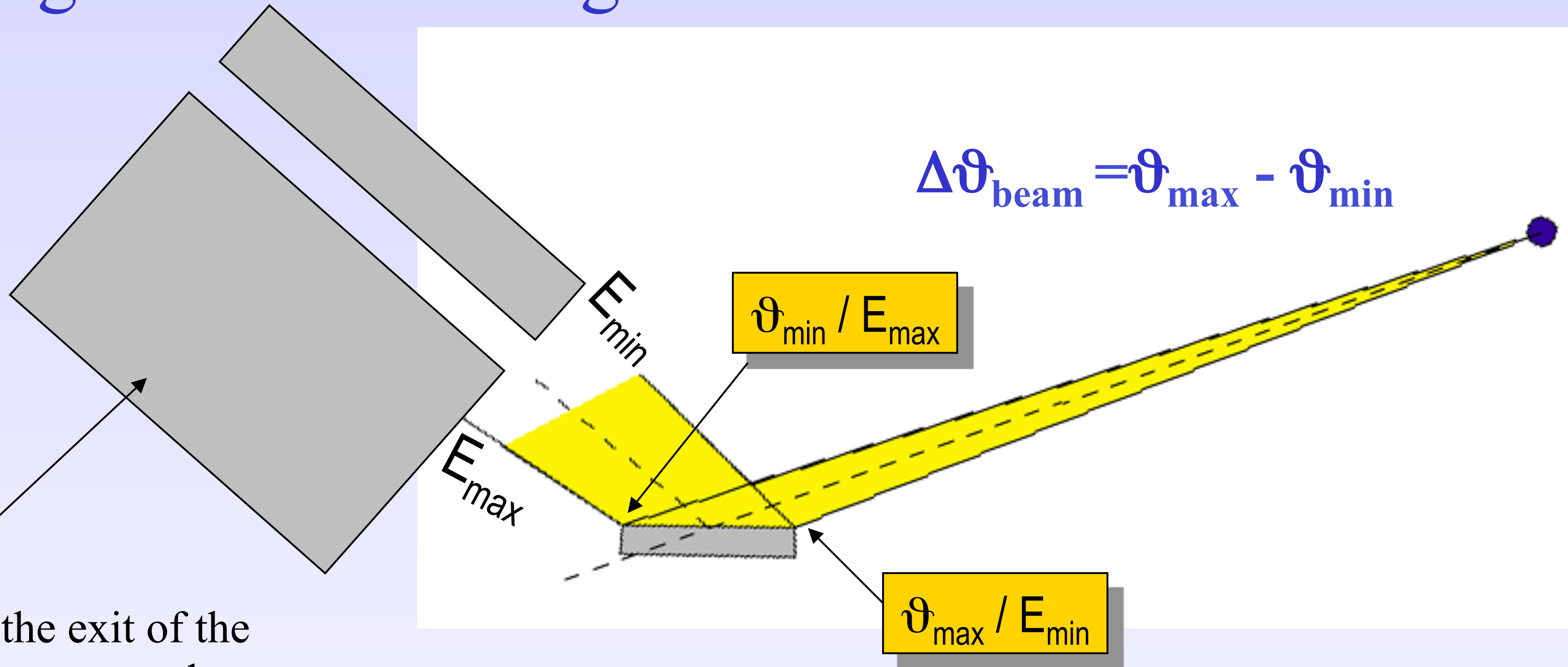
The energy resolution of a crystal monochromator is determined by the angular spread $\Delta\vartheta$ of the diffracted beam and by the Bragg angle ϑ

$\Delta\vartheta$ has two contributions :

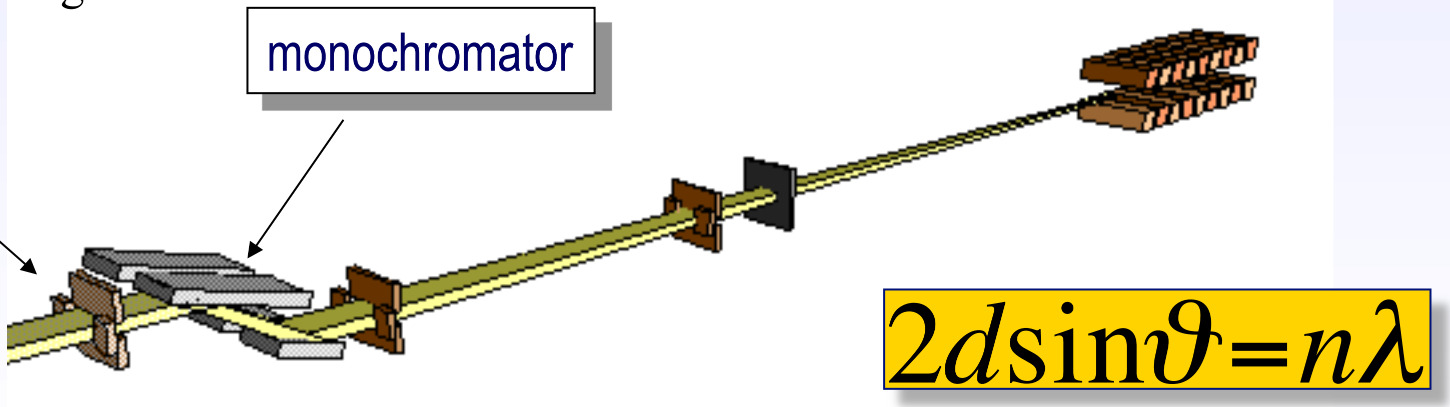
$\Delta\vartheta_{beam}$: angular divergence of the incident beam

$\omega_{crystal}$: intrinsic width of the Bragg reflection

Angular beam divergence

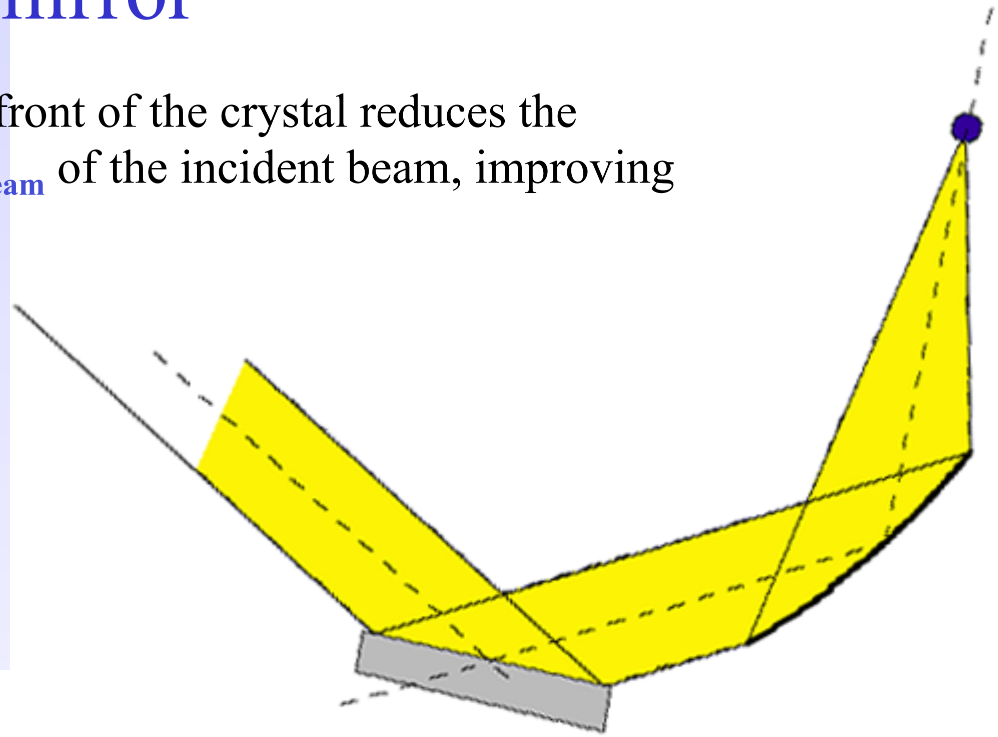


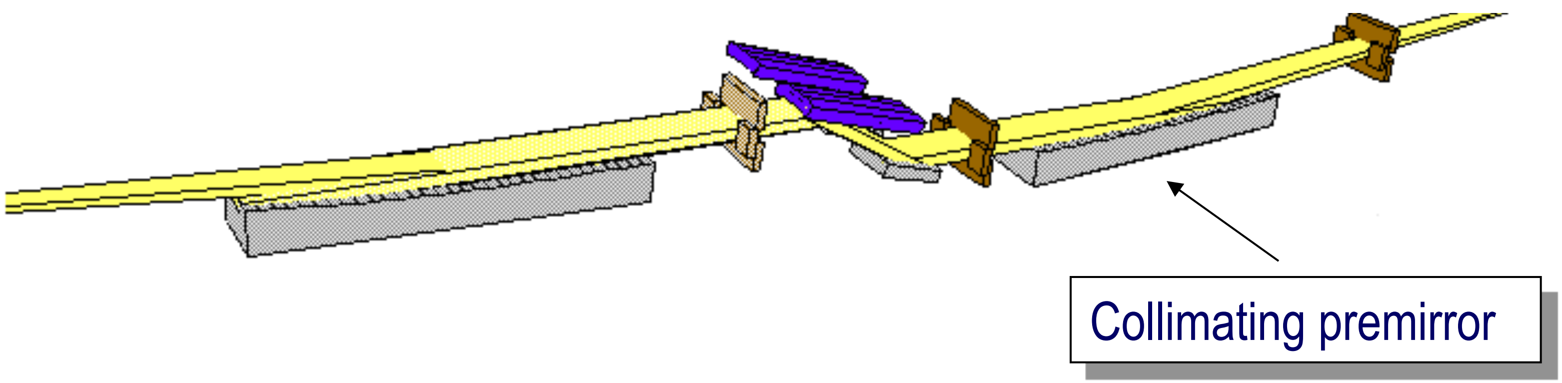
A slit at the exit of the monochromator selects a narrower energy range.



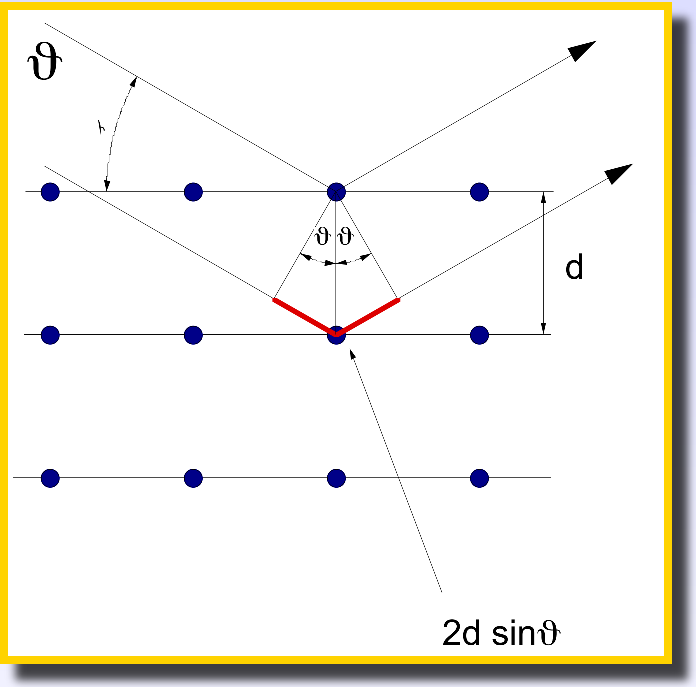
Collimating mirror

A collimating mirror in front of the crystal reduces the angular divergence $\Delta\vartheta_{beam}$ of the incident beam, improving the energy resolution.





Energy resolution



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

The energy resolution of a crystal monochromator is determined by the angular spread $\Delta\vartheta$ of the diffracted beam and by the Bragg angle ϑ

$\Delta\vartheta$ has two contributions :

$\Delta\vartheta_{beam}$: angular divergence of the incident beam

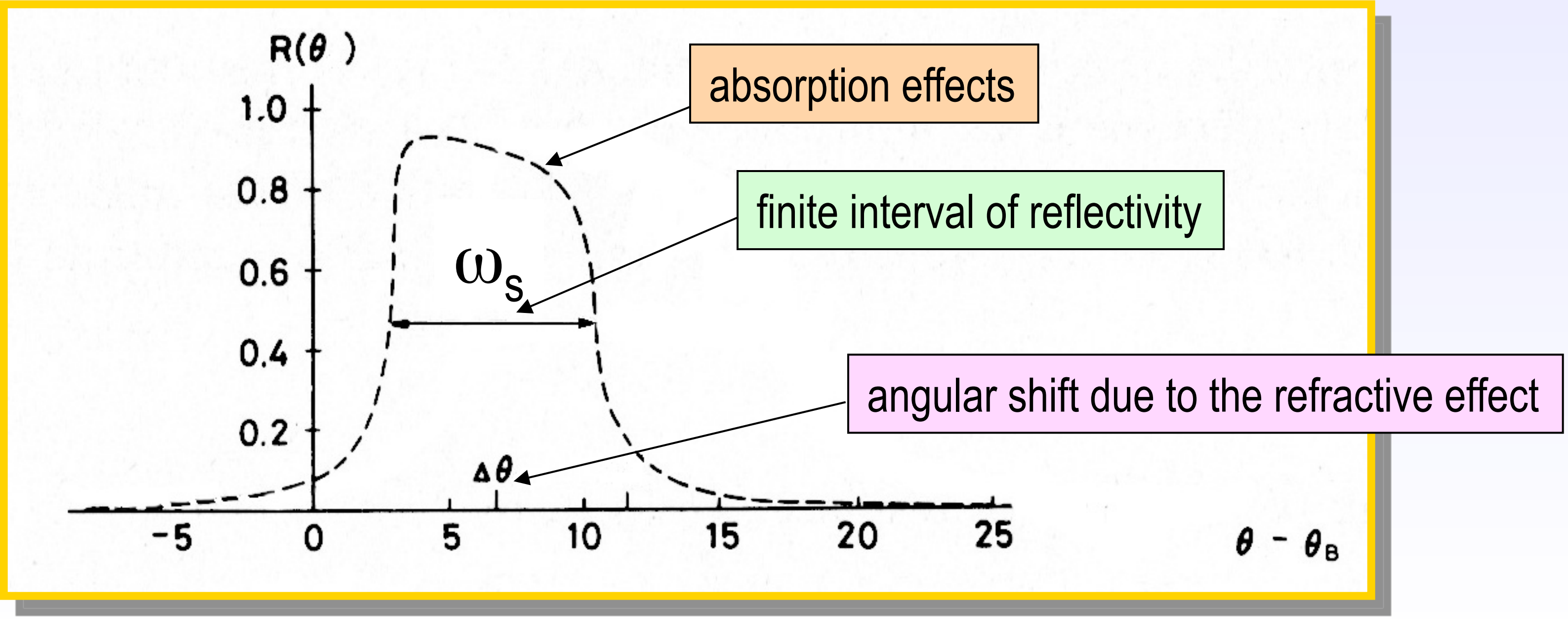
$\omega_{crystal}$: intrinsic width of the Bragg reflection

Darwin Curve

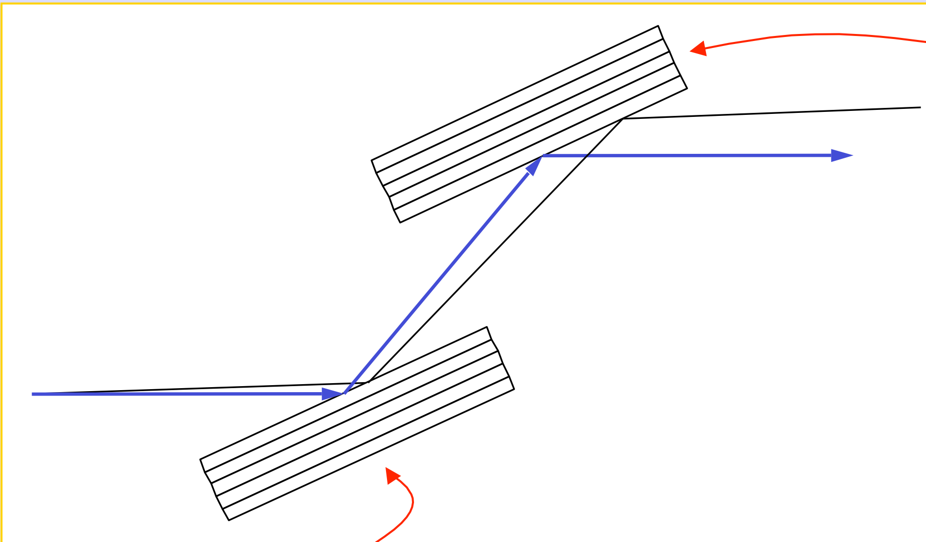
The intrinsic reflection width of the crystal, $\boldsymbol{\omega_s}$, can be obtained measuring the crystal reflectivity for a perfectly collimated monochromatic beam, as a function of the difference between the actual value of the incidence θ angle and the ideal Bragg value: $\Delta\theta = \theta - \theta_B$.

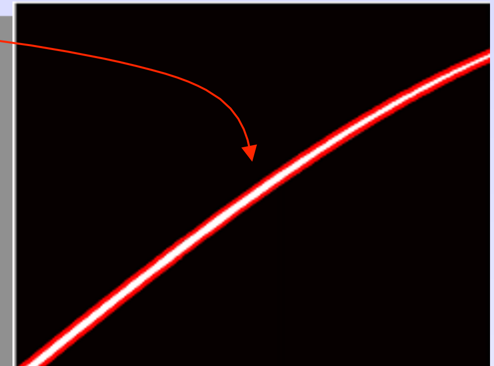
This reflectivity is derived by the dynamic diffraction theory, which includes multiple scattering → **Darwin curve**:

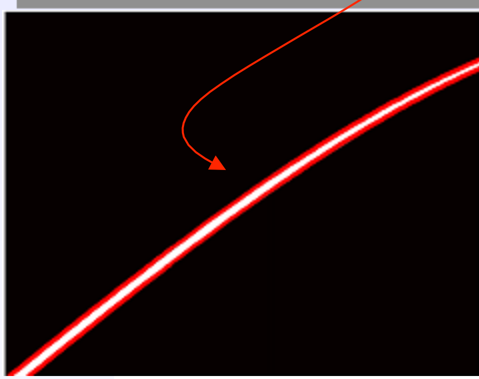
1. there is a finite interval of incidence angles for which the beam is reflected
2. the center of this interval does not coincide with the Bragg angle
3. R < 1 and has a typical asymmetric shape



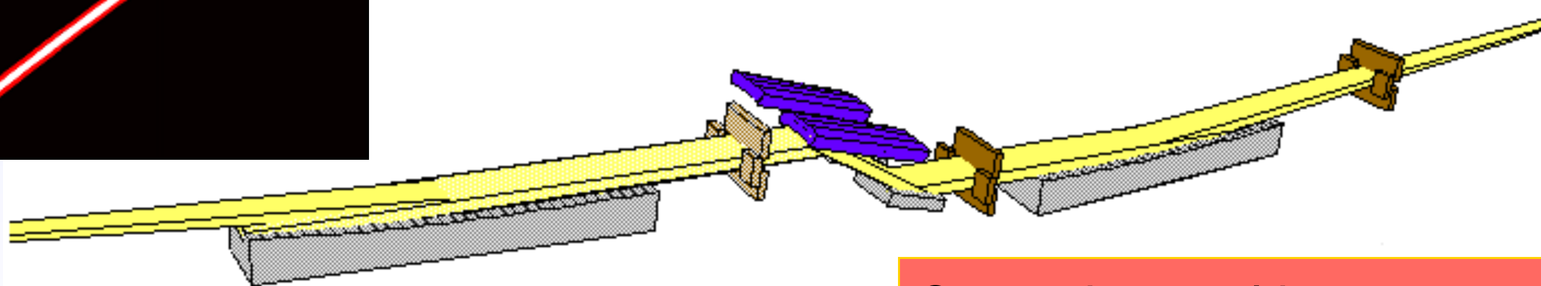
Crystal Monochromators





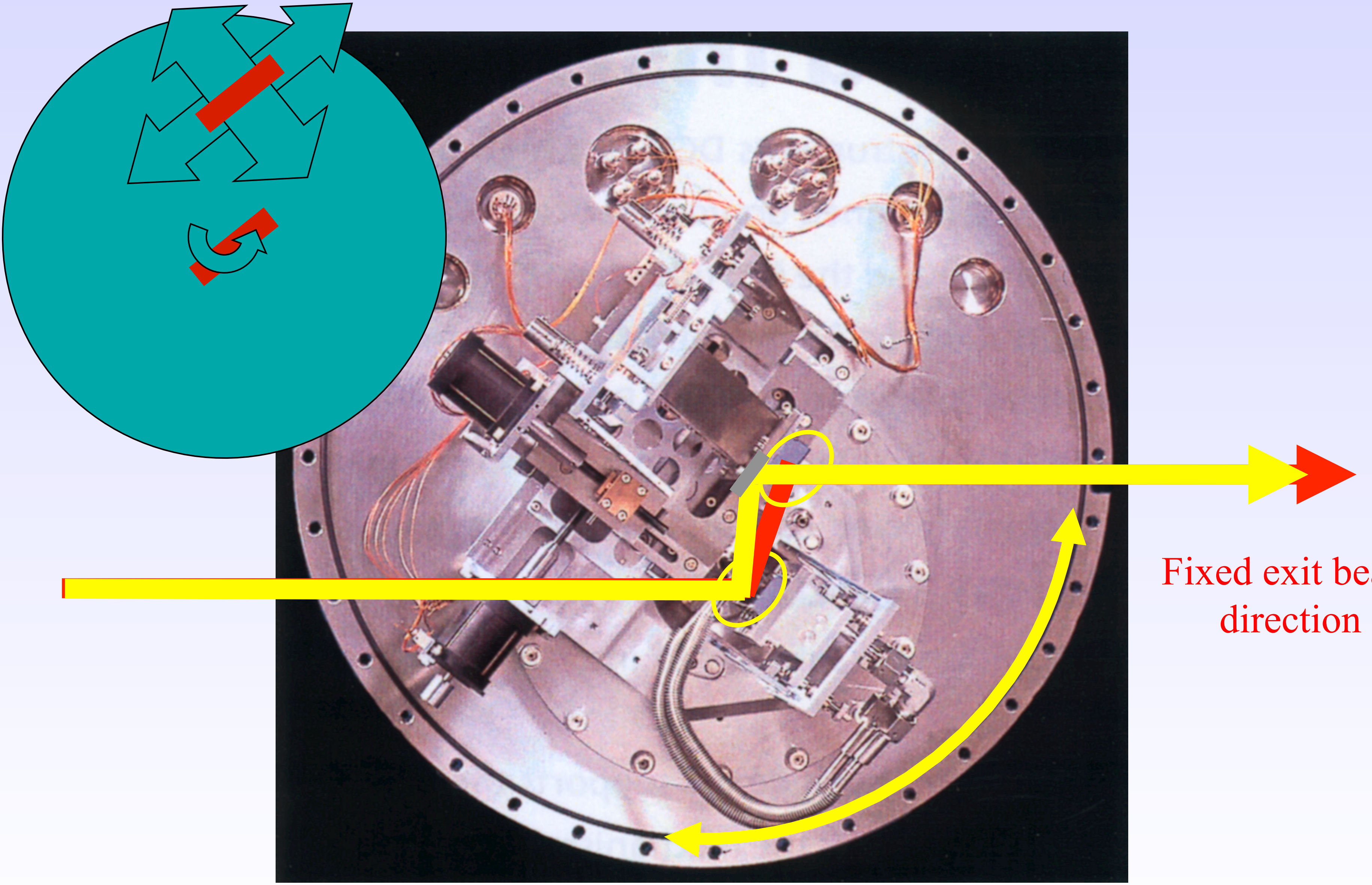


Parallel geometry:
all rays accepted by the first crystal are accepted also by the second.



Second crystal in
non dispersive configuration

Double Crystal Monochromator

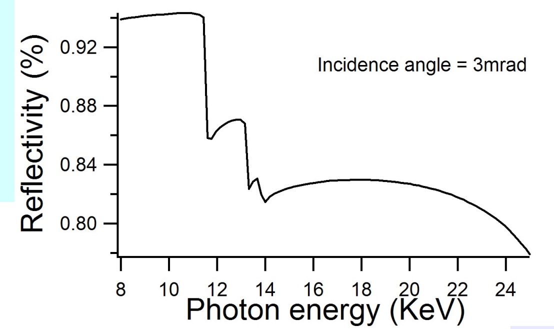


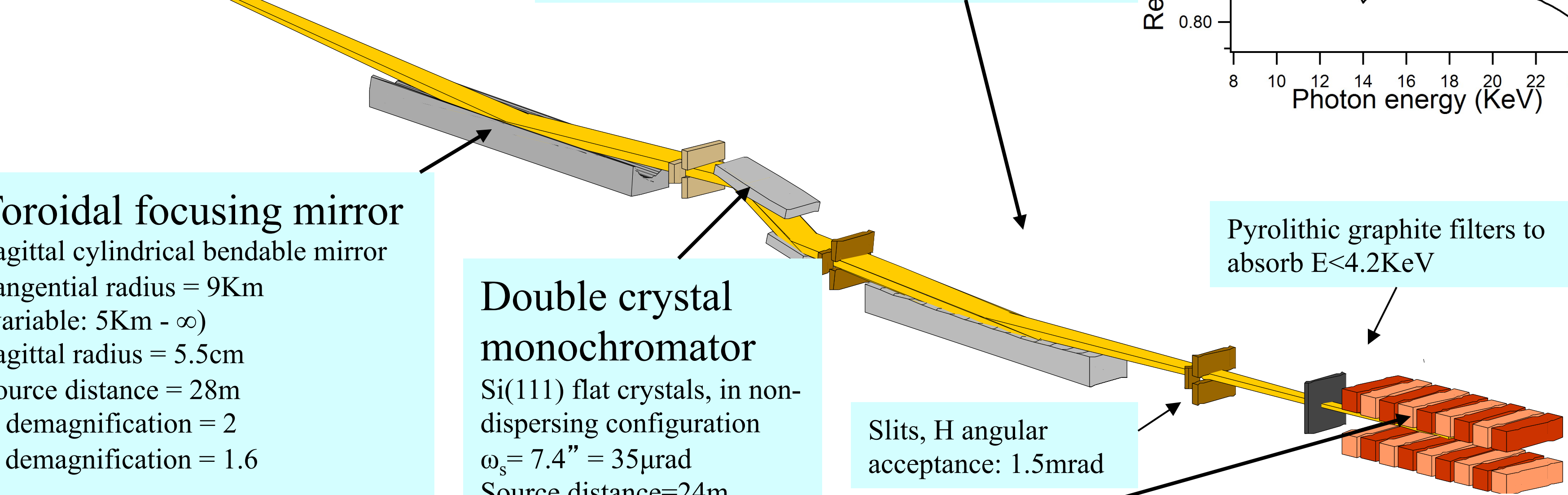
Fixed exit beam direction

Example: the ELETTRA X-ray Diffraction beamline

Experiment
Source distance = 41.5m
Energy range: 4-21KeV
spot size: 0.7x0.2mm^2
Photon flux: 10^{12}ph/s (at λ=1Å)
Resolving power: 3-4000

Cylindrical mirror for vertical collimation
Silicon with 50nm Platinum coating
Mirror length=1.4m
i=3mrad; Vertical angular acceptance =180μrad
Radius=14Km
Source distance d=22m
Collimated beam vertical divergence <10μrad



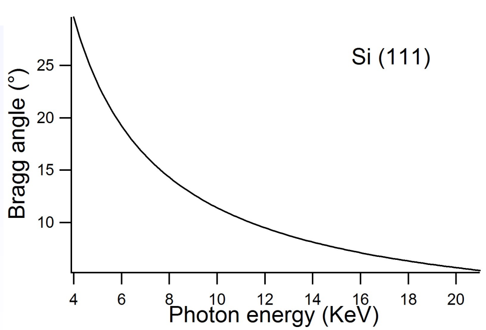


Toroidal focusing mirror
Sagittal cylindrical bendable mirror
Tangential radius = 9Km
(variable: 5Km - ∞)
Sagittal radius = 5.5cm
Source distance = 28m
H demagnification = 2
V demagnification = 1.6

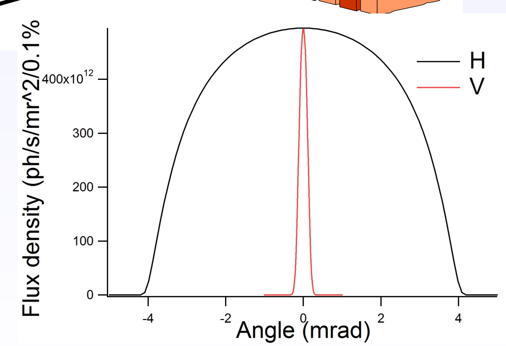
Double crystal monochromator
Si(111) flat crystals, in non-dispersing configuration
ω_s= 7.4” = 35μrad
Source distance=24m

Pyrolithic graphite filters to absorb E<4.2KeV

Slits, H angular acceptance: 1.5mrad



Multi-pole wiggler
57 poles, 1.5T magnetic field,
14cm period length,
5.8KeV critical energy @2.4GeV
5 kW total power @140mA



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These notes have been taken from:

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• B.W.Batterman and D.H.Bilderback, “X-Ray Monocromators and Mirrors” in “Handbook on Synchrotron Radiation”, Vol.3, G.S.Brown and D.E.Moncton, Editors, North Holland, 1991, chapter 4

• “Selected Papers on VUV Synchrotron Radiation Instrumentation: Beam Line and Instrument Development”, D.L.Ederer Editor, SPIE vol. MS 152, 1998

• W.Gudat and C.Kunz, “Instrumentation for Spectroscopy and Other Applications”, in “Syncrotron Radiation”, “Topics in Current Physics”, Vol.10, C.Kunz, Editor, Springer-Verlag, 1979, chapter 3

• M.Howells, “Gratings and monochromators”, Section 4.3 in “X-Ray Data Booklet”, Lawrence Berkeley National Laboratory, Berkeley, 2001

• M.C. Hutley, “Diffraction Gratings”, Academic Press, 1982

References (2)

• R.L. Johnson, “Grating Monochromators and Optics for the VUV and Soft-X-Ray Region” in “Handbook on Synchrotron Radiation”, Vol.1, E.E.Koch, Editor, North Holland, 1983, chapter 3

• G.Margaritondo, “Introduction to Synchrotron Radiation”,Oxford University Press, 1988

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• W.B.Peatman, “Gratings, mirrors and slits”, Gordon and Breach Science Publishers, 1997

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• J.B. West and H.A. Padmore, “Optical Engineering” in “Handbook on Synchrotron Radiation”, Vol.2, G.V.Marr, Editor, North Holland, 1987, chapter 2

• G.P.Williams, “Monocromator Systems”, in “Synchrotron Radiation Research: Advances in Surface and Interface Science”,Vol.2, R.Z.Bachrach, Editor, Plenum Press, 1992, chapter 9

Programs

• **Shadow**

•**http://www.esrf.eu/Instrumentation/software/data-analysis/OurSoftware/raytracing**

• **XOP**

•**http://www.esrf.eu/Instrumentation/software/data-analysis/xop2.3** **(general optical calculations)**

• **SPECTRA**

•**http://radiant.harima.riken.go.jp/spectra/index.html**

(optical properties of synchrotron radiation emitted from bending magnets, wigglers and undulators)

Useful link:

http://www-cxro.lbl.gov/index.php?content=/tools.html/

(general information and on line software)