The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

1936-10

Advanced School on Synchrotron and Free Electron Laser Sources and their Multidisciplinary Applications

7 - 25 April 2008

Introduction to optical beamline design for soft and hard x-rays

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Main properties of Synchrotron Radiation

- Very broad and continuous spectral range, from infrared up to soft and hard x-rays

- High intensity

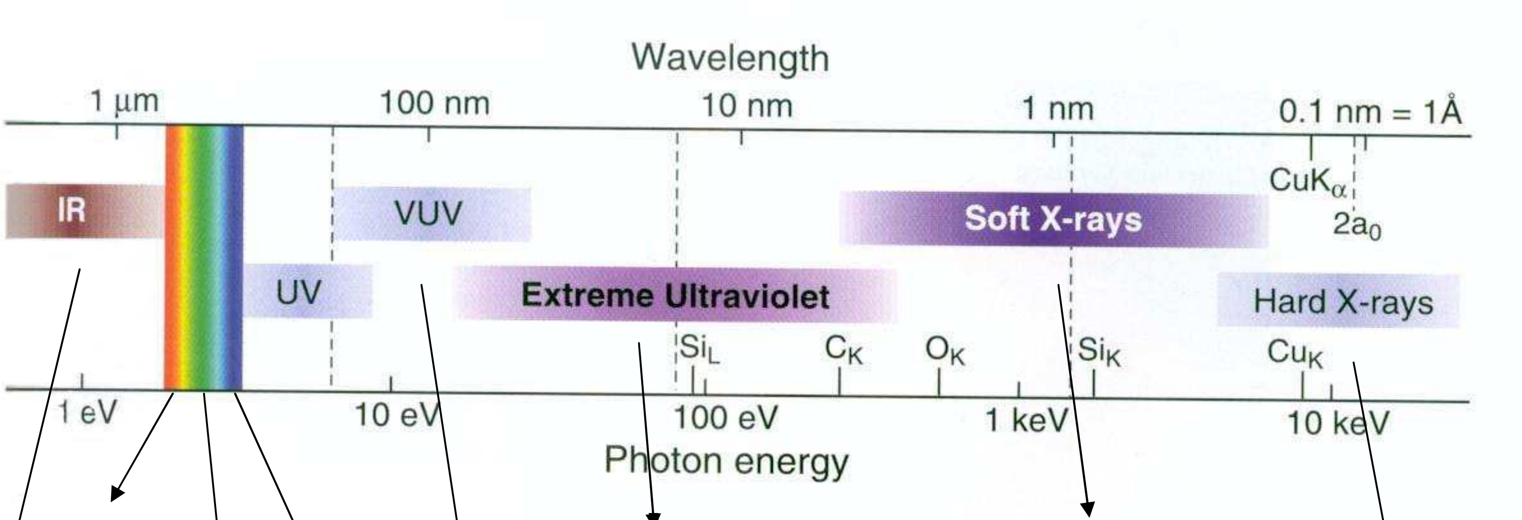
- Highly collimated and emanates from a very small source: the electron beam

- Pulse time structure

- High degree of polarization

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

Spectral brightness

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

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

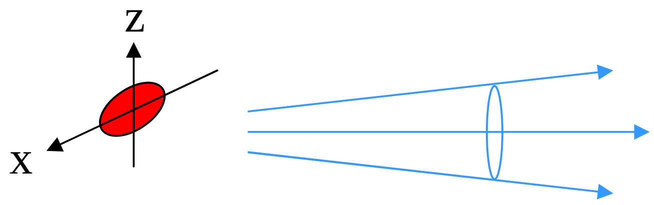
$\sigma_x\sigma_z$ = transverse area from which SR is emitted

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

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

Source size

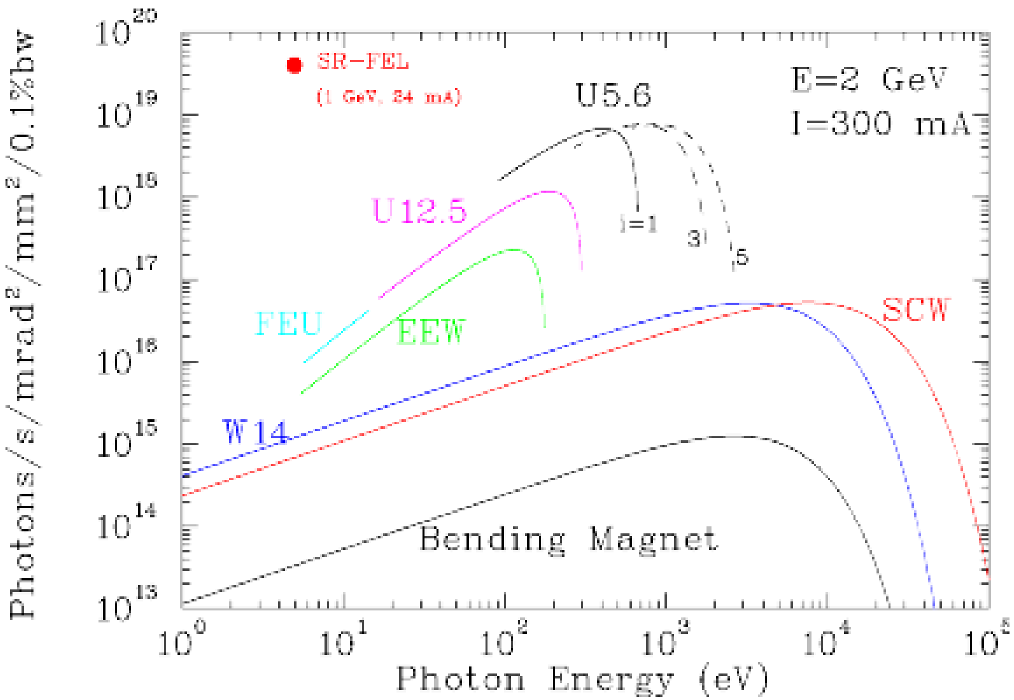
$\sigma_x\sigma_z$



Solid angle

$\sigma'_x\sigma'_z$

SR spectral brightness at ELETTRA



Why is brightness important? (1)

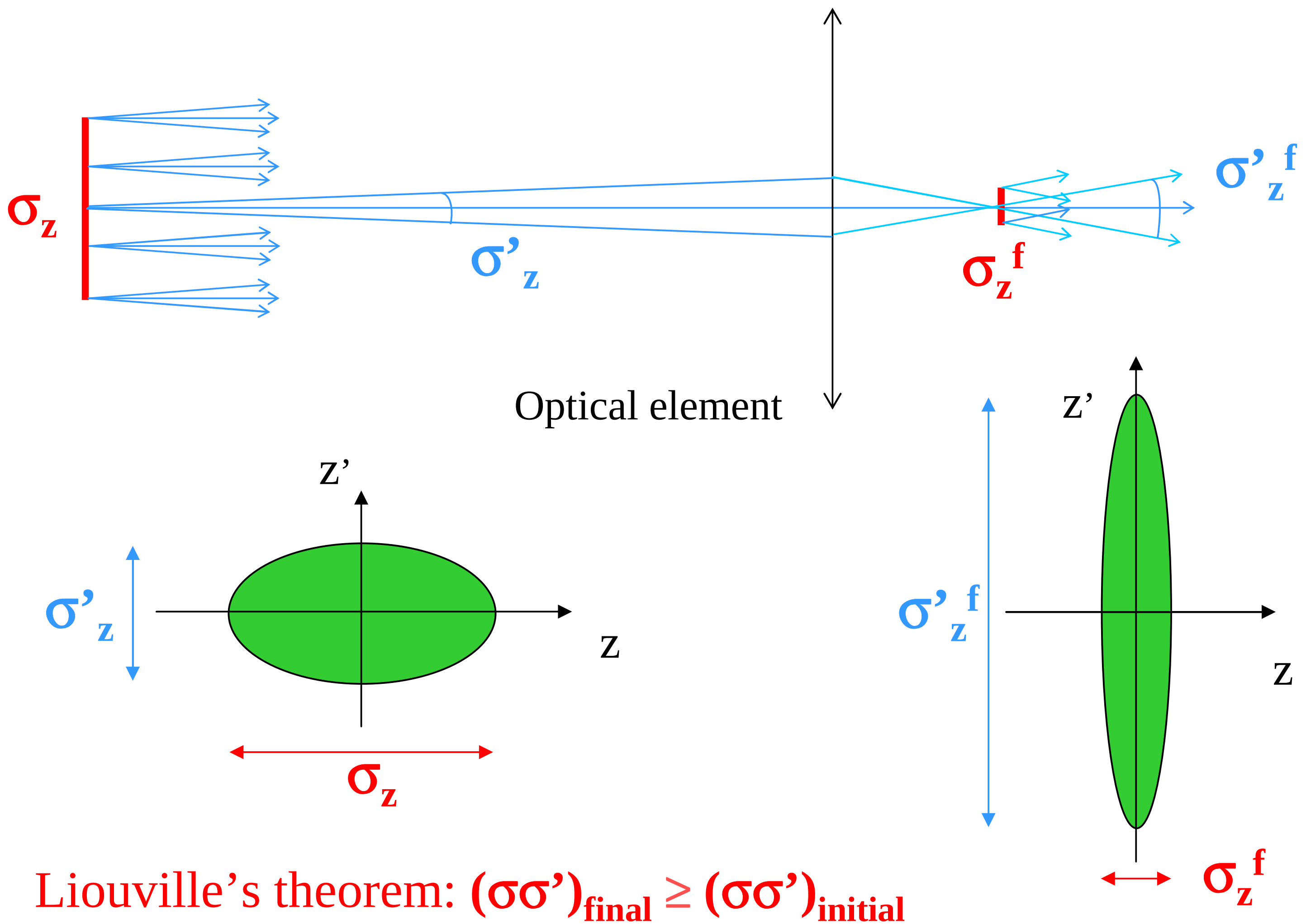
$$\boxed{Spectral\ Brightness = \frac{photon\ \ flux}{I}\frac{1}{\sigma_x\sigma_z\sigma'_x\sigma'_z BW}}$$

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: $\boldsymbol{(\sigma\sigma')_{final} \geq (\sigma\sigma')_{initial}}$

→ 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:

• is the means of bringing radiation from the source to the experiment transforming the phase volume in a controlled way: it de-magnifies, monochromatizes and refocuses the source onto a sample

• must preserve the excellent qualities of the radiation source: it must transfer the high brightness from source up to the experiment

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

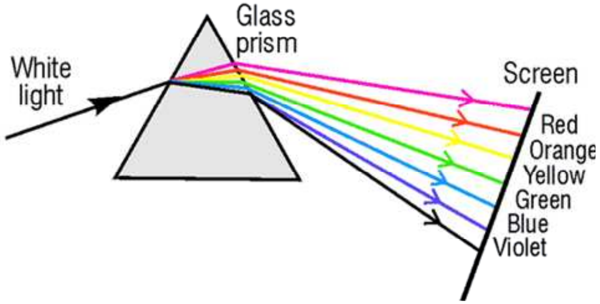
The beamline (2)

Basic elements:

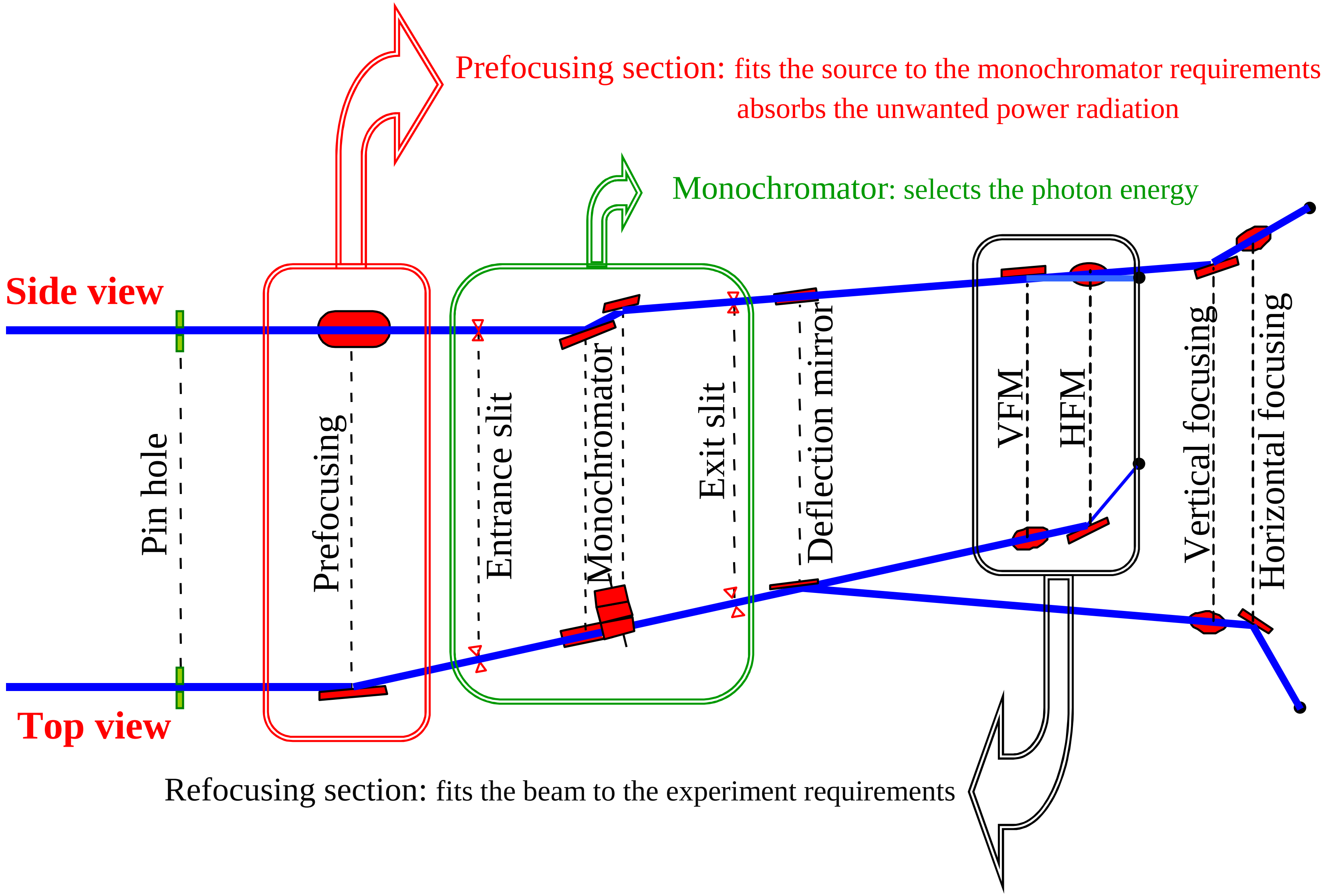
• mirrors, to deflect, focus and filter the radiation

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

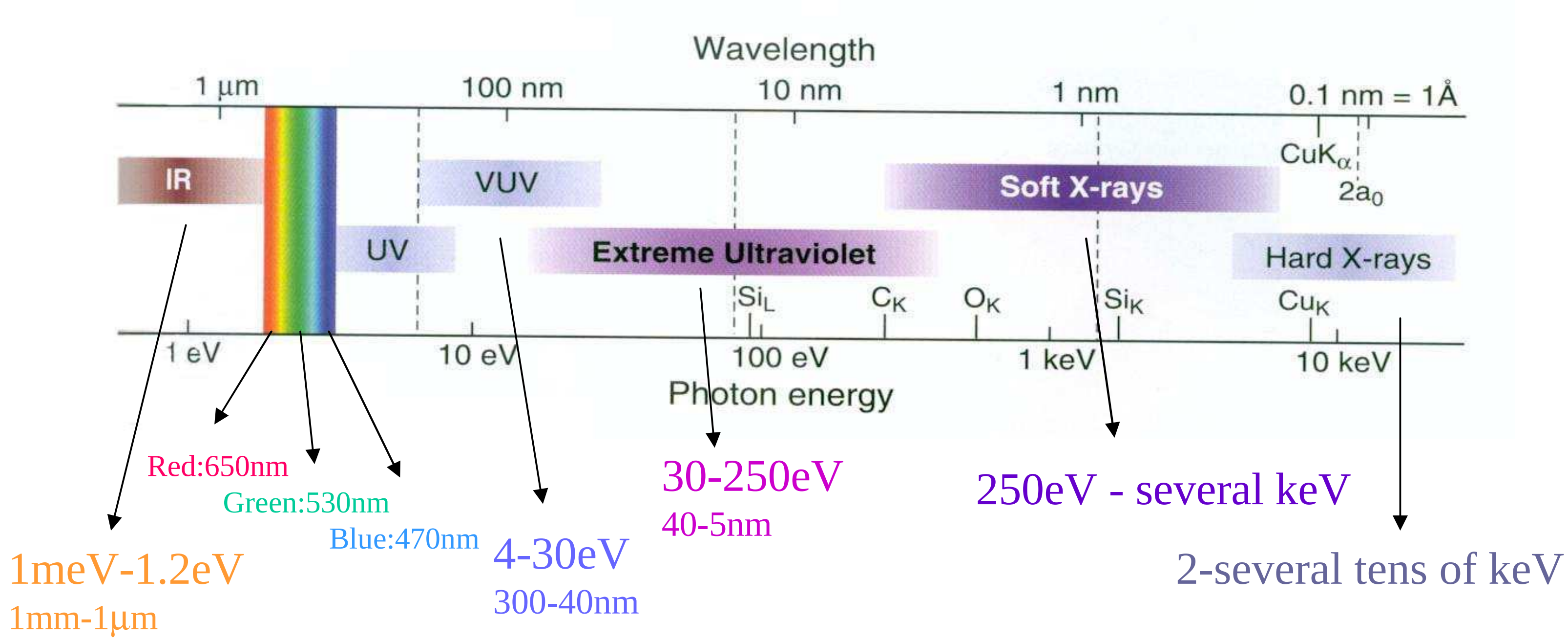
• detectors



Beamline structure



VUV, EUV and soft x-rays



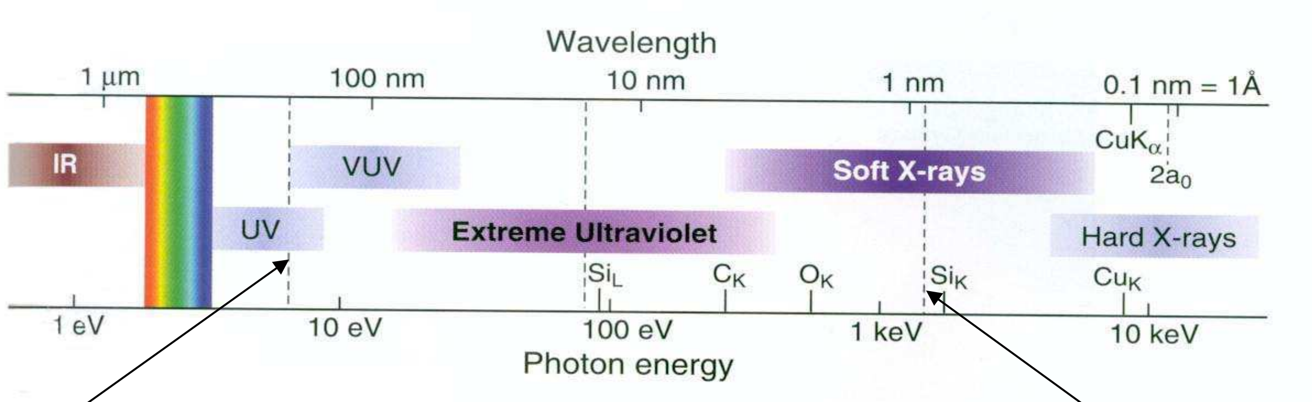
These regions are very interesting because are characterized by the presence of the absorption edges of most low and intermediate Z elements

→ 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

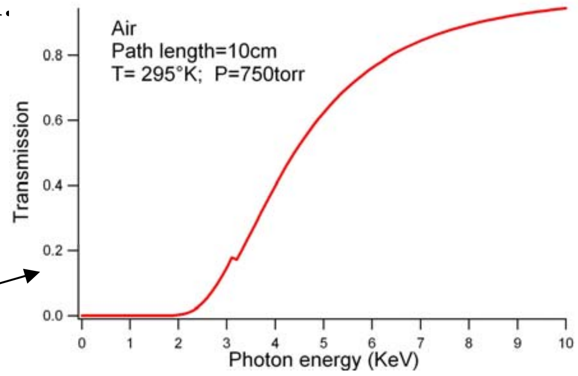
→ No windows

→ The entire optical system must be kept under UH Vacuum

Ultrahigh vacuum conditions (P=1-2x10^{-9} mbar) are required:

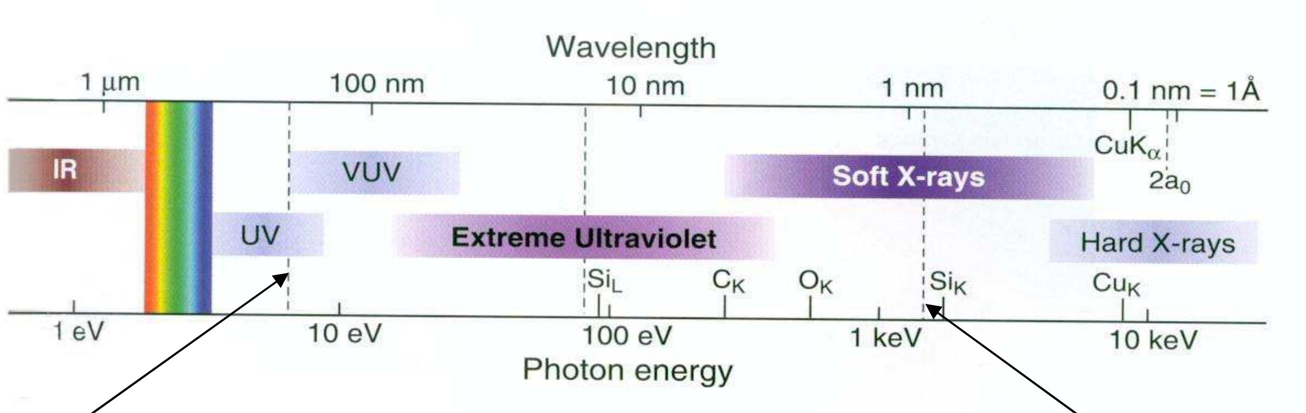
- Not to disturb the storage ring and the experiment
- To avoid photon absorption in air
- To protect optical surfaces from contamination (especially from carbon)

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:



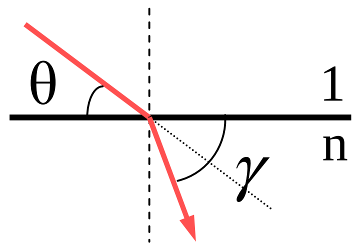
Transmission limit of common fused silica window: ~8eV   Absorption limit of 8µm Be foil: ~1.5keV

→ 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

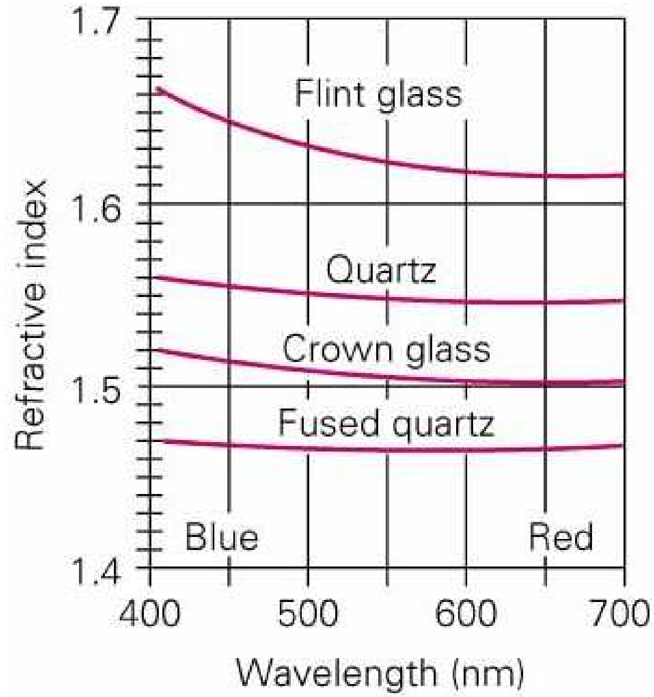
Snell's law, visible light

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

$\rightarrow$ **$\cos\theta = n \cos\gamma$** with $n = n_2/n_1$



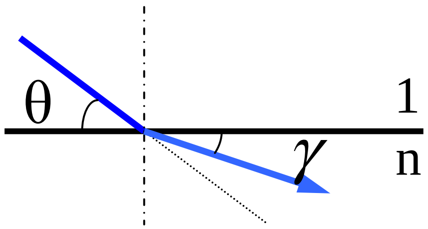
$n > 1 \rightarrow \gamma > \theta$



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 $n = n_2/n_1$

$n < 1$ → $\gamma < \theta$

X-rays have the real part, n, of the refractive index slightly less than unity:

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

Typical values are:

$\delta \approx 10^{-2}$ for 250eV (5nm)

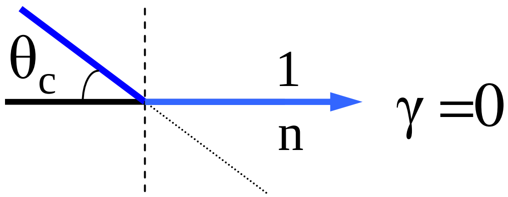
$\delta \approx 10^{-4}$ for 2.5keV (0.5nm)

→ 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: $\cos\theta_c = n$

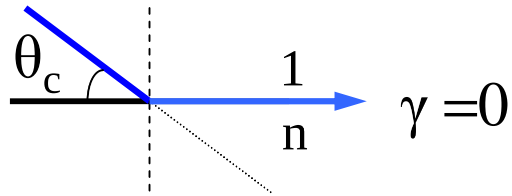
→ $\boxed{\theta_c = \sqrt{2\delta}}$



$n < 1$

Critical angle

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



n < 1

Substituting δ, it can be shown that the major functional dependencies of θ_c are:

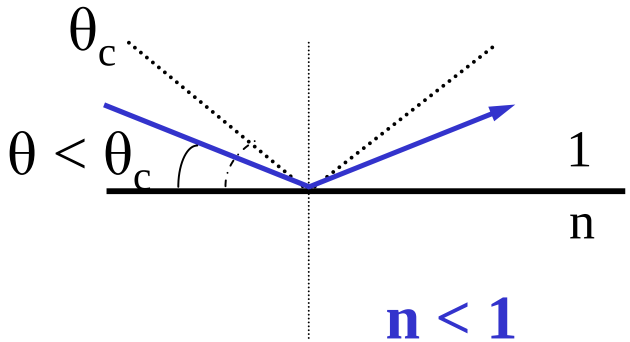
$$\boxed{\theta_c \, \alpha \, \lambda \sqrt{Z}}$$

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

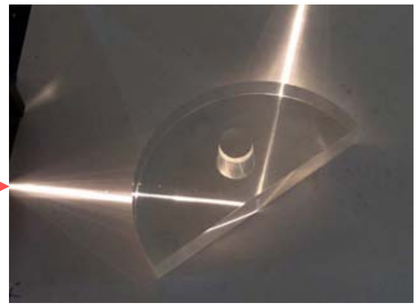
Gold:
600 eV → θc ≈ 7.4°
1200 eV → θc ≈ 3.7°
5 keV → θc ≈ 0.9°

Total external reflection

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



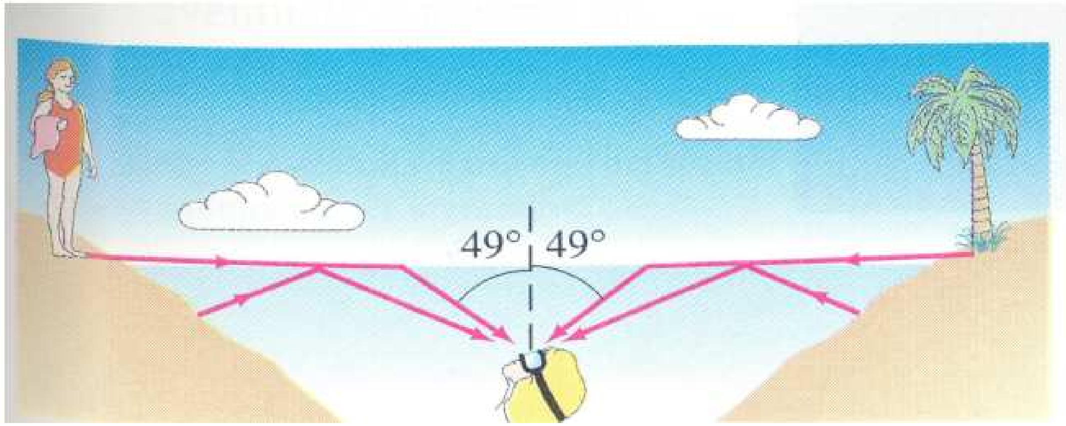
It is the counterpart of total internal reflection of visible light. Visible light is totally reflected at the glass/air boundary if $\theta < \theta_c$.

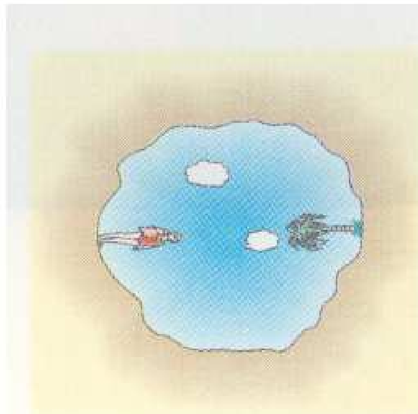


$n * \cos \theta c = 1 \rightarrow \theta c = \arccos(1/n) = 48.2°$

n =1.5 refraction index of glass

Total internal reflection (visible light)



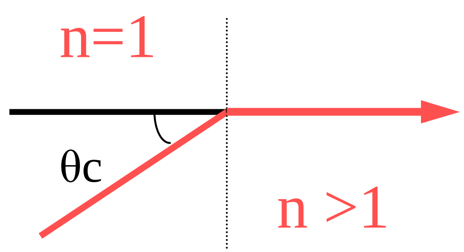


If you are in a swimming pool and look up directly above you within a cone of 49°, will see a compressed view of the outside world. If you look along the water surface beyond the 49° angle, you will not be able to see the world outside but only the reflected sides of the swimming pool.

$n \cdot \cos\theta_c = 1 \rightarrow \theta_c = \arccos(1/n) = 41.4°$

$n = 1.333$ refraction index of water

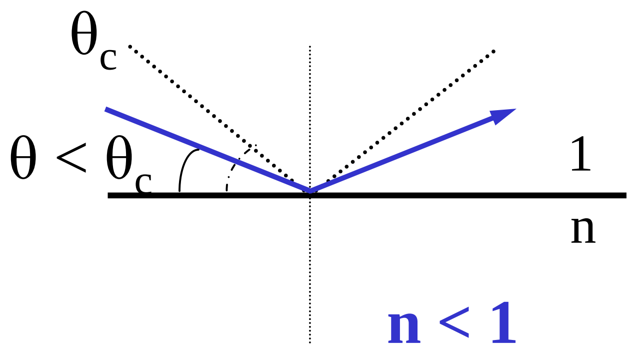
$(90° - 41.4° = 48.6°)$

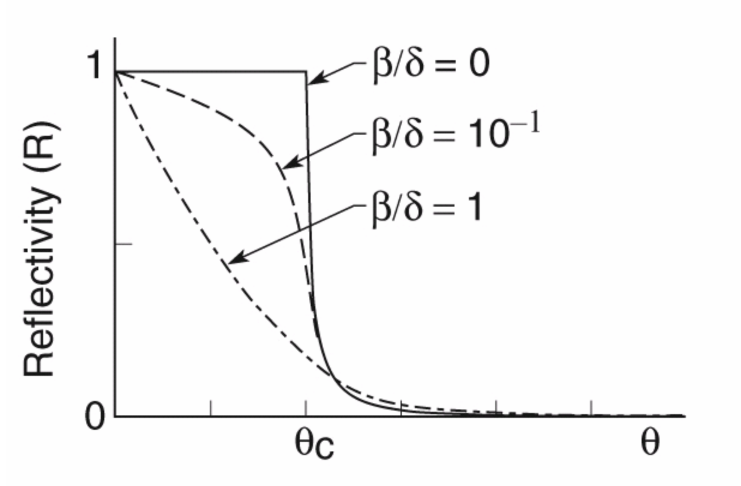


Nearly total external reflection

This model of total reflection is incomplete because it doesn't include the effect of the imaginary part of the refraction index.
The radiation penetrates into the second medium during the reflection process, so that the absorption in this medium decreases the intensity of the reflected beam.

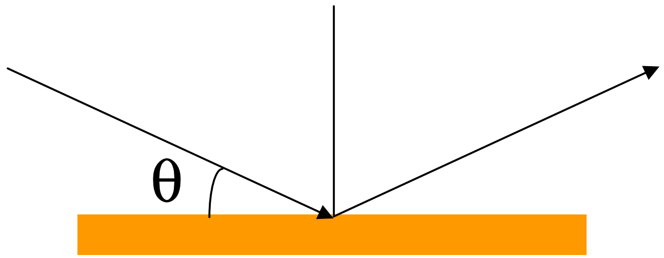
→ The sharpness of the cut-off is reduced



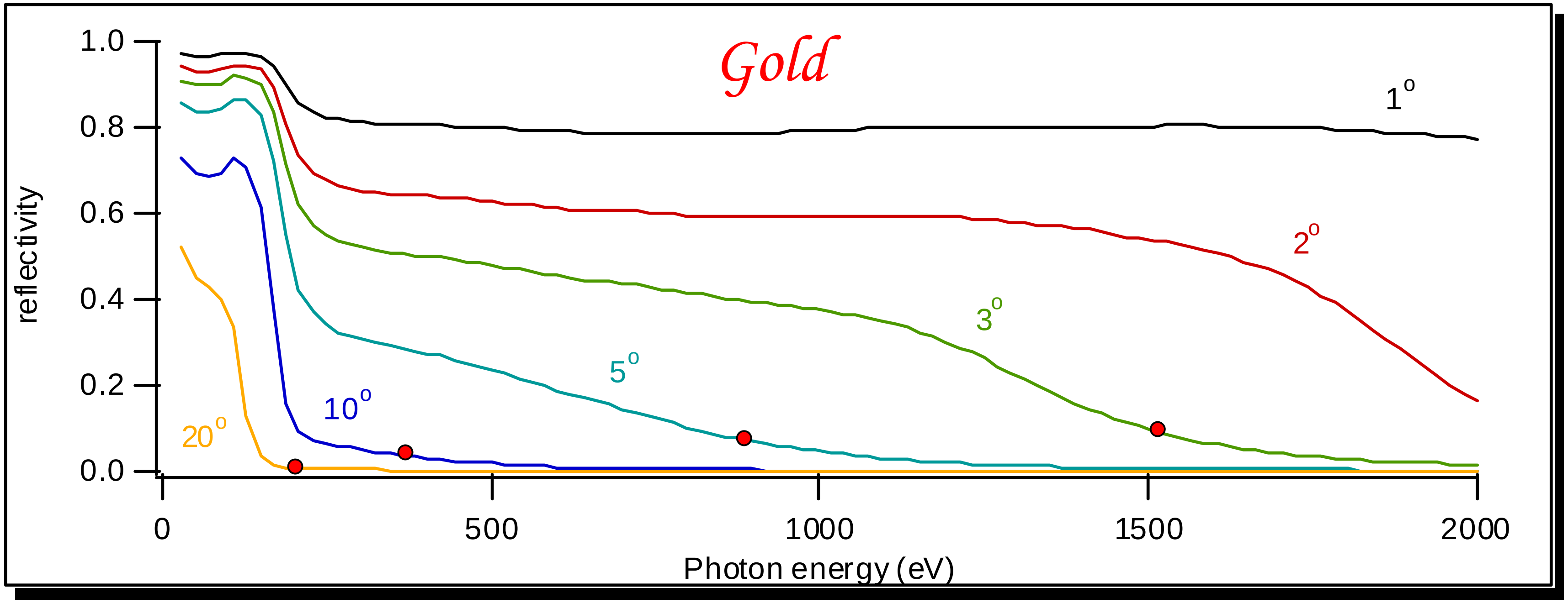


D.Attwood, “Soft x-rays and extreme ultraviolet radiation”, Cambridge University Press, 1999

Mirror reflectivity (1)

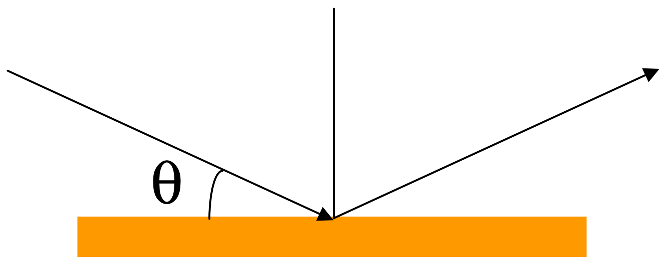


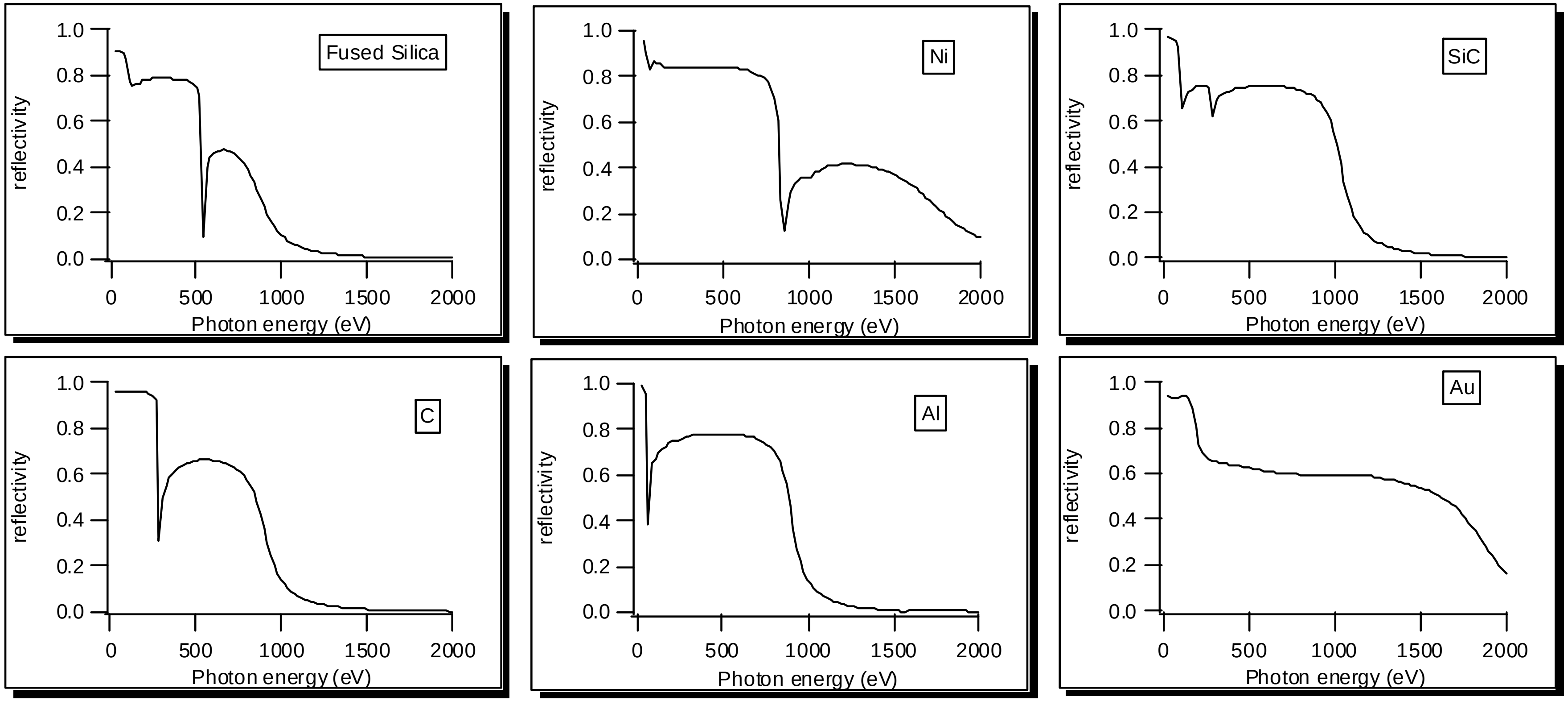
Reflectivity drops down fast with the increasing of the grazing incidence angle
→ only reflective optics at grazing incidence angles
(typically 1°-2° for soft x-rays, few mrad for hard x-rays, 1 mrad= 0.057°)



Mirror reflectivity (2)

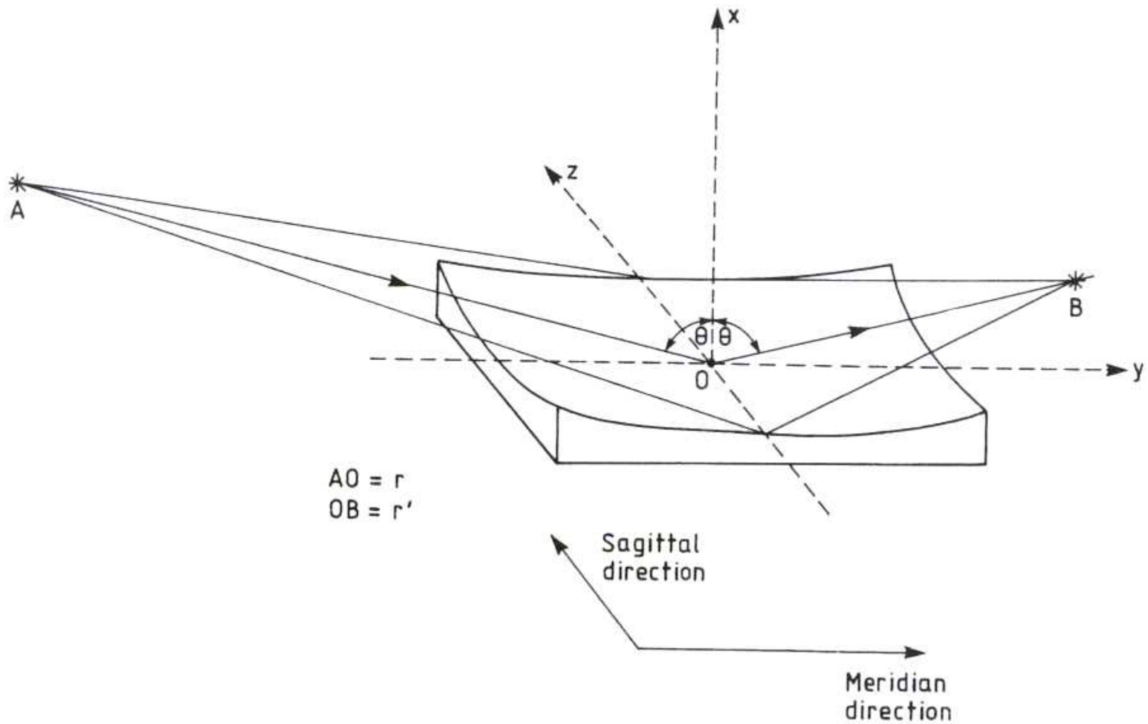
$\theta = 2^{o}$





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.

Paraboloid

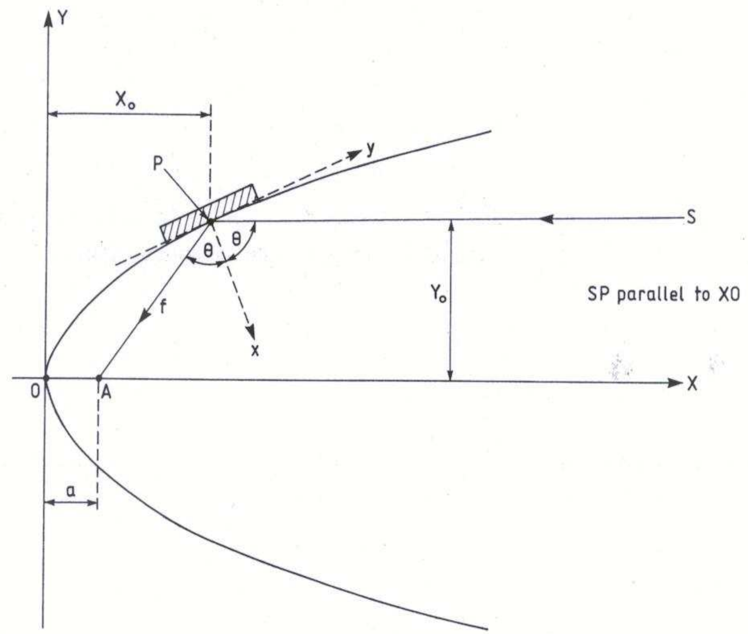
Rays traveling parallel to the symmetry axis OX are all focused to a point A**.**

Conversely, the parabola collimates rays emanating from the focus A.

Line equation: $Y^2 = 4aX$

Paraboloid equation: $Y^2 + Z^2 = 4aX$

where: $a = f\cos^2\vartheta$



Position of the pole P:

$$X_o = a\tan^2\vartheta$$
$$Y_o = 2a\tan\vartheta$$

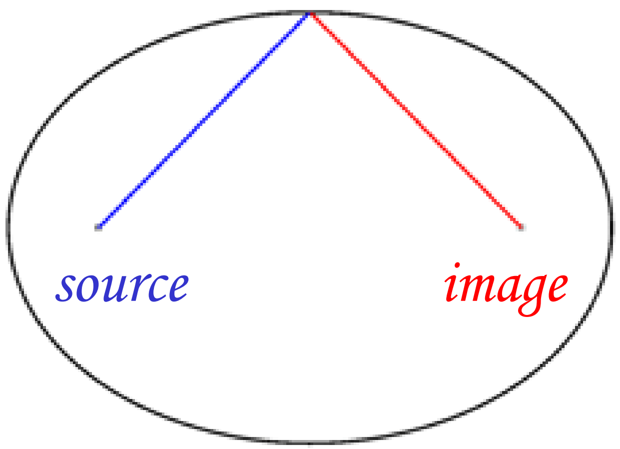
Paraboloid equation:

$$x^2\sin^2\vartheta + y^2\cos^2\vartheta + z^2 - 2xy\sin\vartheta\cos\vartheta - 4ax\sec\vartheta = 0$$

J.B. West and H.A. Padmore, Optical Engineering, 1987

Ellipse

The ellipse has the property that rays from one point focus F_1 will always be perfectly focused to the second point focus F_2



Ellipsoid

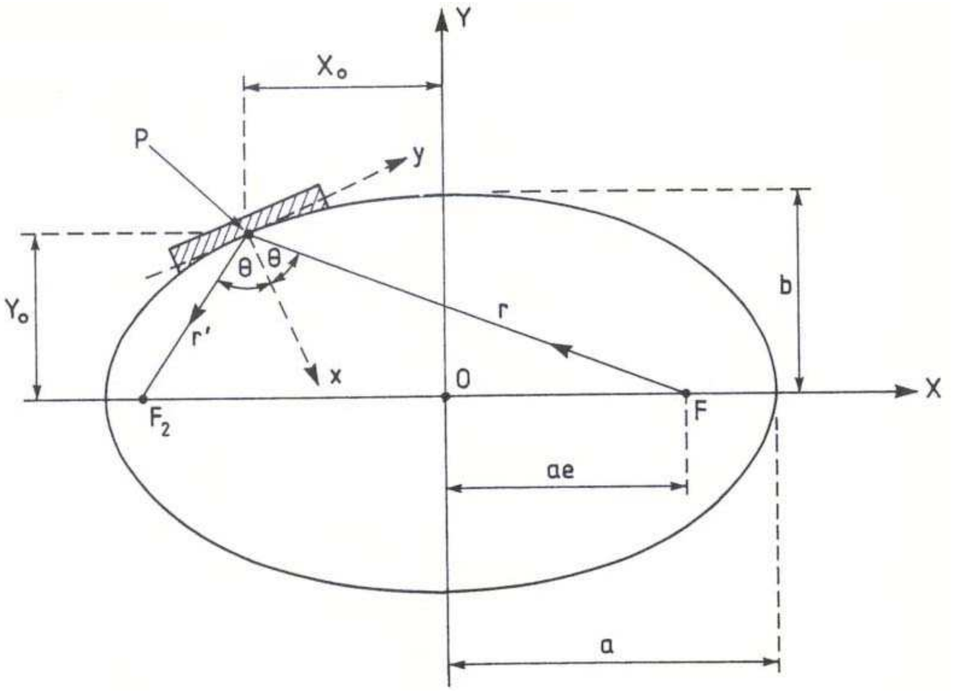
Line equation: $$\frac{X^2}{a^2}+\frac{Y^2}{b^2}=1$$

Ellipsoid equation:

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

where: $a=\frac{r+r'}{2}$; $b=a\sqrt{1-e^2}$

$$e=\frac{1}{2a}\sqrt{r^2+r'^2-2rr'\cos(2\vartheta)}$$



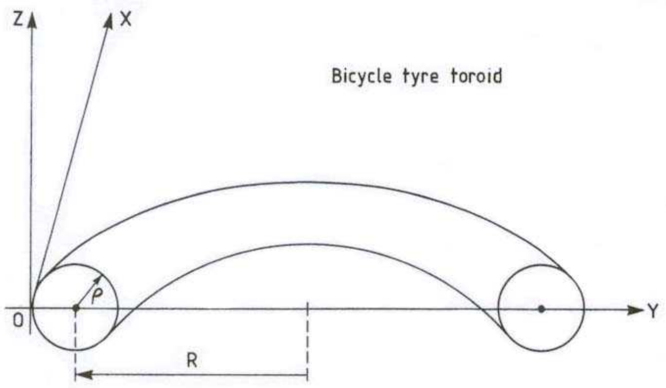
Rays from one focus F_1 will always be perfectly focused to the second focus F_2.

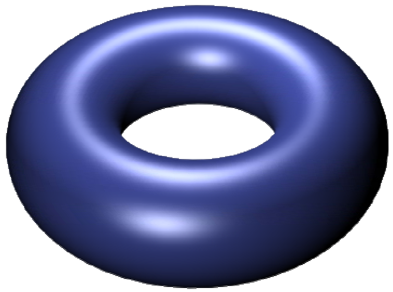
$$x^2\left(\frac{\sin^2\vartheta}{b^2}+\frac{1}{a^2}\right)+y^2\left(\frac{\cos^2\vartheta}{b^2}\right)+\frac{z^2}{b^2}-x\left(\frac{4f\cos\vartheta}{b^2}\right)-xy\left[\frac{2\sin\vartheta\sqrt{e^2-\sin^2\vartheta}}{b^2}\right]=0$$

where: $$f=\left(\frac{1}{r}+\frac{1}{r'}\right)^{-1}$$

J.B. West and H.A. Padmore, Optical Engineering, 1987

Toroid (1)

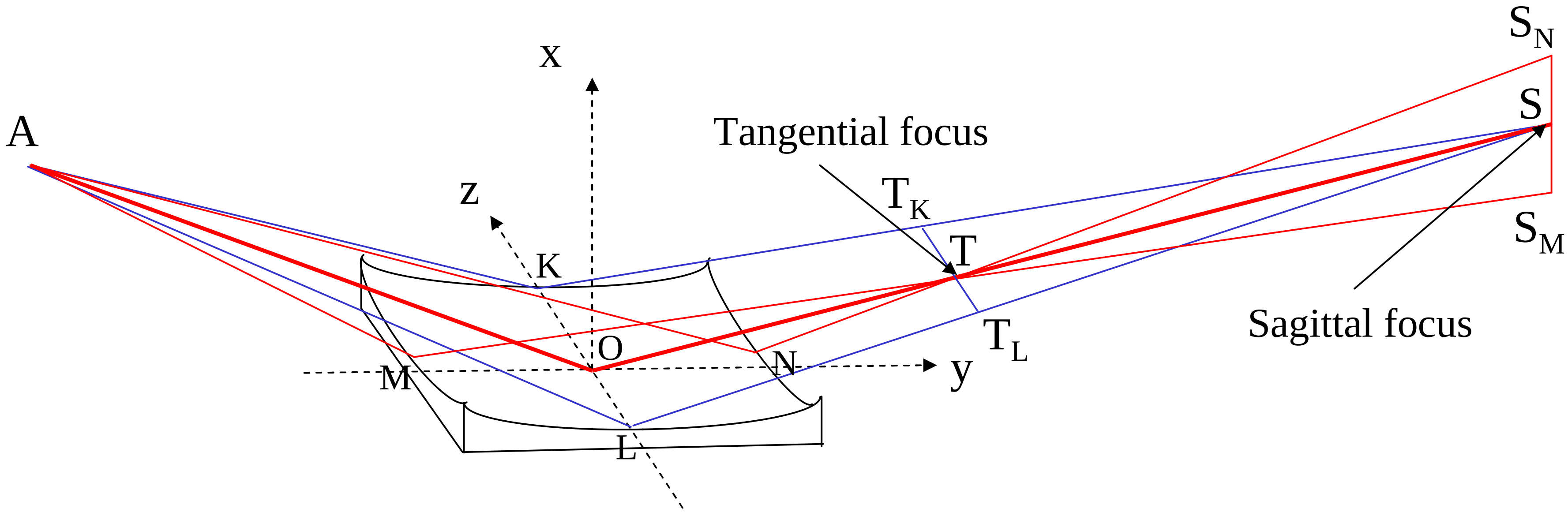




$$x^2 + y^2 + z^2 = 2Rx - 2R(R-\rho) + 2(R-\rho)\sqrt{(R-x)^2 + y^2}$$

The bicycle tyre toroid is generated rotating a circle of radius ρ in an arc of radius R.

Toroid (2)



In general, a toroid produces two non-coincident focii: one in the tangential focal plane and one in the sagittal focal plane

Tangential focus T:

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

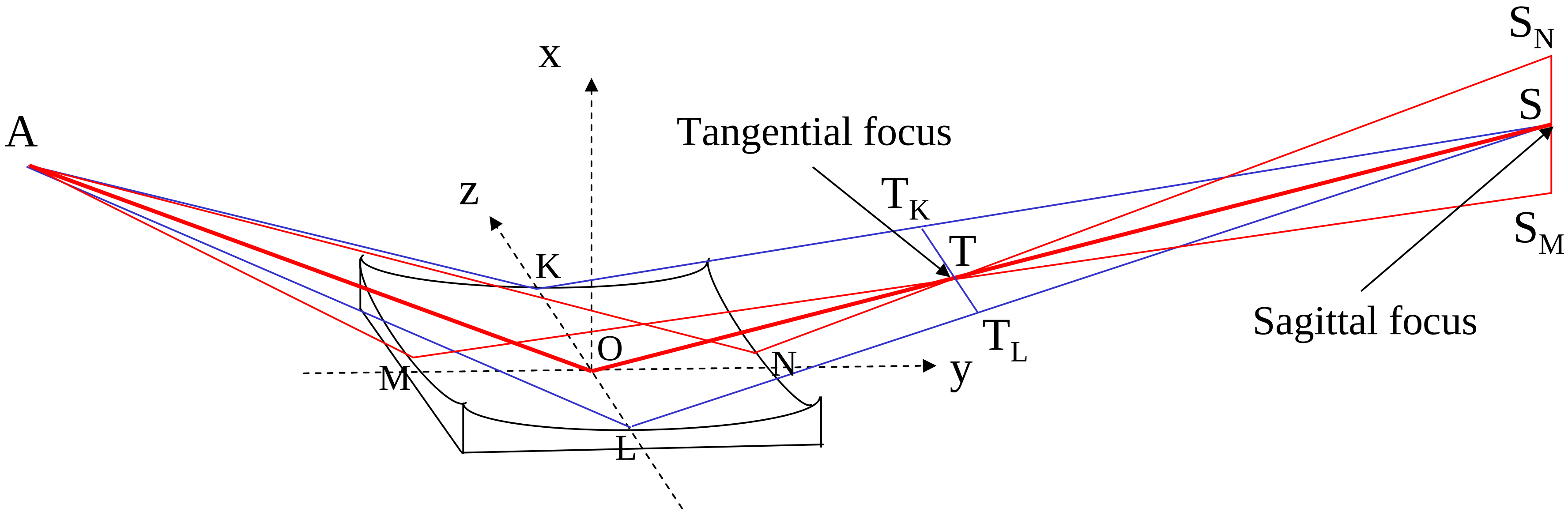
Sagittal focus S:

$$\left(\frac{1}{r}+\frac{1}{r'_s}\right)\frac{1}{2\cos\vartheta}=\frac{1}{\rho}$$

Stigmatic image:

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

Spherical mirror

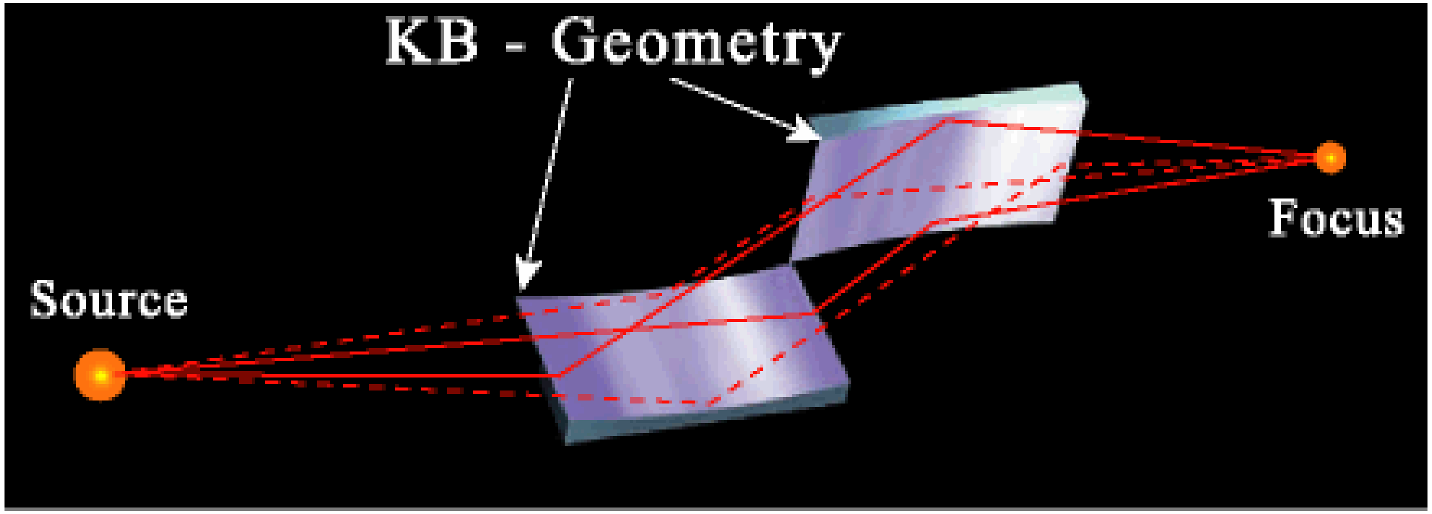


For $\rho = R$ → spherical mirror :

A stigmatic image can only be obtained at normal incidence.

For a vertical deflecting spherical mirror at grazing incidence the horizontal sagittal focus is always further away from the mirror than the vertical tangential focus. The mirror only weakly focalizes in the sagittal direction.

Kirkpatrick-Baez focusing system

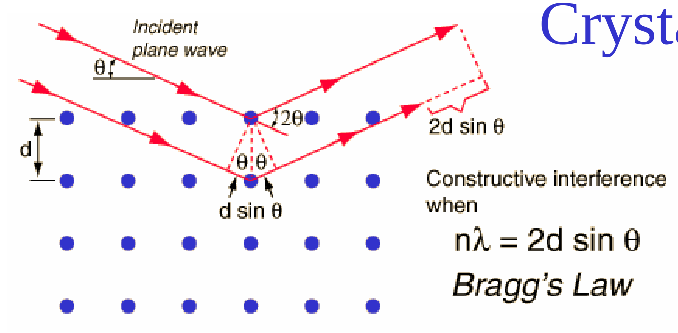


This configuration, originally suggested by Kirkpatrick and Baez in 1948, is based on two mutually perpendicular concave spherical mirrors.

Monochromators

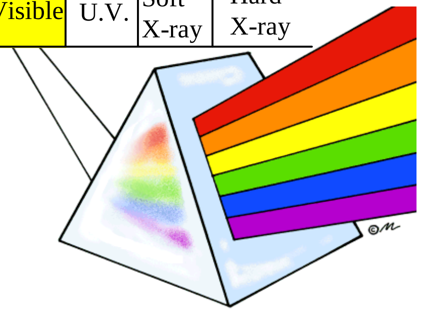
Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Crystal

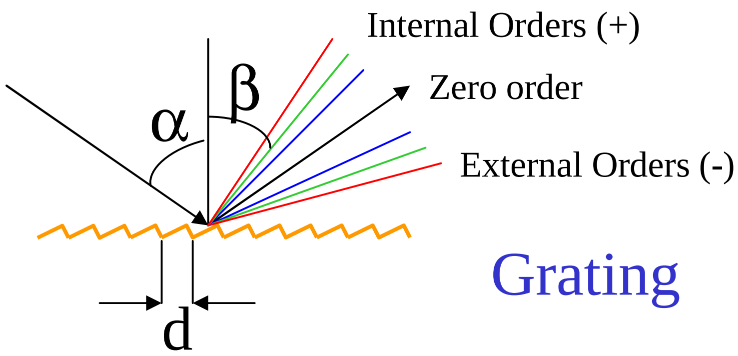


Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Prism



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

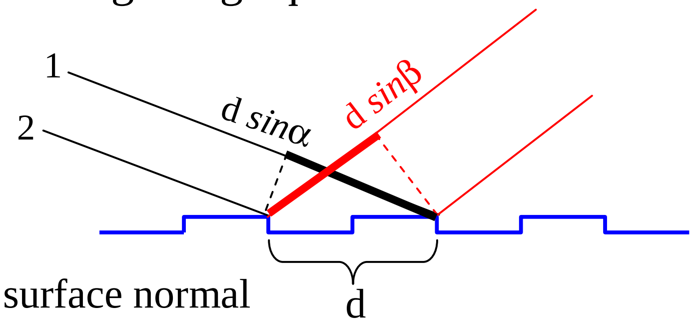


Grating

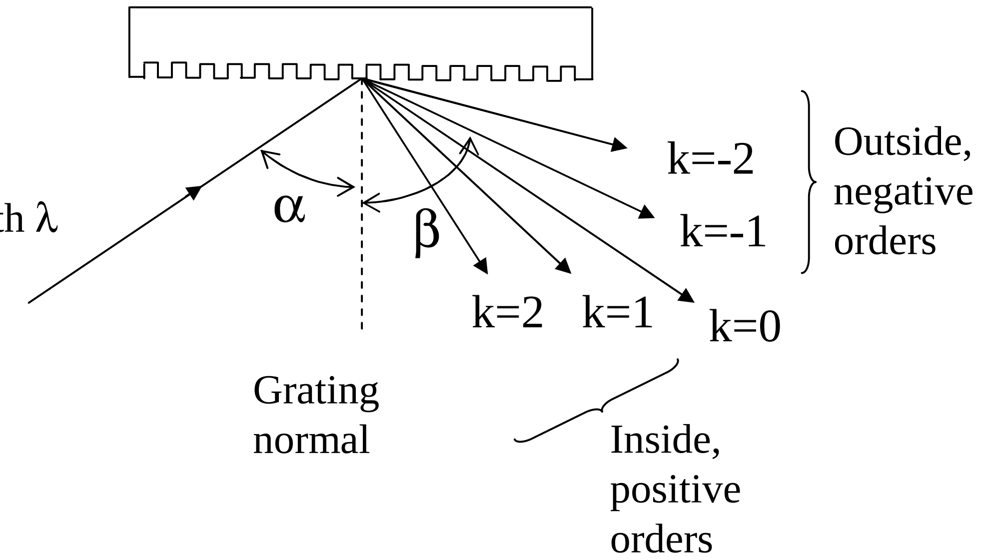
Gratings

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:

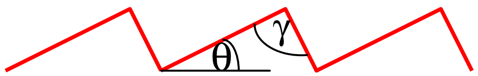
$$\boxed{\sin\alpha + \sin\beta = Nk\lambda}$$



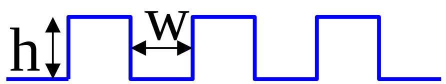
α and β are of opposite sign if on opposite sides of the surface normal
N=1/d is the groove density, k is the order of diffraction (±1,±2,...)



Gratings profiles (1)

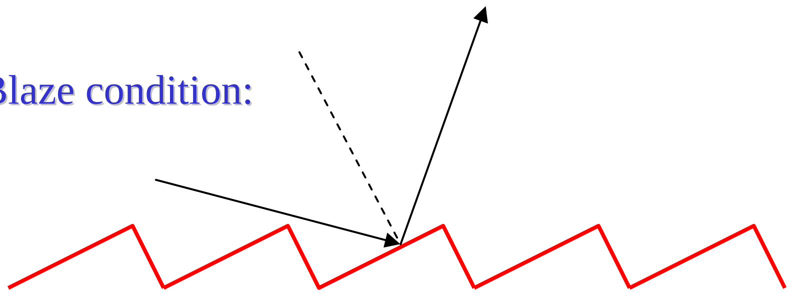


Blaze profile

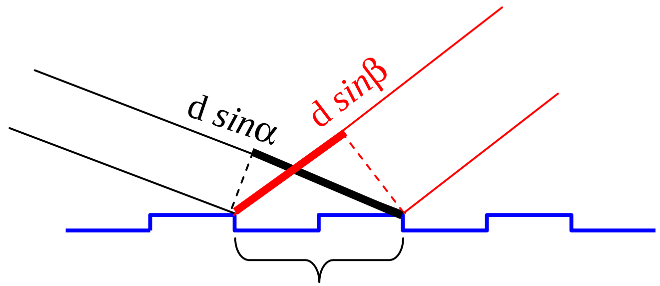


Laminar profile

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

1λ

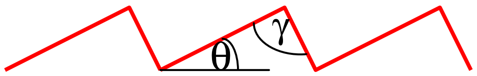
$$k\lambda = d\left(\sin\alpha + \sin\beta\right)$$

$2\frac{\lambda}{2}$

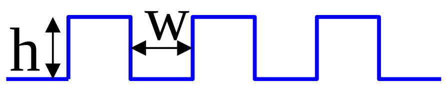
Blaze gratings: higher efficiency

Laminar gratings: higher spectral purity

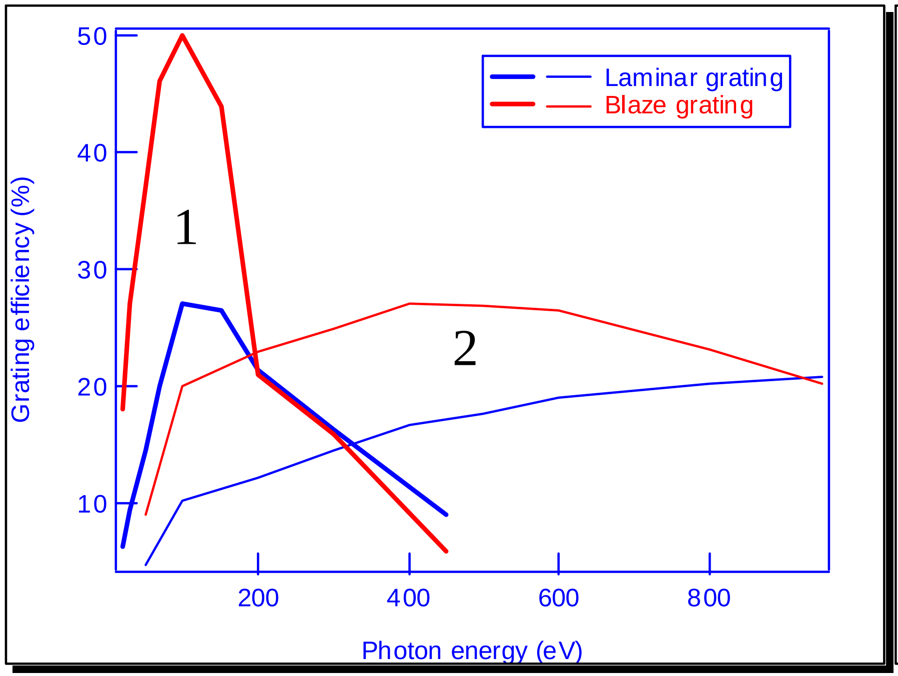
Gratings profiles (2)

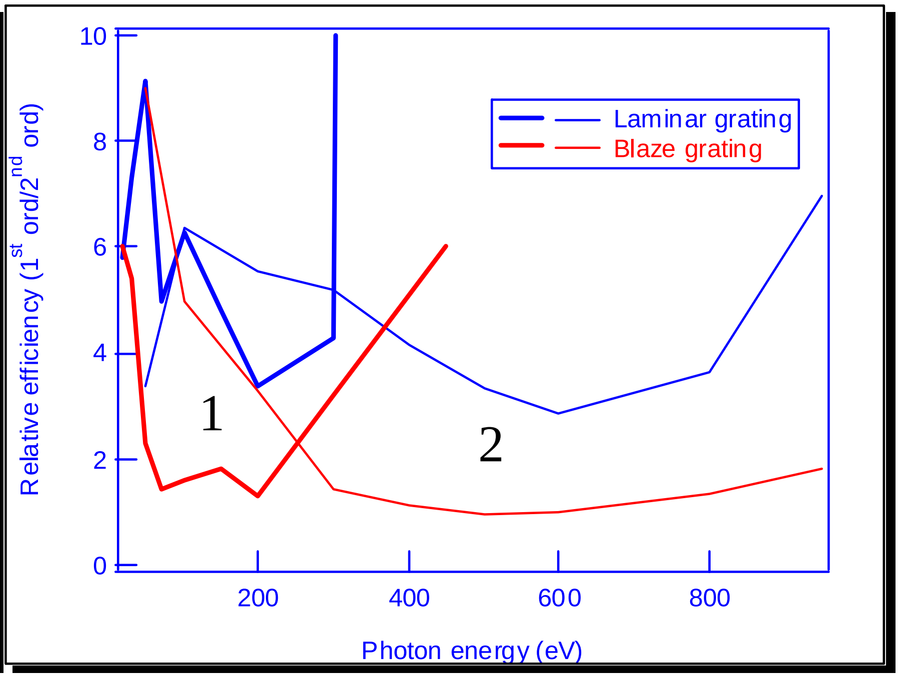


Blaze profile



Laminar profile



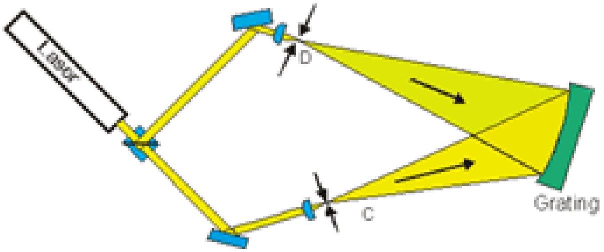


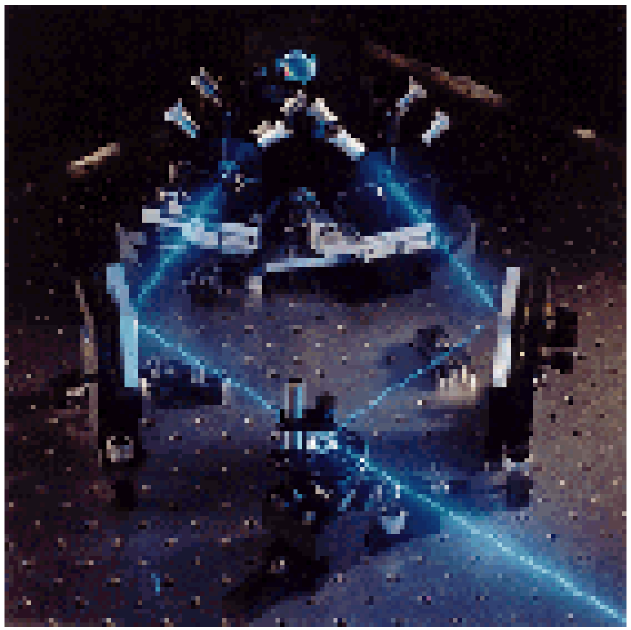
$$d(\sin\alpha + \sin\beta) = k\lambda$$

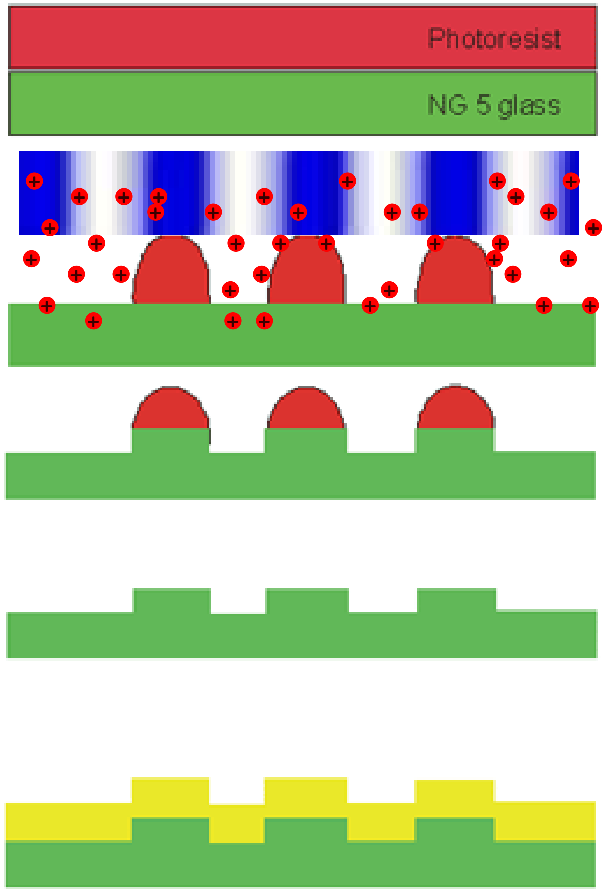
Grating 1: N=200 g/mm (d=5µm)

Grating 2: N=400 g/mm (d=2.5µm)

Holographically recorded grating







Exposure

Development

Ion-beam etching

Photoresist removal

Coating

Grating resolving power (1)

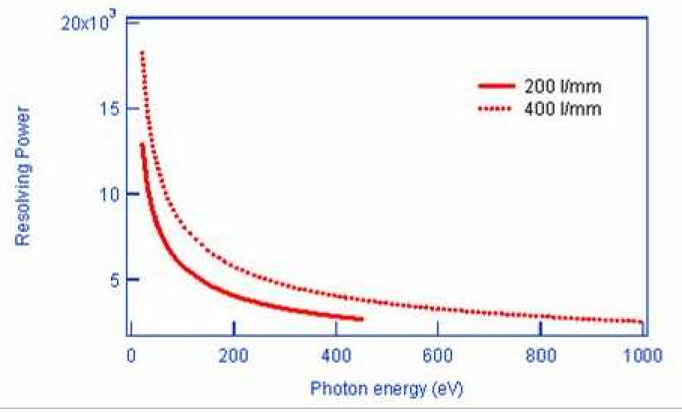
Differentiating the grating equation: $\sin\alpha + \sin\beta = Nk\lambda$
the **angular dispersion** of the grating is obtained:

(higher groove density → higher angular dispersion)

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

The **resolving power** is defined as:

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



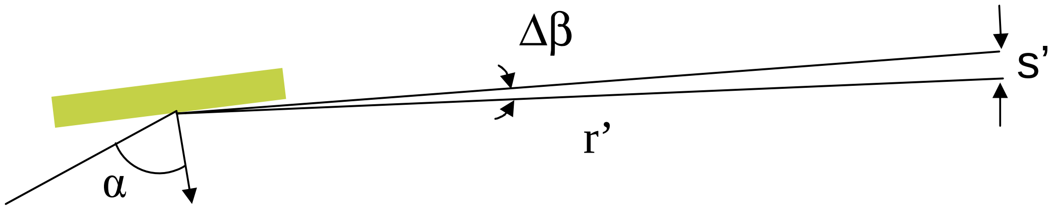
R=10000 @100eV → ΔE=100eV/10000=10meV

Grating resolving power (2)

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

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

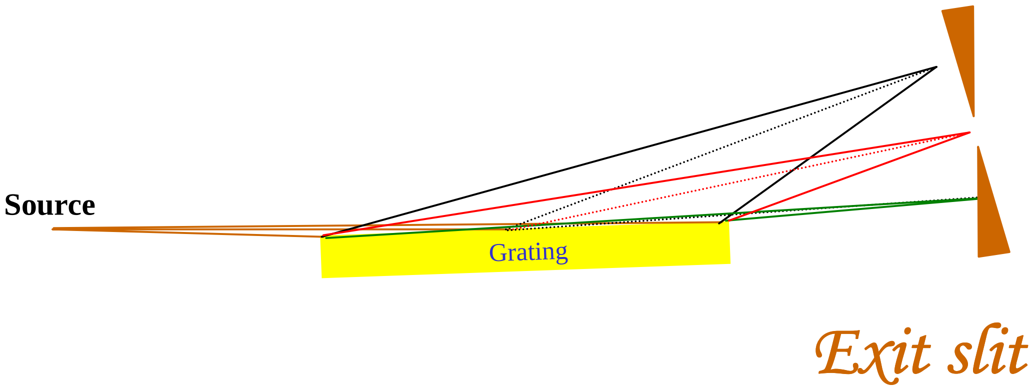
$$\boxed{\frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda} = \frac{\lambda\, N\, k\, r'}{(\cos\beta)s'}}$$

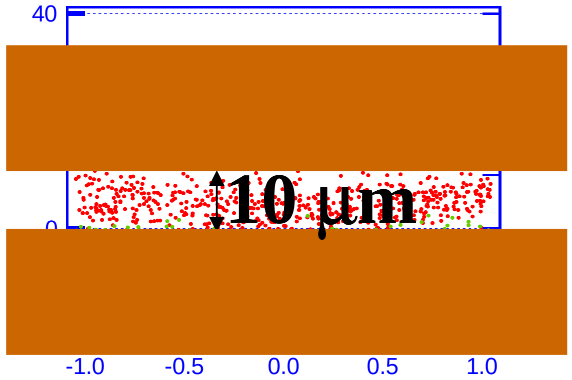


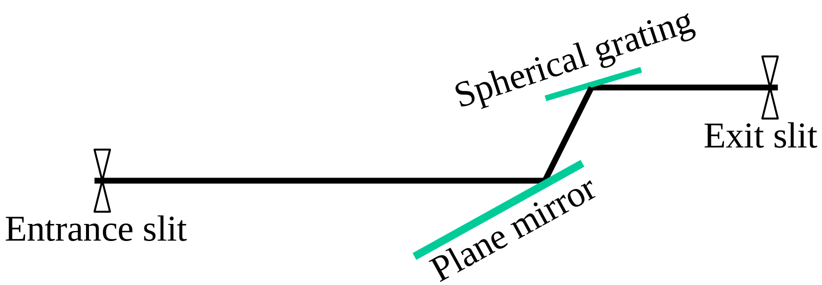
The entrance slit contribution is similar:

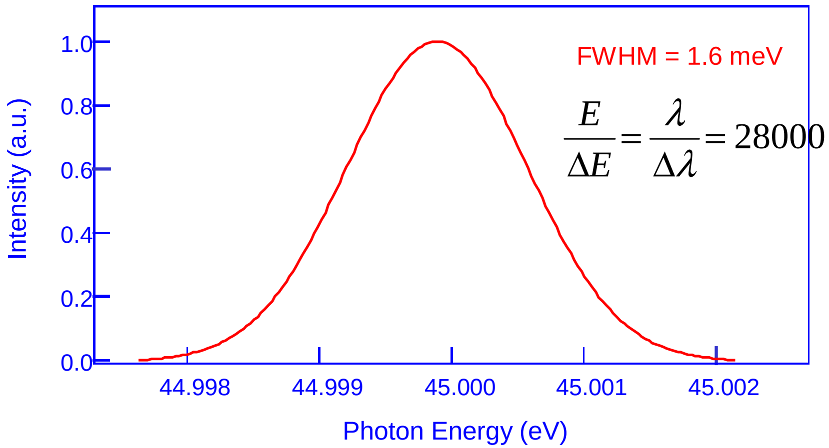
$$\boxed{\frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda} = \frac{\lambda\, N\, k\, r}{(\cos\beta)s}}$$

Grating resolving power (3)





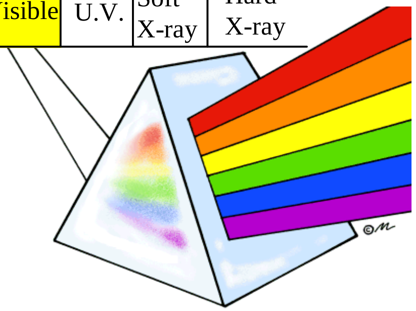




Monochromators

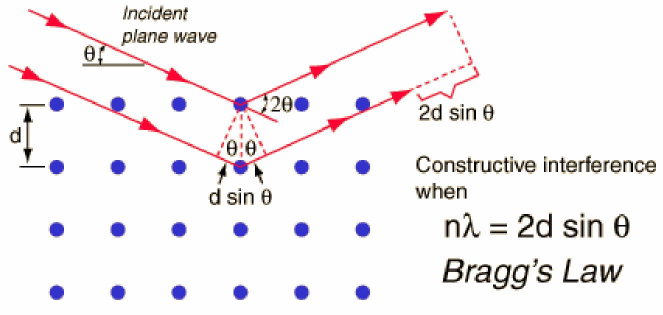
Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Prism

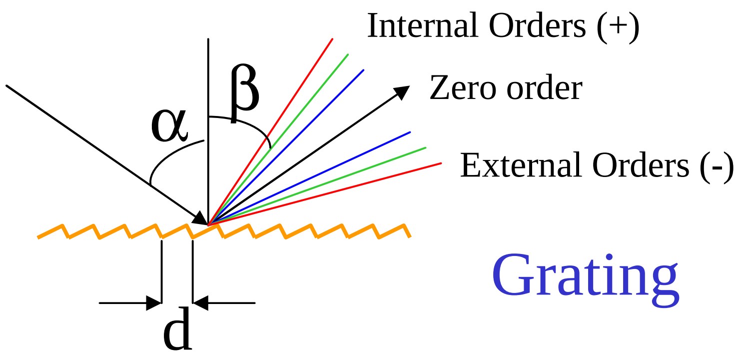


Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Crystal

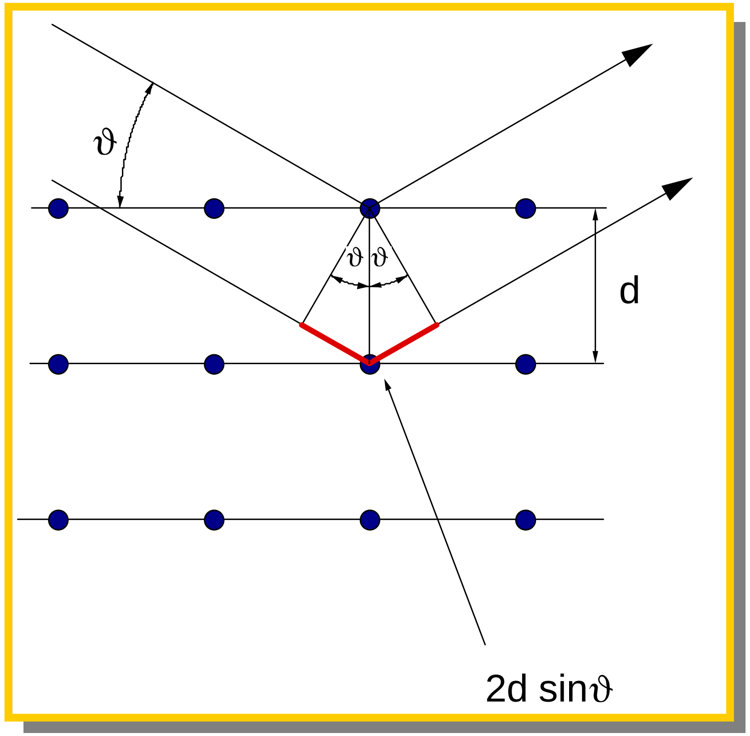


Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray



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:

$$\boxed{2d\sin\vartheta = n\lambda}$$

d is the distance between crystal planes.

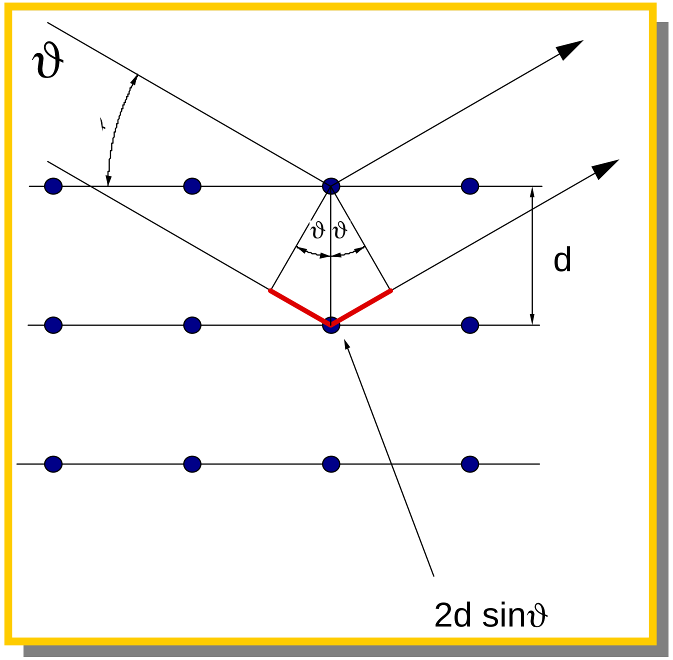
$$\sin\vartheta \le 1 \Rightarrow \lambda \le \lambda_{max} = 2d$$

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



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

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

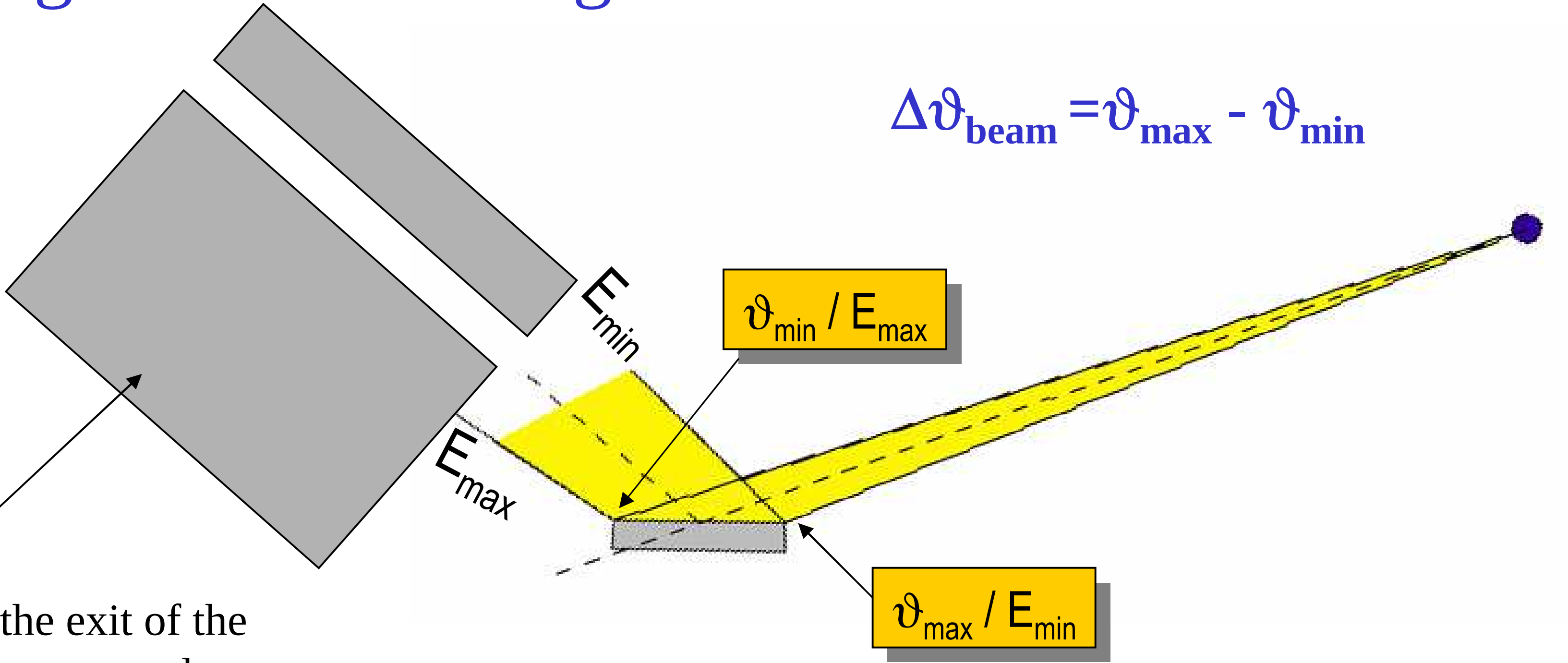
$\Delta\vartheta$ has two contributions :

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

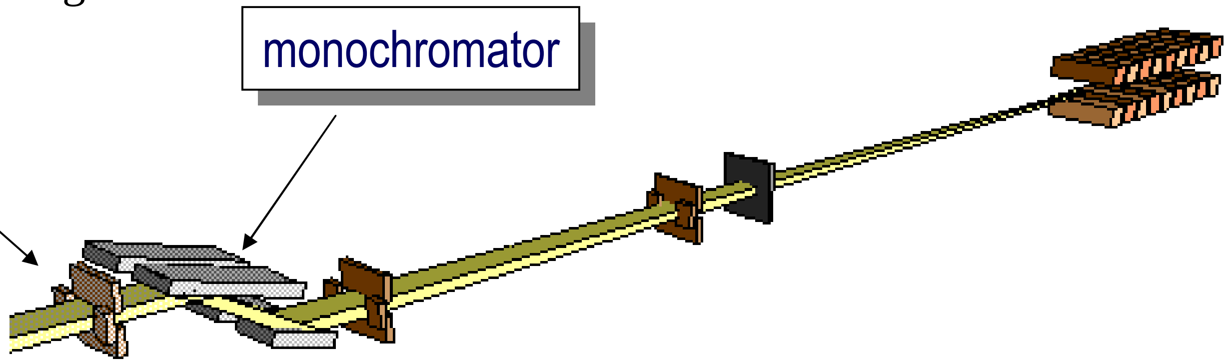
ω_{crystal} : intrinsic width of the Bragg reflection

Angular beam divergence

$$\Delta\vartheta_{beam} = \vartheta_{max} - \vartheta_{min}$$

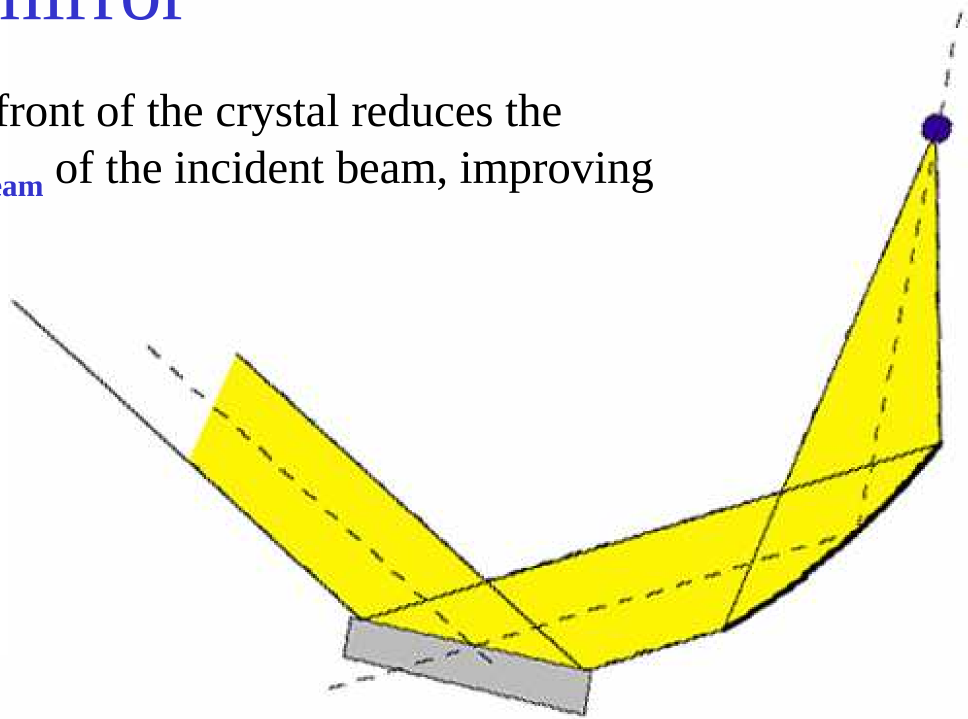


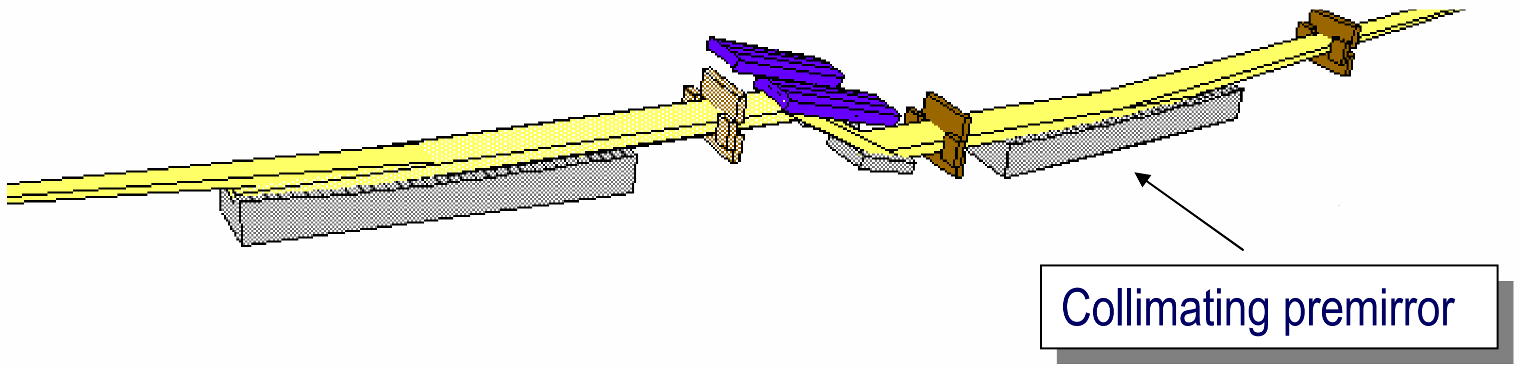
A slit at the exit of the monochromator selects a narrower energy range.



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.



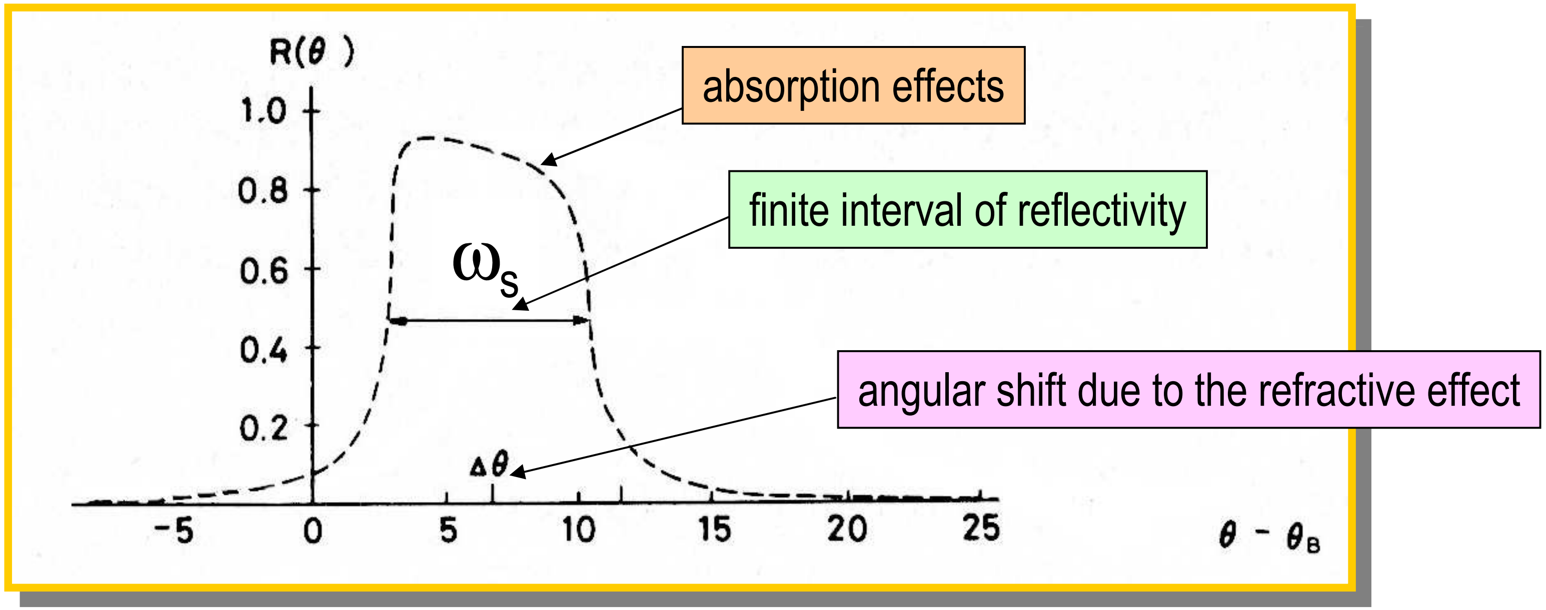


Darwin Curve

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 incident 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

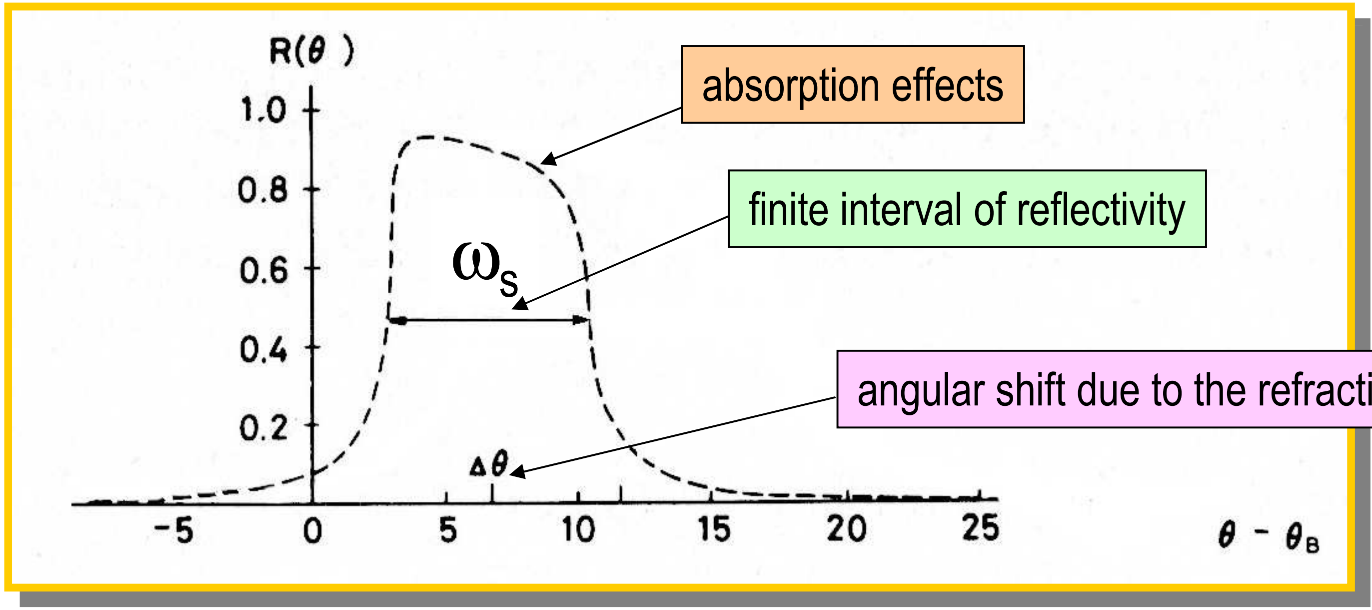


Intrinsic width of the Bragg reflection

$$\omega_S = \frac{2}{\sin(2\vartheta_B)} \frac{r_e \lambda^2}{\pi V} C \left| F_{hr} \right| e^{-M}$$

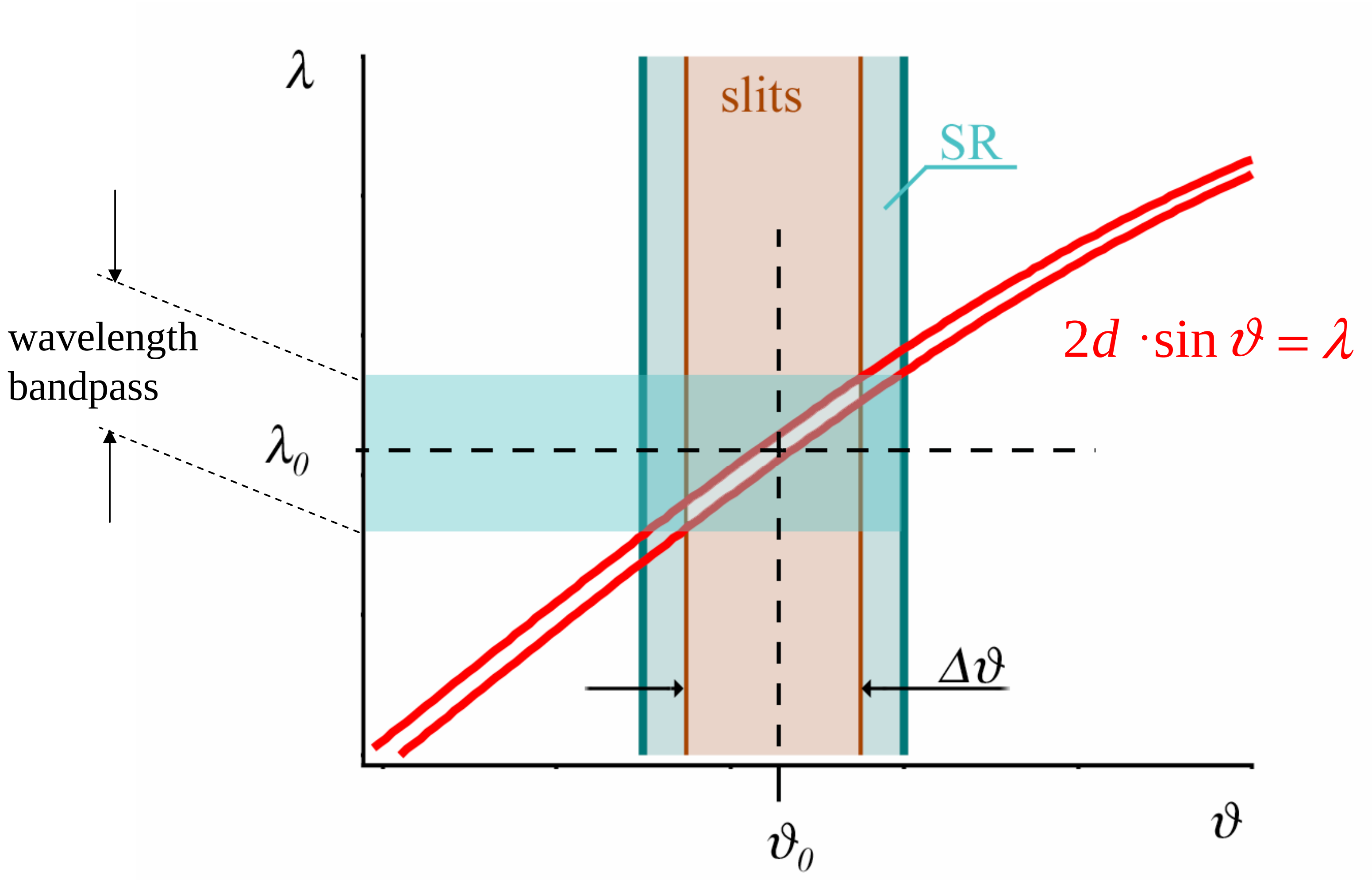
Dynamic diffraction theory

θ_B	**Bragg angle**
λ	**wavelength of radiation**
r_e	radius of the electron e^2/mc^2
V	volume of the unit cell
C	polarization factor
$\vert F_{hr}\vert$	amplitude of the **crystal structure factor F_r related to the (hkl) diffraction**
e^{-M}	temperature factor



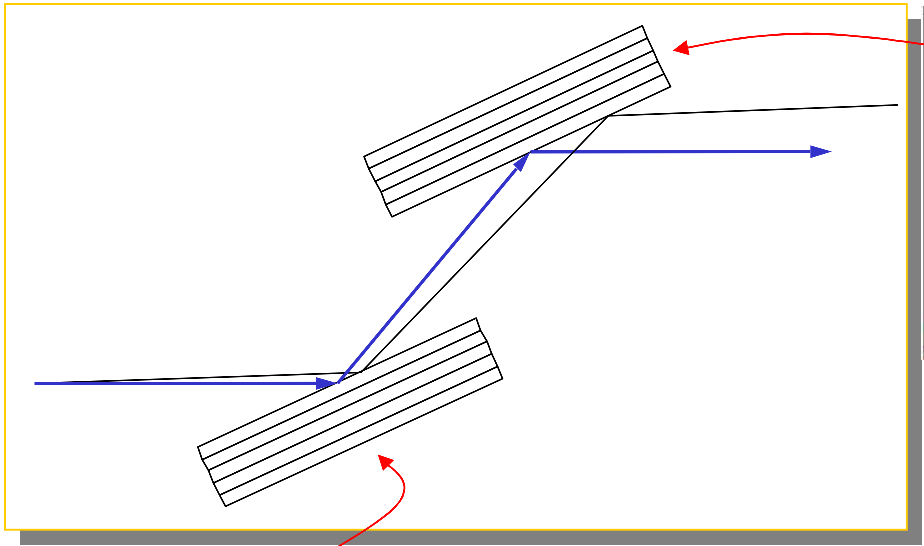
Du Mond diagram

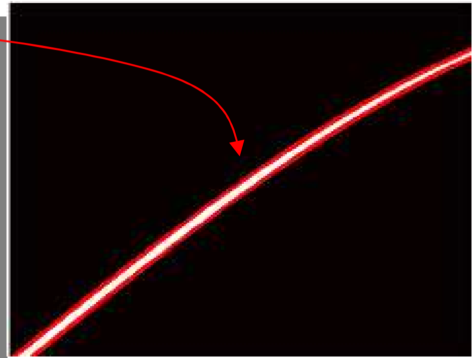
$\Delta\vartheta$ = angular acceptance of the slit

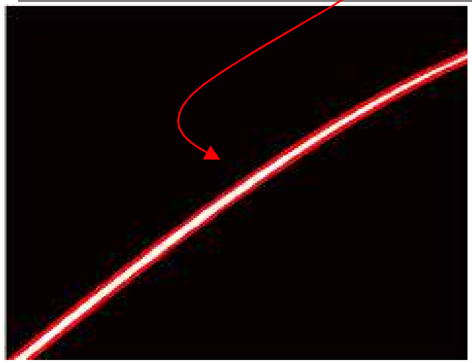


The Du Mond diagram describes the reflection of radiation by the crystal in the $\vartheta - \lambda$ space.

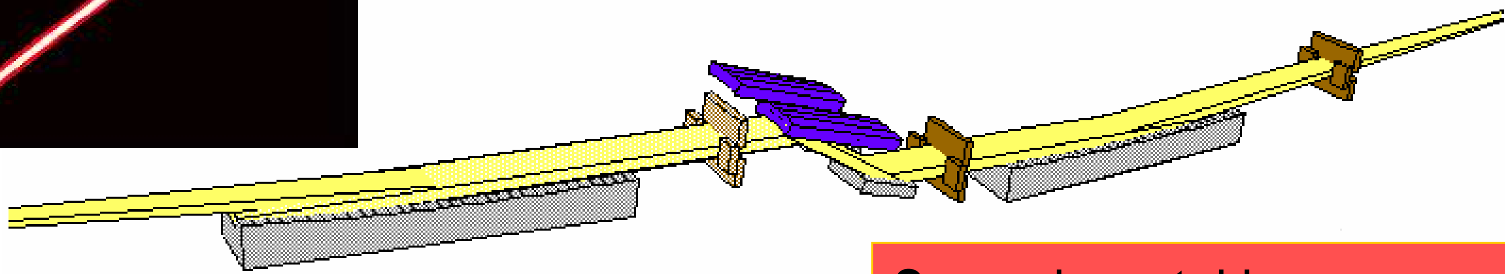
Crystal Monochromators





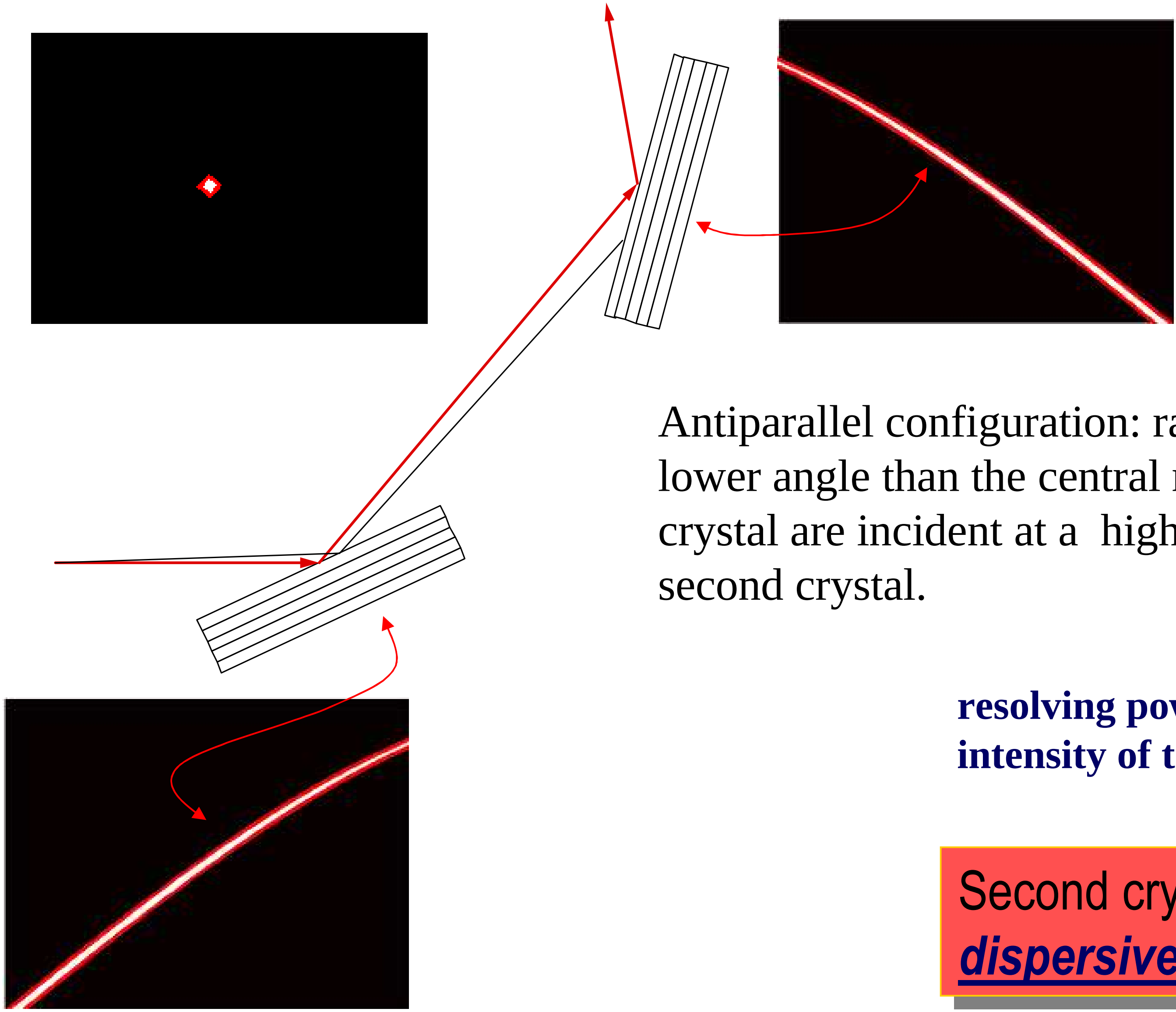


Parallel geometry:
all rays accepted by the first crystal are accepted also at the second.



Second crystal in
non dispersive configuration

Crystal Monochromators

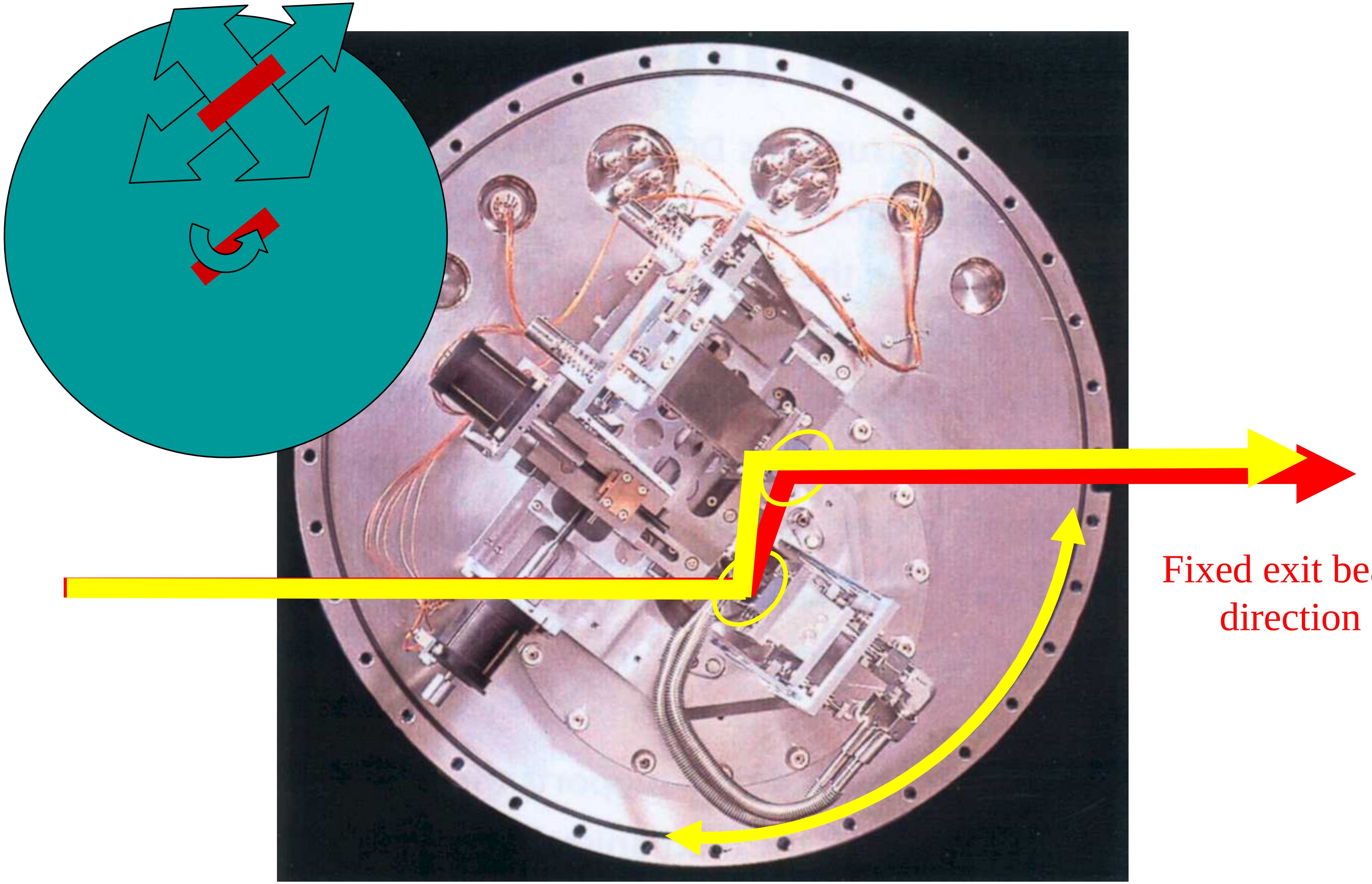


Antiparallel configuration: rays incident at a lower angle than the central ray on the first crystal are incident at a higher angle on the second crystal.

resolving power ↑
intensity of the reflection ↓

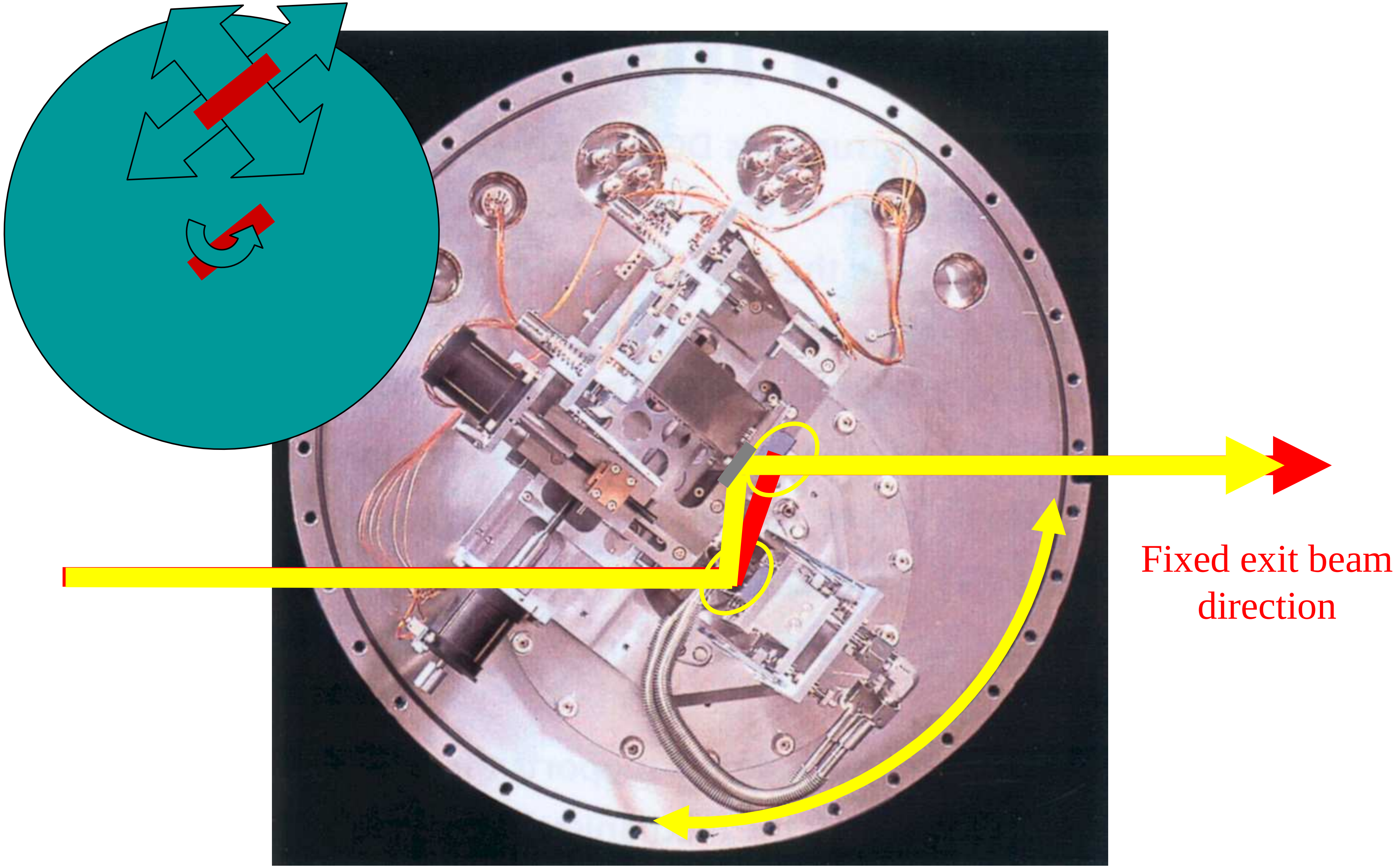
Second crystal in ***<u>dispersive</u>*** configuration

Double Crystal Monochromator

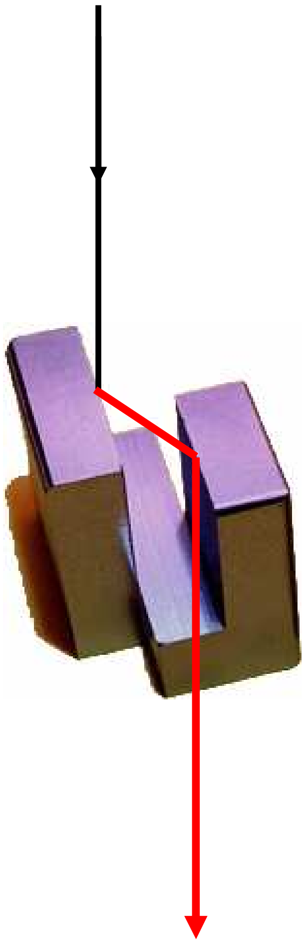


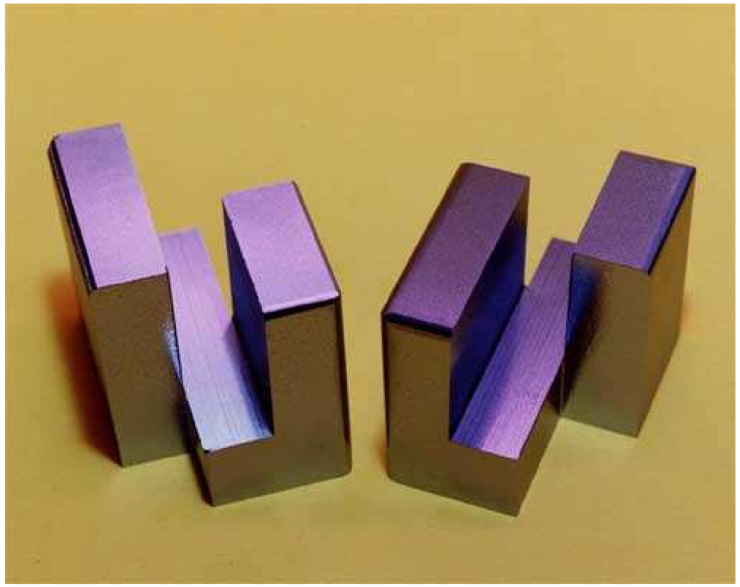
Fixed exit beam direction

Double Crystal Monochromator

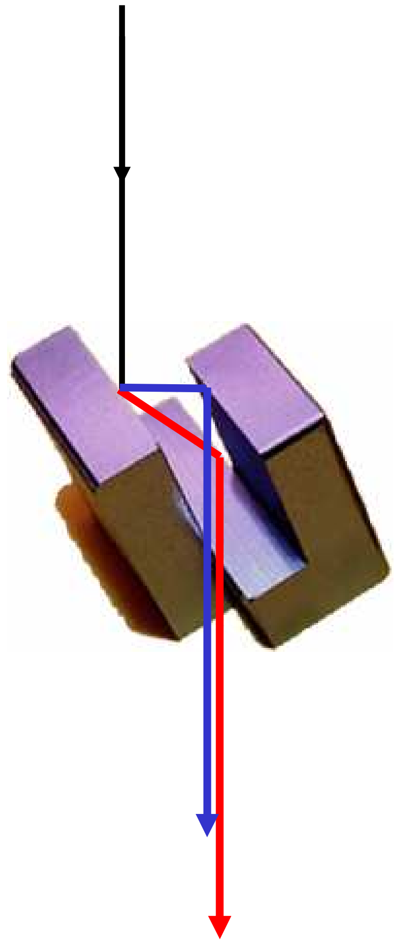


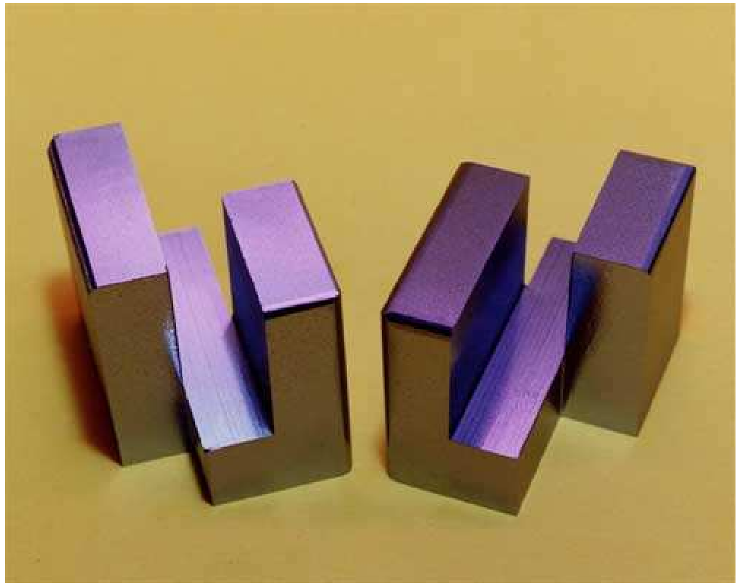
Channel-cut



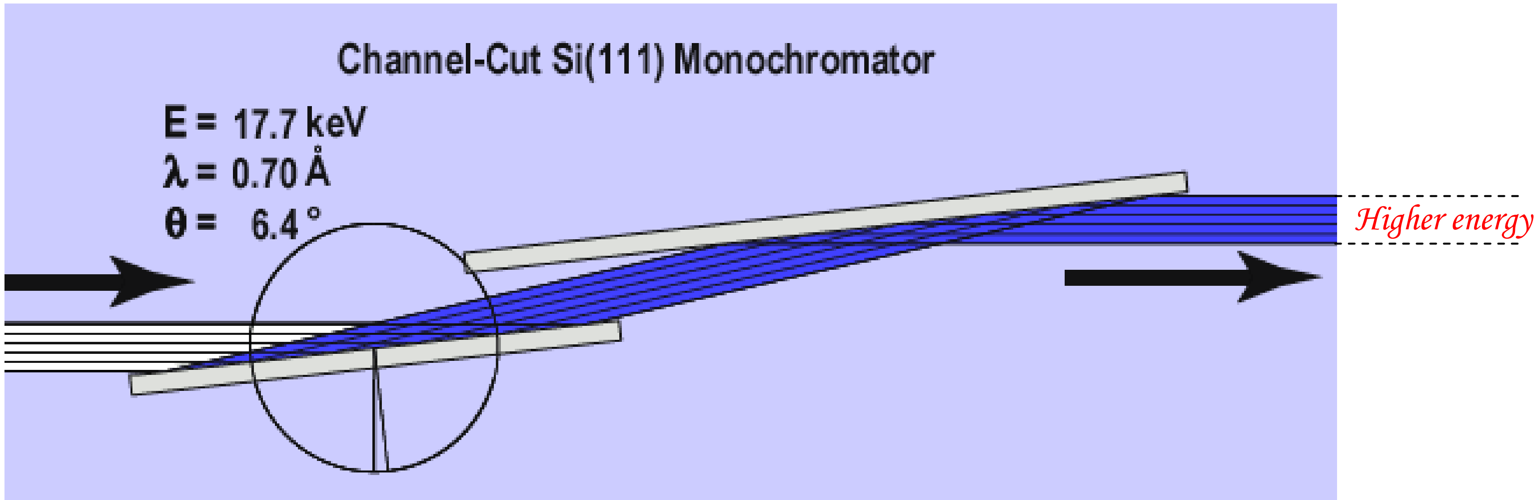


Channel-cut



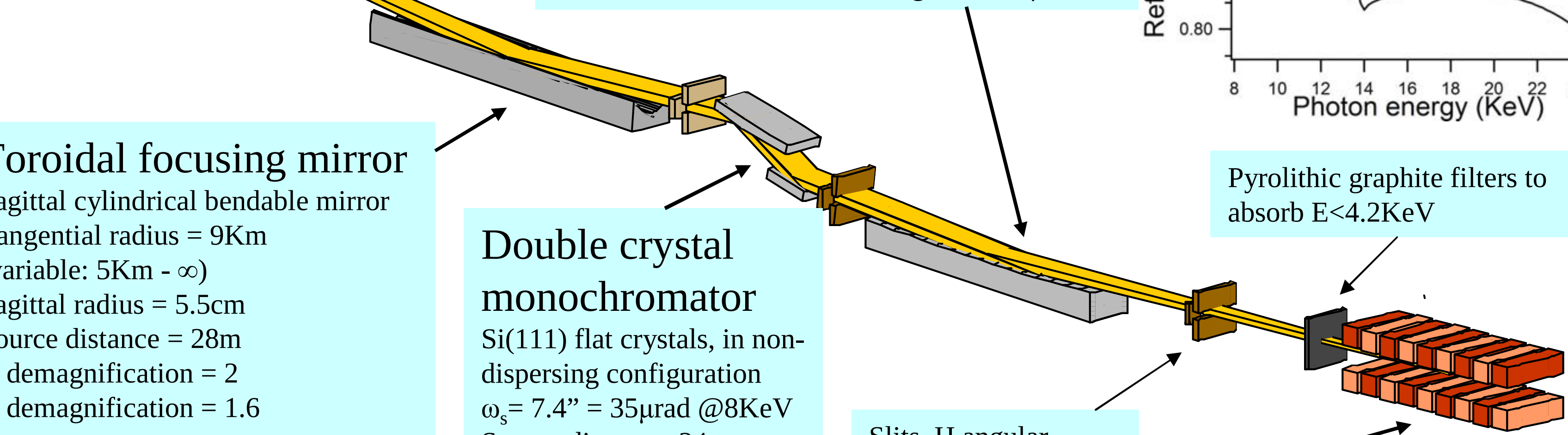


Channel-cut



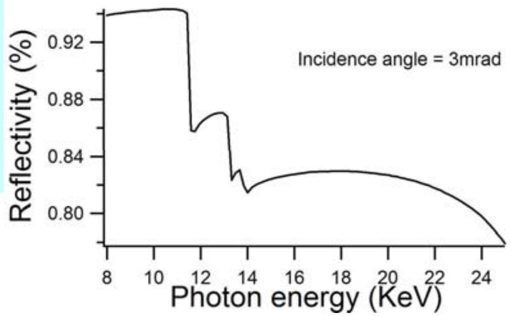
Much easy to align
Exit beam displacement

Example: the ELETTRA X-ray Diffraction beamline



Experiment
Source distance = 41.5m
Energy range: 4-21KeV
spot size: 0.4x0.2mm^2
Photon flux: 10^{12}ph/s (at λ=1Å)
Energy resolution: 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

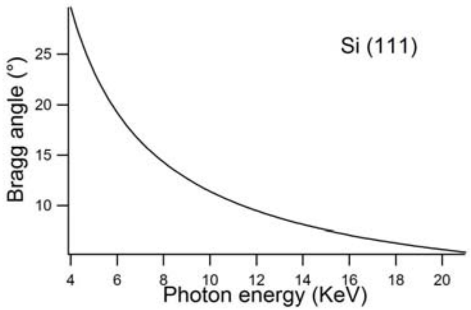


Toroidal focusing mirror
Sagittal cylindrical bendable mirror
Tangential radius = 9Km
(variable: 5Km - ∞)
Sagittal radius = 5.5cm
Source distance = 28m
H demagnification = 2
V demagnification = 1.6

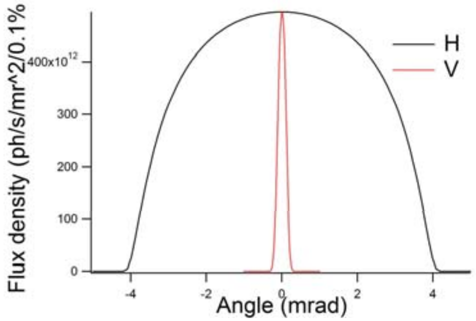
Double crystal monochromator
Si(111) flat crystals, in non-dispersing configuration
ω_s= 7.4” = 35μrad @8KeV
Source distance=24m
250W absorbed by the 1° crystal

Pyrolithic graphite filters to absorb E<4.2KeV

Slits, H angular acceptance: 1.5mrad



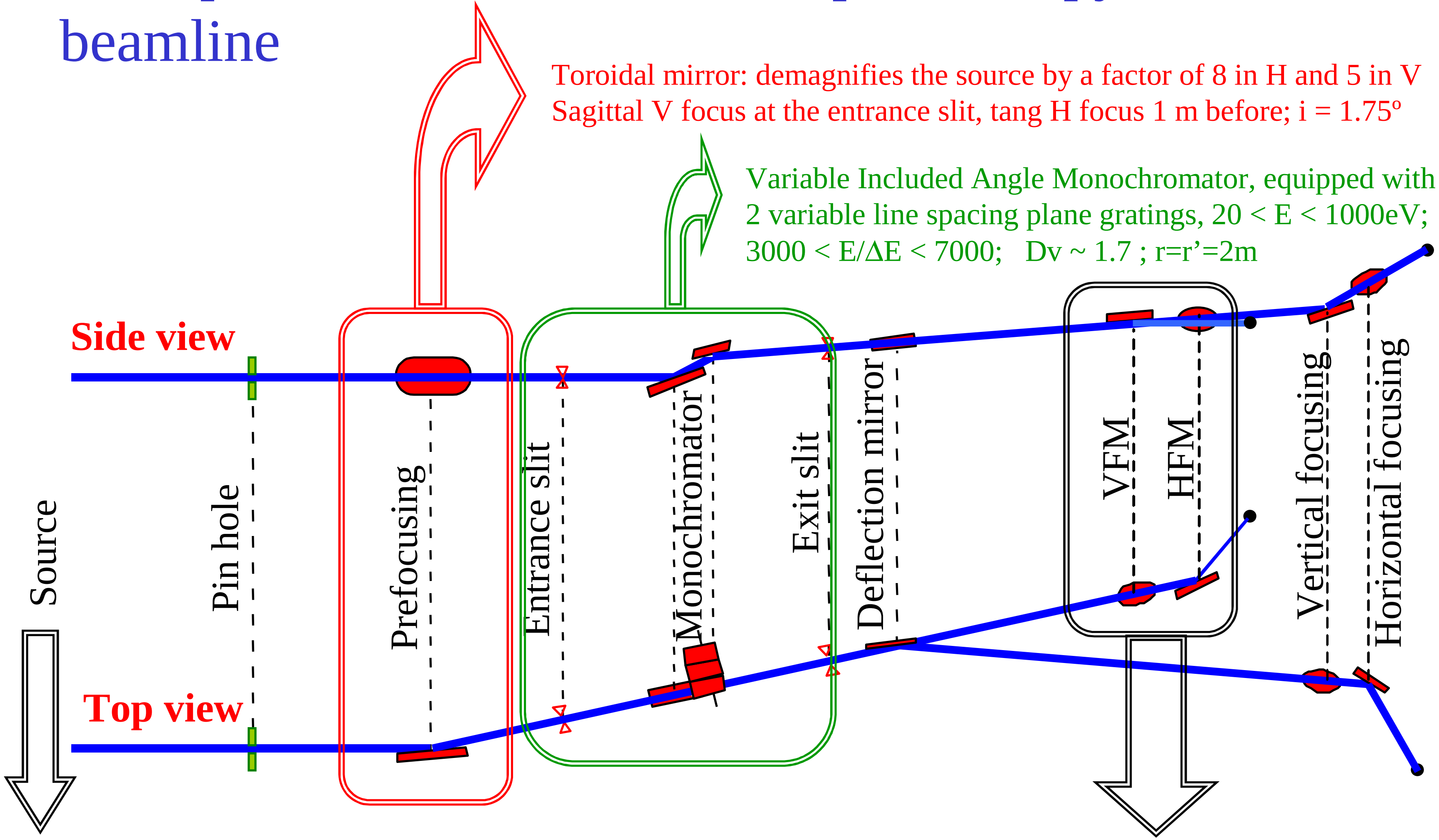
Multi-pole wiggler
57 poles, 1.5T magnetic field,
14cm period length,
5.8KeV critical energy @2.4GeV
5 kW total power @140mA



Example: the ELETTRA Nanospectroscopy beamline

Toroidal mirror: demagnifies the source by a factor of 8 in H and 5 in V
Sagittal V focus at the entrance slit, tang H focus 1 m before; i = 1.75°

Variable Included Angle Monochromator, equipped with
2 variable line spacing plane gratings, 20 < E < 1000eV;
3000 < E/ΔE < 7000;   Dv ~ 1.7 ; r=r'=2m



two APPLE-II helical undulators,
Photon energy: 20 - 1000eV
Size @400eV: 560µm×50µm;
110µrad×85µrad (FWHM)

Two bendable elliptical cylinder mirrors, in KB geometry:
demagnification factors are 10 in H and 5 in V, i = 2°
About 1x10^{12} photons/s are focused in a 7µm x 2µm spot.

Conserving brightness

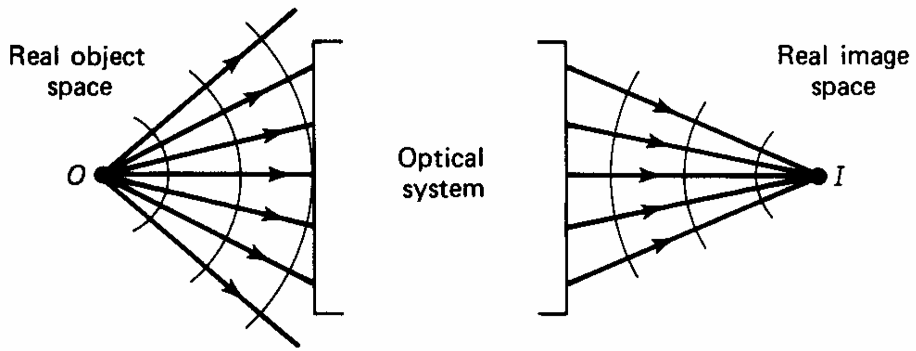
Brilliance decreases because of:

- 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

In the following we will consider OEs with theoretical surface shapes.

Perfect imaging and aberrations

An ideal optical element is able to perform perfect imaging if all the rays originating from a single object point cross at a single image point.



Deviations from perfect imaging are called aberrations.

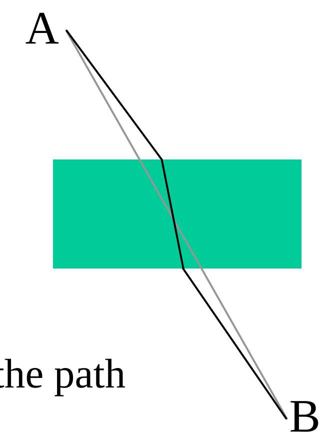
Aberrations theory

Aberration theory shows what the different aberration terms are and how they play a role in the image formation → it teaches how aberrations can be reduced

We will study the case of a concave grating.

The general theory of aberrations of diffraction gratings derives mathematical expressions for the aberration terms applying Fermat's principle.

Fermat's principle



A light-ray going from A to B chooses the path with the minimum optical pathlength:

$$\int_A^B n(\vec{r})\,dl$$

$n(\vec{r})$: index of refraction of the medium; dl: line segment along the path

$$\int_A^B n(\vec{r})\,dl = \int_A^B \frac{c}{v}\,dl = c\int_A^B dt$$

A more accurate statement:

a light-ray going from A to B chooses the path for which the optical pathlength between the two points is an extremum :

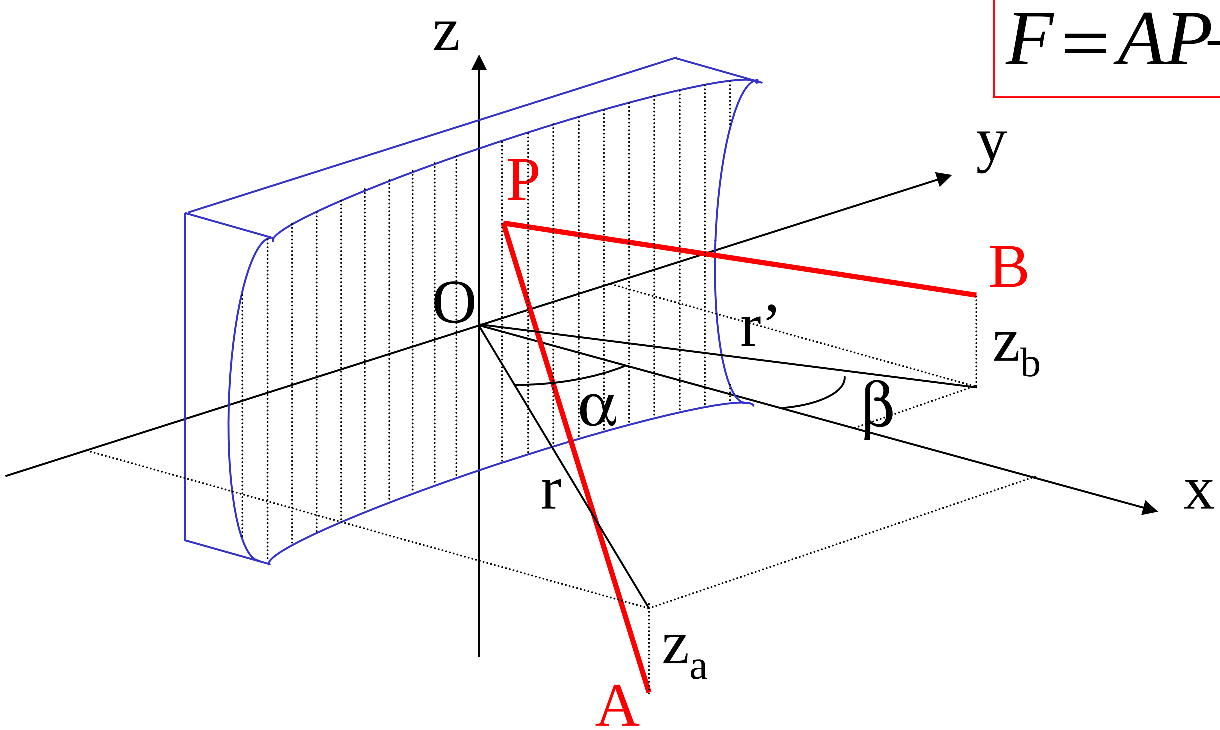
$$\delta\int_A^B n(\vec{r})\,dl = 0$$

where the delta variation of the integral means that is a variation of the path of the integral such that the endpoints A and B are fixed.

Theory of conventional diffraction gratings

For a classical grating with rectilinear grooves parallel to z with constant spacing d, the optical path length is:

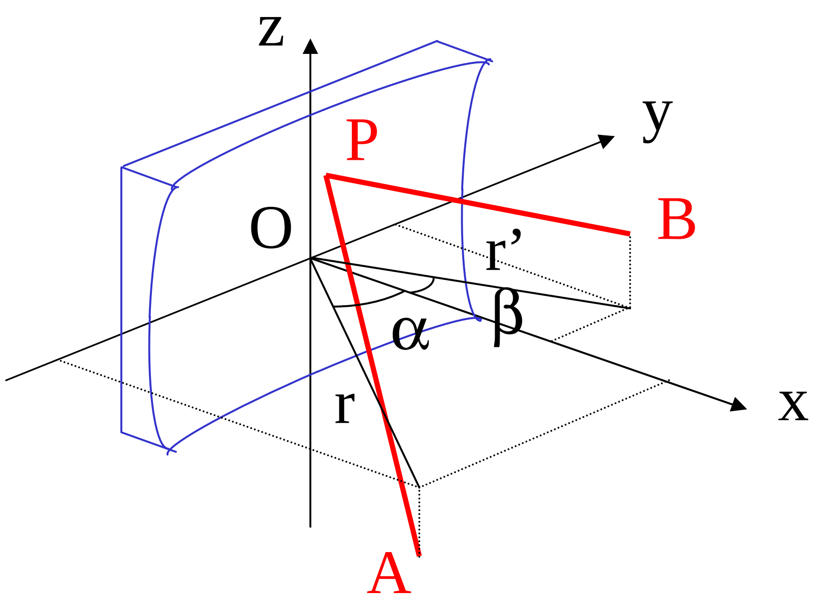
$$F = \overline{AP} + \overline{PB} + kN\lambda y$$



where λ is the wavelength of the diffracted light, k is the order of diffraction (±1,±2,...), N=1/d is the groove density

Perfect focus condition (1)

Let us consider some number of light rays starting from A and impinging on the grating at different points P. Fermat's principle states that if the point A is to be imaged at the point B, then all the optical path lengths from A via the grating surface to B will be the same.



B is the point of a perfect focus if:

$$\boxed{\frac{\partial F}{\partial y}=0 \qquad \frac{\partial F}{\partial z}=0}$$

for any pair of (y,z)

Perfect focus condition (2)

Equations:

$$\boxed{F = \overline{AP} + \overline{PB} + kN\lambda y} \quad \mathbf{+} \quad \boxed{\frac{\partial F}{\partial y} = 0 \quad \frac{\partial F}{\partial z} = 0 \quad \textit{for any pair of } (y,z)}$$

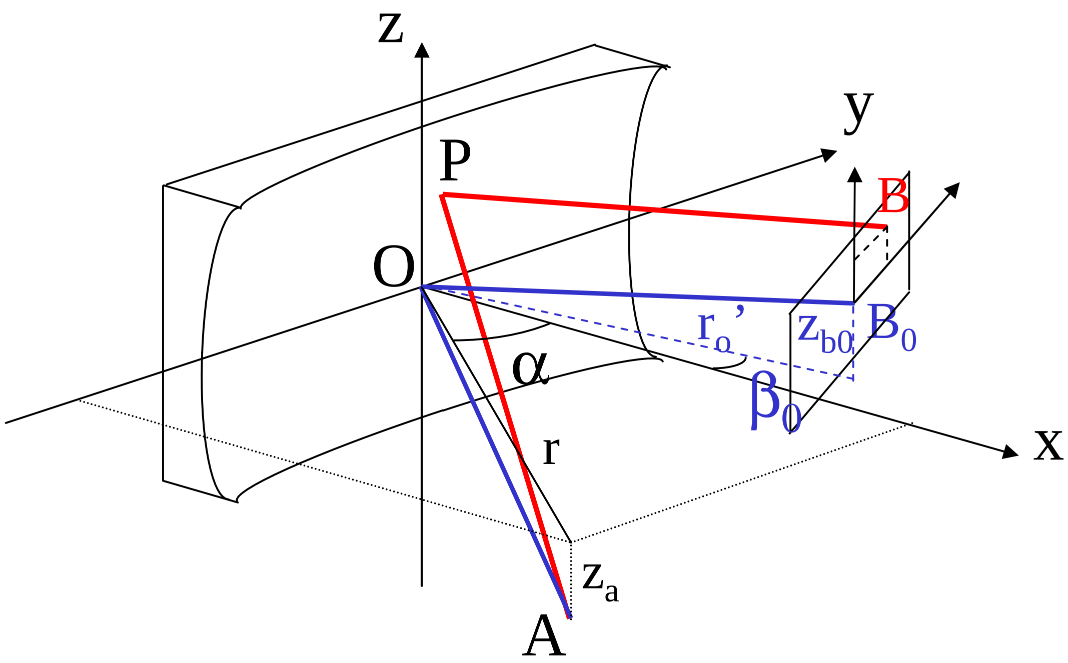
can be used to decide on the required characteristics of the diffraction grating:

•the shape of the surface
•the grooves density
•the object and image distances

Aberrated image

In general, $\dfrac{\partial F}{\partial y}$ and $\dfrac{\partial F}{\partial z}$ are functions of y and z and can not be made zero for any y,z

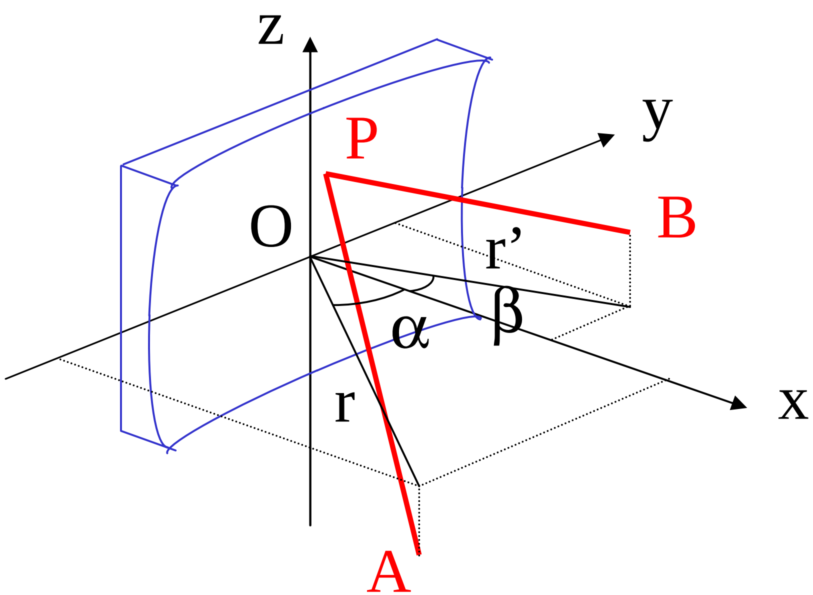
→ when the point P wanders over the grating surface, diffracted rays fall on slightly different points on the focal plane and an aberrated image is formed



- B_0: gaussian image, produced by the central ray
- B: ray diffracted by the generic point P on the grating surface
- Aberrations: displacements of B with respect to B_0

Grating surface

The grating surface can in general be described by a **series expansion**:



$$x = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} a_{ij} y^i z^j$$

$a_{00} = a_{10} = a_{01} = 0$ because of the choice of origin

j = even if the xy plane is a symmetry plane

Giving suitable values to the coefficients a_{ij}'s we obtain the expressions for the various geometrical surfaces.

a_{ij} coefficients (1)

Toroid

$$a_{02} = \frac{1}{2\rho}; \quad a_{20} = \frac{1}{2R}; \quad a_{22} = \frac{1}{4R^2\rho}; \quad a_{40} = \frac{1}{8R^3};$$

$$a_{04} = \frac{1}{8\rho^3}; \quad a_{12} = 0; \quad a_{30} = 0$$

Sphere, cylinder and plane are special cases of toroid:

- $R=\rho$ → **sphere**
- $R=\infty$ → **cylinder**
- $R=\rho=\infty$ → **plane**

Paraboloid

$$a_{02} = \frac{1}{4f\cos\vartheta}; \quad a_{20} = \frac{\cos\vartheta}{4f}; \quad a_{22} = \frac{3\sin^2\vartheta}{32f^3\cos\vartheta};$$

$$a_{12} = -\frac{\tan\vartheta}{8f^2}; \quad a_{30} = -\frac{\sin\vartheta\cos\vartheta}{8f^2}$$

$$a_{40} = \frac{5\sin^2\vartheta\cos\vartheta}{64f^3}; \quad a_{04} = \frac{\sin^2\vartheta}{64f^3\cos^3\vartheta}$$

a_{ij} coefficients (2)

Ellipsoid

$$a_{02} = \frac{1}{4f\cos\vartheta}; \quad a_{20} = \frac{\cos\vartheta}{4f}; \quad a_{04} = \frac{b^2}{64f^3\cos^3\vartheta}\left[\frac{\sin^2\vartheta}{b^2} + \frac{1}{a^2}\right];$$

$$a_{12} = \frac{\tan\vartheta}{8f^2\cos\vartheta}\sqrt{e^2 - \sin^2\vartheta}; \quad a_{30} = \frac{\sin\vartheta}{8f^2}\sqrt{e^2 - \sin^2\vartheta} \;;$$

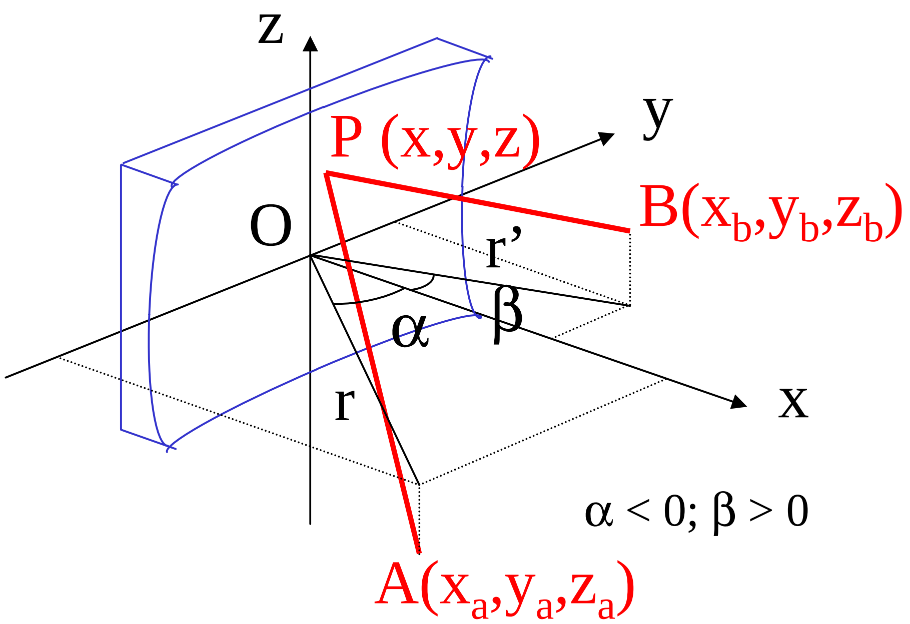
$$a_{40} = \frac{b^2}{64f^3\cos^3\vartheta}\left[\frac{5\sin^2\vartheta\ \cos^2\vartheta}{b^2} - \frac{5\sin^2\vartheta}{a^2} + \frac{1}{a^2}\right];$$

$$a_{22} = \frac{\sin^2\vartheta}{16f^3\cos^3\vartheta}\left[\frac{3}{2}\cos^2\vartheta - \frac{b^2}{a^2}\left(1 - \frac{\cos^2\vartheta}{2}\right)\right]$$

$$where \quad f = \left[\frac{1}{r} + \frac{1}{r'}\right]^{-1}$$

http://xdb.lbl.gov/Section4/Sec_4-3Extended.pdf

Optical path function (1)



$$F = \overline{AP} + \overline{PB} + kN\lambda y$$

$$\overline{AP} = \sqrt{(x_a - x)^2 + (y_a - y)^2 + (z_a - z)^2}$$

$$\overline{PB} = \sqrt{(x_b - x)^2 + (y_b - y)^2 + (z_b - z)^2}$$

$$x_a = r\cos\alpha \qquad y_a = r\sin\alpha$$

$$x_b = r'\cos\beta \qquad y_b = r'\sin\beta$$

Optical path function (2)

$$\boxed{F = \sum_{ijk} F_{ijk} y^i z^j}$$

power series in the aperture coordinates y and z

$$= F_{000} + yF_{100} + zF_{011} + \frac{1}{2} y^2 F_{200} + \frac{1}{2} z^2 F_{020} + \frac{1}{2} y^3 F_{300}$$

$$+ \frac{1}{2} yz^2 F_{120} + \frac{1}{8} y^4 F_{400} + \frac{1}{4} y^2 z^2 F_{220} + \frac{1}{8} z^4 F_{040}$$

$$+ yzF_{111} + \frac{1}{2} yF_{102} + \frac{1}{4} y^2 F_{202} + \frac{1}{2} y^2 zF_{211} + \ldots$$

$$F_{ijk} = z_a^k C_{ijk}(\alpha, r) + z_b^k C_{ijk}(\beta, r') + Nk\lambda f_{ijk}$$

$$f_{ijk} = \begin{cases} 1 & \text{when ijk} = 100 \\ 0 & \text{otherwise} \end{cases}$$

Perfect focus condition (3)

$$\frac{\partial F}{\partial y}=0 \quad \frac{\partial F}{\partial z}=0 \quad \text{for any pair of } (y,z)$$

$$\Downarrow$$

$$\boxed{F_{ijk}=0 \quad \text{for all } ijk \neq (000)}$$

Each term $F_{ijk}\, y^i z^j$ in the series (except F_{000} and F_{100}) represents a particular type of aberration

F_{ijk} coefficients (1)

for r,r' >> z_a,z_b

$$F_{000} = r + r'$$

$$F_{100} = Nk\lambda - (\sin\alpha + \sin\beta)$$

$$F_{200} = \left(\frac{\cos^2\alpha}{r} + \frac{\cos^2\beta}{r'}\right) - 2a_{20}(\cos\alpha + \cos\beta)$$

$$F_{020} = \frac{1}{r} + \frac{1}{r'} - 2a_{02}(\cos\alpha + \cos\beta)$$

$$F_{300} = \left[\frac{T(r,\alpha)}{r}\right]\sin\alpha + \left[\frac{T(r',\beta)}{r'}\right]\sin\beta - 2a_{30}(\cos\alpha + \cos\beta)$$

$$F_{120} = \left[\frac{S(r,\alpha)}{r}\right]\sin\alpha + \left[\frac{S(r',\beta)}{r'}\right]\sin\beta - 2a_{12}(\cos\alpha + \cos\beta)$$

where $T(r,\alpha) = \dfrac{\cos^2\alpha}{r} - 2a_{20}\cos\alpha$ and $S(r,\alpha) = \dfrac{1}{r} - 2a_{02}\cos\alpha$

and analogous expressions for $T(r',\beta)$ and $S(r',\beta)$

F_{ijk} coefficients (2)

$$F_{400} = \left[\frac{4T(r,\alpha)}{r^2}\right]\sin^2\alpha - \left[\frac{T^2(r,\alpha)}{r}\right] + \left[\frac{4T(r',\beta)}{r'^2}\right]\sin^2\beta - \left[\frac{T^2(r',\beta)}{r'}\right]$$
$$-8a_{30}\left[\frac{\sin\alpha\cos\alpha}{r} + \frac{\sin\beta\cos\beta}{r'}\right] - 8a_{40}\left(\cos\alpha + \cos\beta\right) + 4a_{20}^2\left[\frac{1}{r} + \frac{1}{r'}\right]$$

$$F_{220} = \left[\frac{2S(r,\alpha)}{r^2}\right]\sin^2\alpha + \left[\frac{2S(r',\beta)}{r'^2}\right]\sin^2\beta - \left[\frac{T(r,\alpha)S(r,\alpha)}{r}\right] - \left[\frac{T(r',\beta)S(r',\beta)}{r'}\right]$$
$$+4a_{20}a_{02}\left[\frac{1}{r} + \frac{1}{r'}\right] - 4a_{22}\left(\cos\alpha + \cos\beta\right) - 4a_{12}\left[\frac{\sin\alpha\cos\alpha}{r} + \frac{\sin\beta\cos\beta}{r'}\right]$$

$$F_{040} = 4a_{02}^2\left[\frac{1}{r} + \frac{1}{r'}\right] - 8a_{04}\left(\cos\alpha + \cos\beta\right) - \left[\frac{S^2(r,\alpha)}{r}\right] - \left[\frac{S^2(r',\beta)}{r'}\right]$$

F_{ijk} coefficients (3)

$$F_{011} = -\frac{z_a}{r} - \frac{z_b}{r'}$$

$$F_{111} = -\frac{z_a \sin\alpha}{r^2} - \frac{z_b \sin\beta}{r'^2}$$

$$F_{102} = \frac{z_a{}^2 \sin\alpha}{r^2} + \frac{z_b{}^2 \sin\beta}{r'^2}$$

$$F_{202} = \left(\frac{z_a}{r}\right)^2 \left[\frac{2\sin^2\alpha}{r} - T(r,\alpha)\right] + \left(\frac{z_b}{r'}\right)^2 \left[\frac{2\sin^2\beta}{r'} - T(r',\beta)\right]$$

$$F_{211} = \frac{z_a}{r^2}\left[T(r,\alpha) - \frac{2\sin^2\alpha}{r}\right] + \frac{z_b}{r'^2}\left[T(r',\beta) - \frac{2\sin^2\beta}{r'}\right]$$

Gaussian image point (1)

If we apply Fermat's principle to the central ray: $\left(\frac{\partial F}{\partial y}\right)_{y=0,z=0}=0 \quad \left(\frac{\partial F}{\partial z}\right)_{y=0,z=0}=0$

$F_{100}=0 \Rightarrow \sin\alpha+\sin\beta_0 = Nk\lambda$ **grating equation**

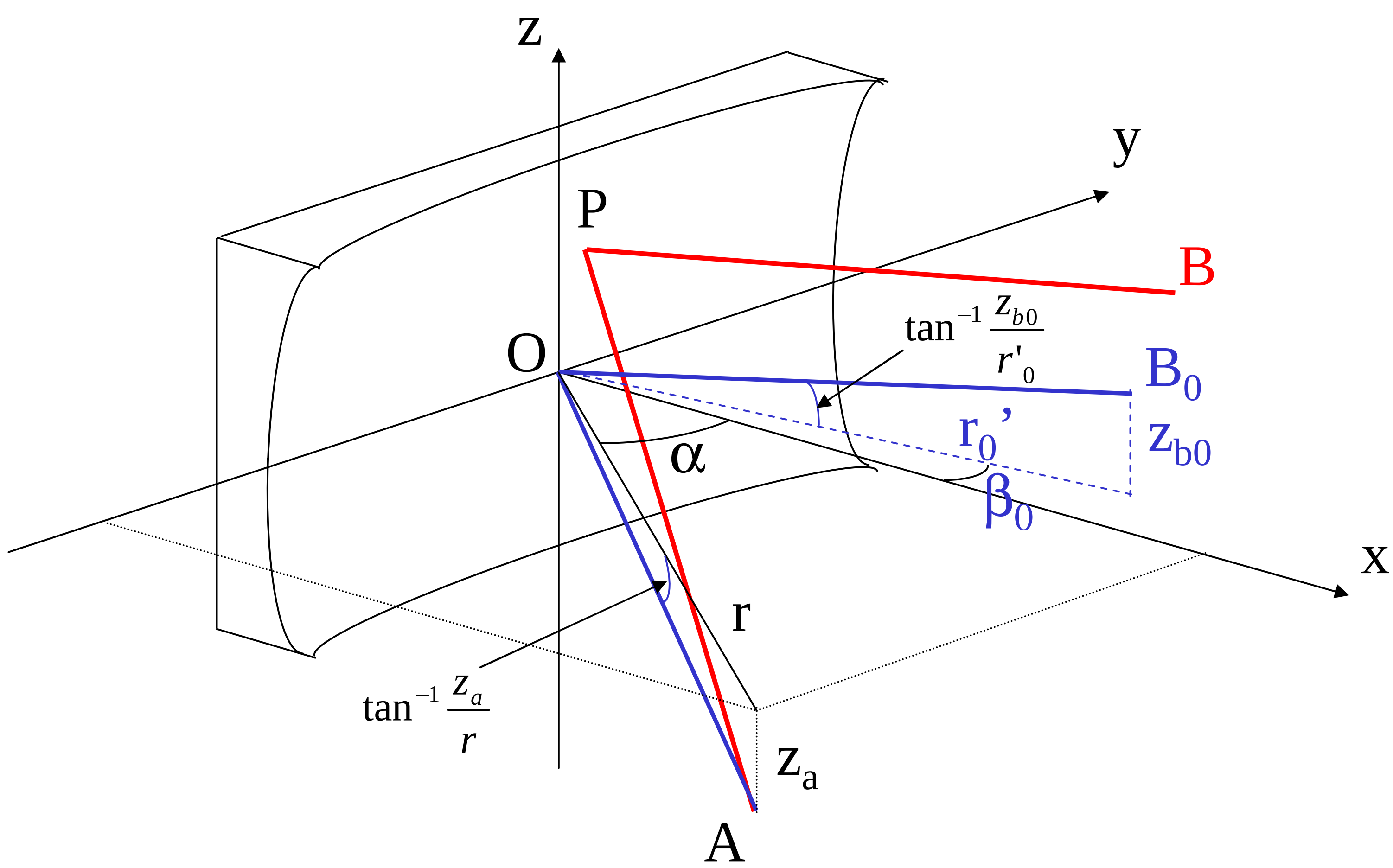
$F_{011}=0 \Rightarrow \frac{z_a}{r}=-\frac{z_{b0}}{r'_0}$ law of magnification in the sagittal direction

The tangential focal distance r'_0 is obtained by setting:

$F_{200}=0 \Rightarrow \left(\frac{\cos^2\alpha}{r}+\frac{\cos^2\beta_0}{r'_0}\right)-2a_{20}(\cos\alpha+\cos\beta_0)=0$ **tangential focusing**

The three above equations determine the Gaussian image point $B_0(r'_0,\beta_0,z_{b0})$

Gaussian image point (2)



Sagittal focusing

While the second order aberration term F_{200} governs the tangential focusing, the second order term F_{020} governs the sagittal focusing:

$$F_{020} = 0 \quad \Rightarrow \quad \frac{1}{r} + \frac{1}{r'} - 2a_{02}(\cos\alpha + \cos\beta) = 0$$

sagittal focusing

Example: toroidal mirror

Substituting $a_{02} = \dfrac{1}{2\rho}$; $a_{20} = \dfrac{1}{2R}$ in $F_{200} = 0$; $F_{020} = 0$

and imposing $\alpha = -\beta = \theta$

$$\Rightarrow \quad \left(\frac{1}{r} + \frac{1}{r_t'}\right)\frac{\cos\vartheta}{2} = \frac{1}{R} \qquad \left(\frac{1}{r} + \frac{1}{r_s'}\right)\frac{1}{2\cos\vartheta} = \frac{1}{\rho}$$

Aberrations terms

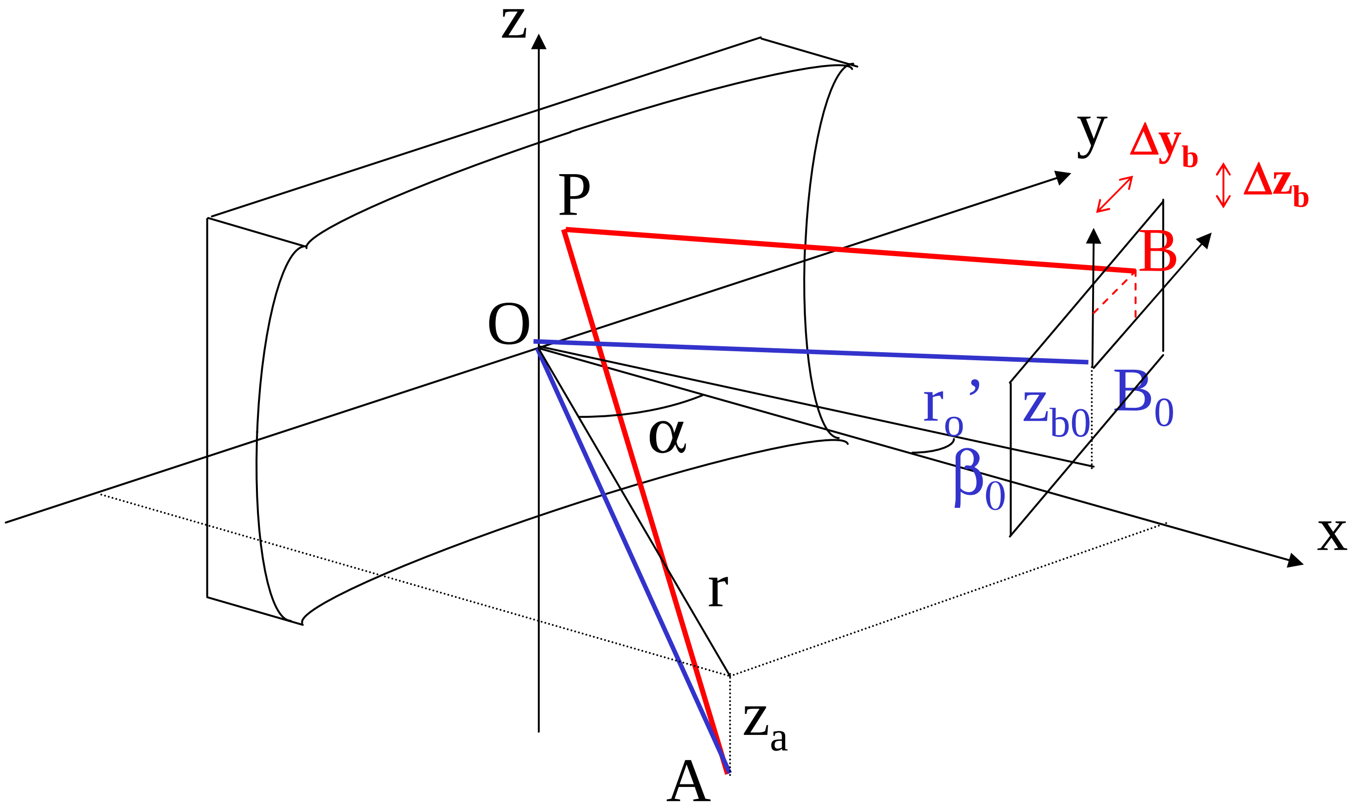
Most important imaging errors:

F_{200}	defocus
F_{020}	astigmatism
F_{300}	primary coma (aperture defect)
F_{120}	astigmatic coma
F_{400} F_{220} F_{040}	spherical aberration

There is an ambiguity in the naming of the aberrations in the grazing incidence case!

Ray aberrations (1)

The generic ray starting from A will arrive at the focal plane at a point B displaced from the Gaussian image point B_0 by the ray aberrations Δy_b and Δz_b:



$$\Delta y_b = \frac{r_0'}{\cos \beta_0} \frac{\partial F}{\partial y}$$

$$\Delta z_b = r_0' \frac{\partial F}{\partial z}$$

Ray aberrations (2)

Substituting the expansion of F , the ray aberrations for each aberration type can be calculated separately:

$$\boxed{\Delta y_b^{\;ijk} = \frac{r_0'}{\cos\beta_0} F_{ijk}\; i\; y^{i-1}\; z^{j}}$$

$$\boxed{\Delta z_b^{\;ijk} = r_0'\, F_{ijk}\;\; y^{i}\; j\; z^{j-1}}$$

each coefficient F_{ijk} represents a particular form of aberration and is related to the strength of that aberration

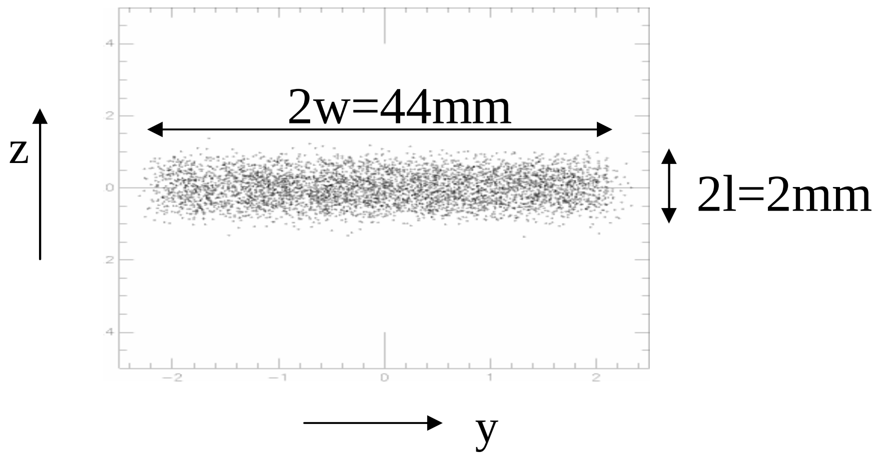
Provided the aberrations are not too large, they are additive: they may either reinforce or cancel.

$$\boxed{\Delta y_b = \sum_{ijk} \Delta y_b^{\;ijk}} \qquad \boxed{\Delta z_b = \sum_{ijk} \Delta z_b^{\;ijk}}$$

Aberrated image size

The most important contributions are from the rays which are more distant from the pole of the grating

Example of footprint on the grating:



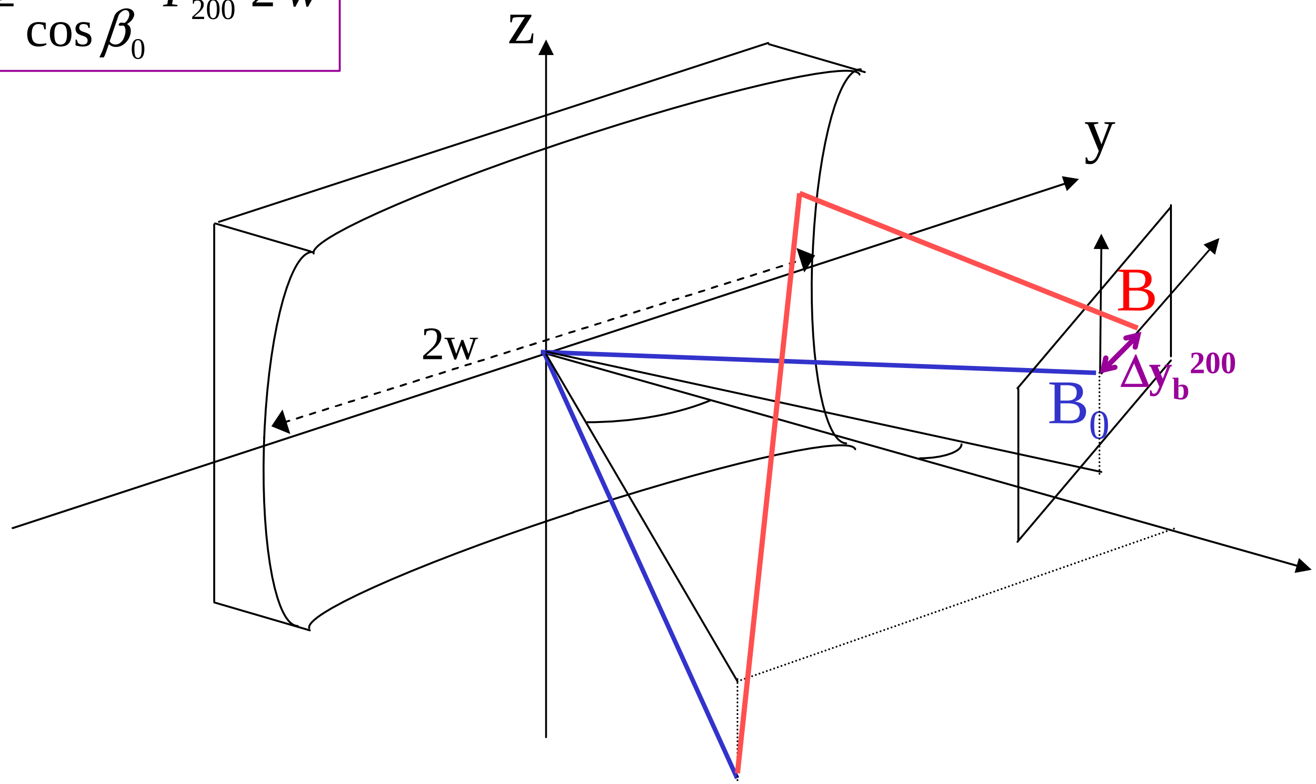
Substituting y=±w and z=±l in the ray aberrations Δy_b^{ijk} and Δz_b^{ijk} :

→ size ($\Delta y_b * \Delta z_b$) of the resulting aberrated image

Defocus contribution

The **defocus** contribution is in the dispersive direction and is proportional to the length (± w) of the grating footprint. The error is symmetric about the Gaussian image point:

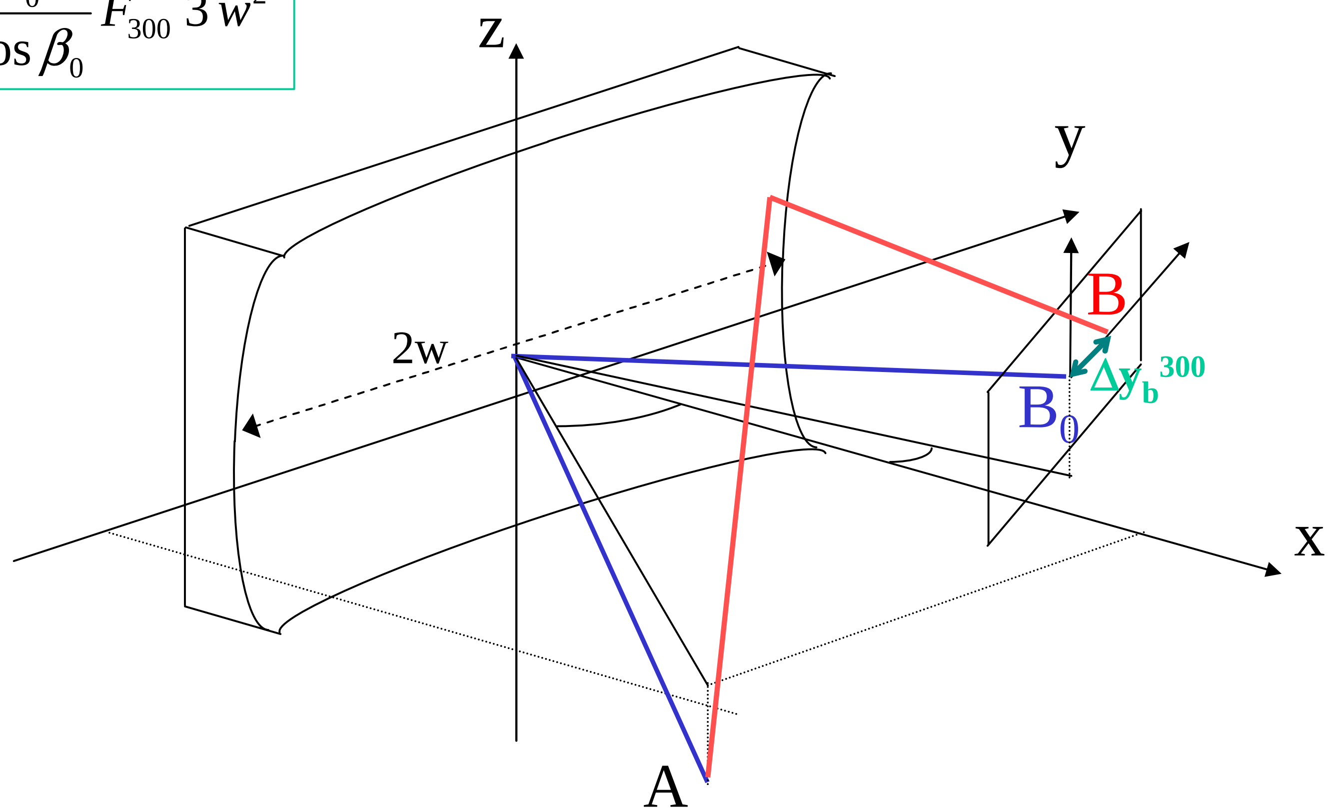
$$\boxed{\Delta y_b^{\;200}(\pm w) = \pm \frac{r_0'}{\cos\beta_0} F_{200}\, 2\, w}$$



Coma contribution

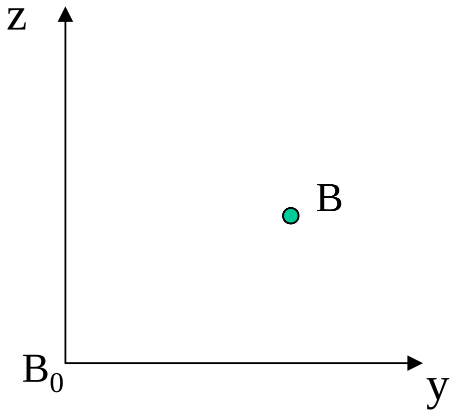
The **coma** contribution is proportional to w^2, giving a dispersive error which only occurs on one side of the Gaussian image point for rays from both the top and the bottom of the grating (y=±w):

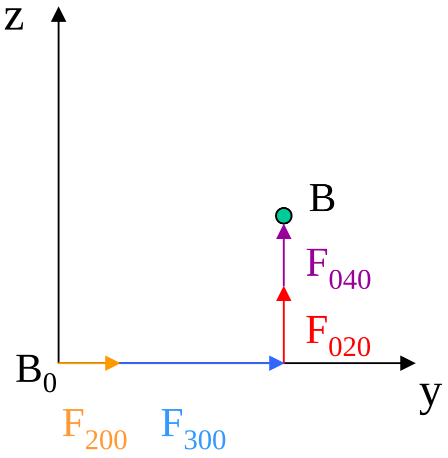
$$\boxed{\Delta y_b^{300}(\pm w) = \frac{r_0'}{\cos\beta_0} F_{300}\, 3\, w^2}$$



Comparison ray trace - aberration calculations

Example:





Ray trace simple tells us that the ray arrives in a certain point

Aberration-based calculations specify the different contributions

Knowing the expression of the different contributions, we can try to minimize the resulting aberration

Aberrations contribution to resolution

$$\Delta\lambda = \left(\frac{\partial\lambda}{\partial\beta}\right)_{\alpha=const} \Delta\beta$$

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

Substituting: $\Delta\beta = \frac{\Delta y_b}{r'}$ $\rightarrow$ $\Delta\lambda = \frac{\cos\beta}{Nk}\frac{\Delta y_b}{r'}$

Substituting: $\Delta y_b = \frac{r_0'}{\cos\beta_0}\frac{\partial F}{\partial y}$ $\rightarrow$ $\Delta\lambda = \frac{1}{Nk}\frac{\partial F}{\partial y}$

$$\boxed{\Delta\lambda = \frac{1}{Nk}\sum_{ijk} F_{ijk}\ i\ y^{i-1}\ z^{j}}$$

aberration-limited wavelength resolution

Aberration theory: conclusions

• Perfect focus condition: $\frac{\partial F}{\partial y} = 0 \quad \frac{\partial F}{\partial z} = 0$ for each pair (y,z)

→ all the coefficients F_{ijk} must be zero

• Non-zero values for the coefficients F_{ijk} lead to displacements of the rays arriving in the image plane from the ideal Gaussian image point.

• We have found the expressions for these rays displacements and the corresponding contributions to wavelength resolution. In this way the impact on the imaging and energy resolution properties of a given grating can be evaluated.

• By a proper choice of the grating shape, groove density, object and image distances, the sum of the aberrations may be reduced to a minimum.

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Programs

- **Shadow** **(ray tracing)** http://www.nanotech.wisc.edu/CNT_LABS/shadow.html
- **XOP** **(general optical calculations)** http://www.esrf.eu/computing/scientific/xop2.1/intro.html
- **SPECTRA** **(optical properties of synchrotron radiation emitted from bending magnets, wigglers and undulators)** http://radiant.harima.riken.go.jp/spectra/index_e.html

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