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Introduction to X-ray optics: photon transport and focusing

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Introduction to X-ray optics: photon transport and focusing

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School on Synchrotron and Free-Electron-Laser Sources and their Multidisciplinary Applications , Trieste, Italy, 26 April-7 May 2010

Outline

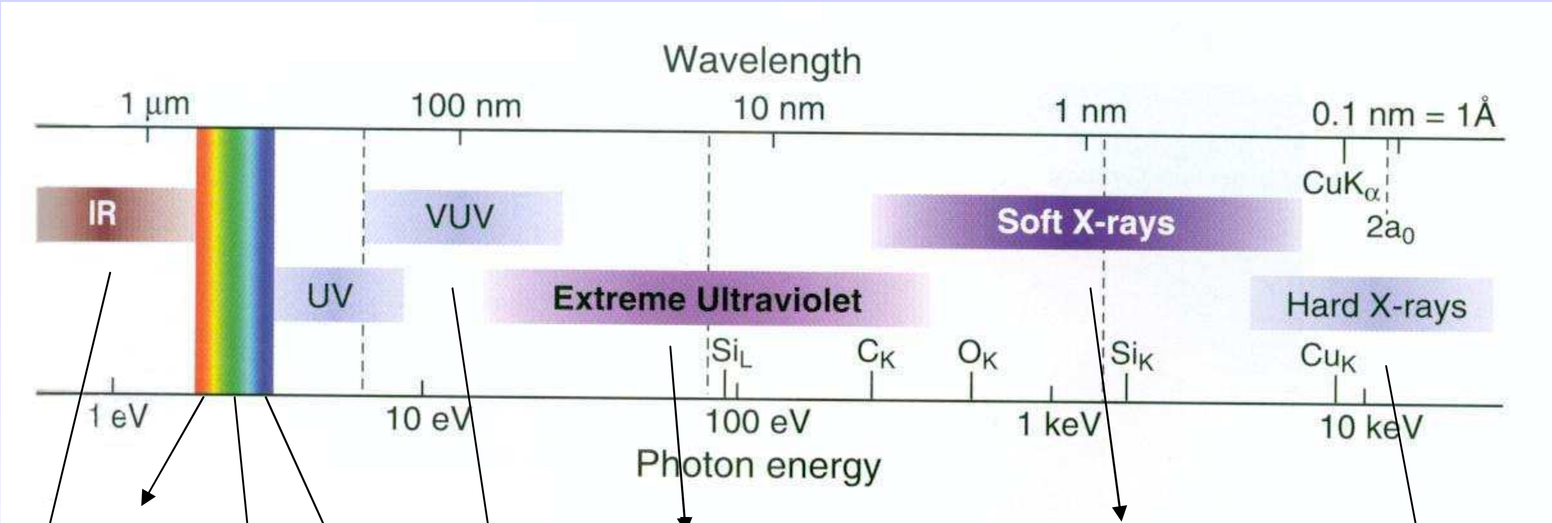
- SL properties, spectral brightness
- x-ray beamline: tasks, structure, main optical elements
- VUV, EUV and soft x-rays characteristics, properties of reflection
- x-rays mirrors reflectivity
- x-rays mirrors focusing properties
- x-rays mirrors defects

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=30 ps, separation=2 ns (60 cm))
- 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

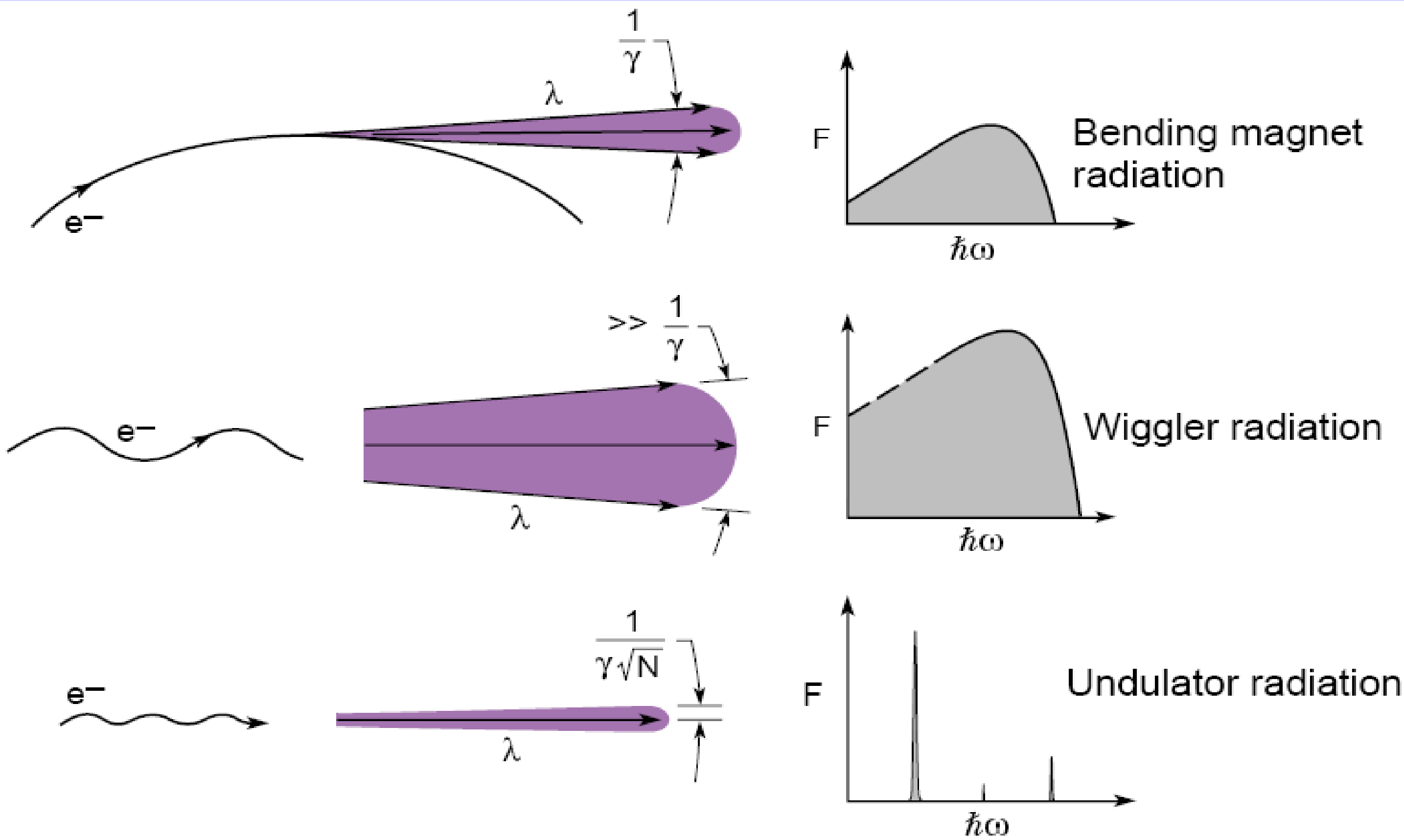
30-250eV
40-5nm

250eV-several keV

2-several tens of keV

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

Three Synchrotron Light sources



from D.Attwood

the spectrum is continuus only for bending magnets and wigglers!

Spectral brightness

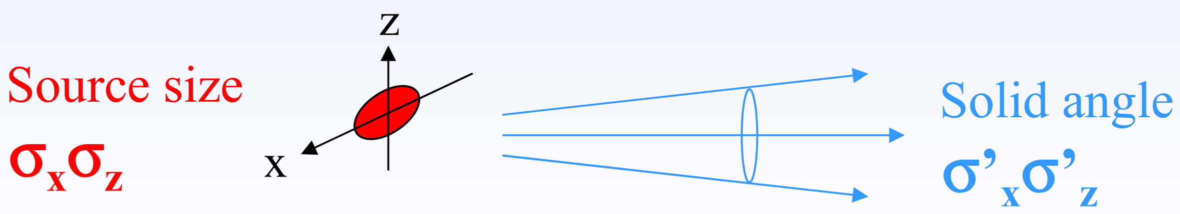
$$Spectral\ Brightness = \frac{photon\ flux}{I} \frac{1}{\sigma_x \sigma_z \sigma'_x \sigma'_z BW}$$

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

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

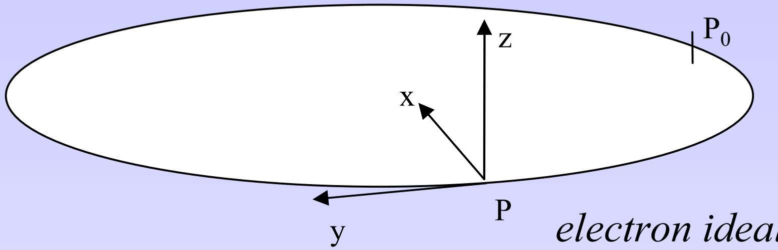
$\sigma'_x \sigma'_z$ = solid angle into which SR is emitted

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

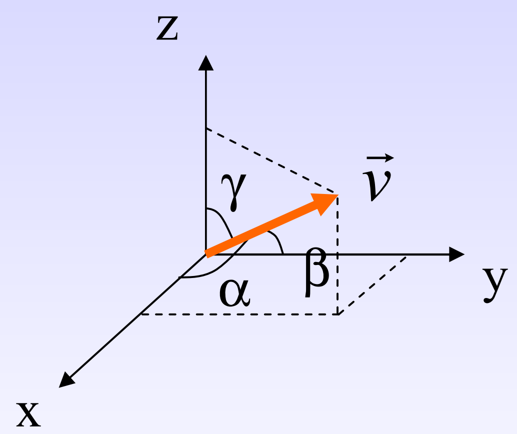


Coordinate system

Electron beam coordinate system:



electron ideal orbit



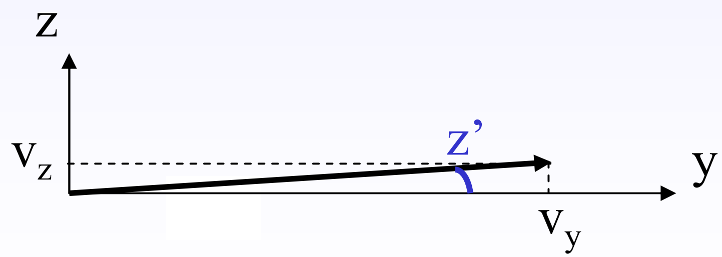
$$x' = \cos\alpha = \frac{dx}{ds}$$

$$z' = \cos\gamma = \frac{dz}{ds}$$

$v_y >> v_x, v_z$ $\longrightarrow$

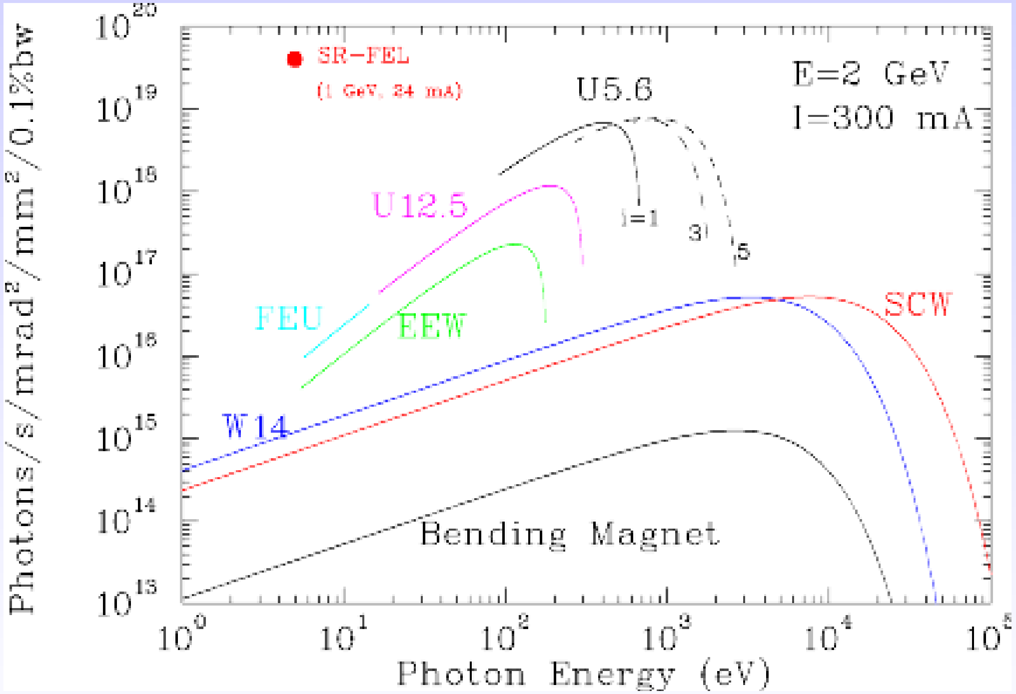
$$x' = \cos\alpha = \frac{v_x}{v} \cong \frac{v_x}{v_y}$$

$$z' = \cos\gamma = \frac{v_z}{v} \cong \frac{v_z}{v_y}$$



v_x, v_z are proportional to x' and z'

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)

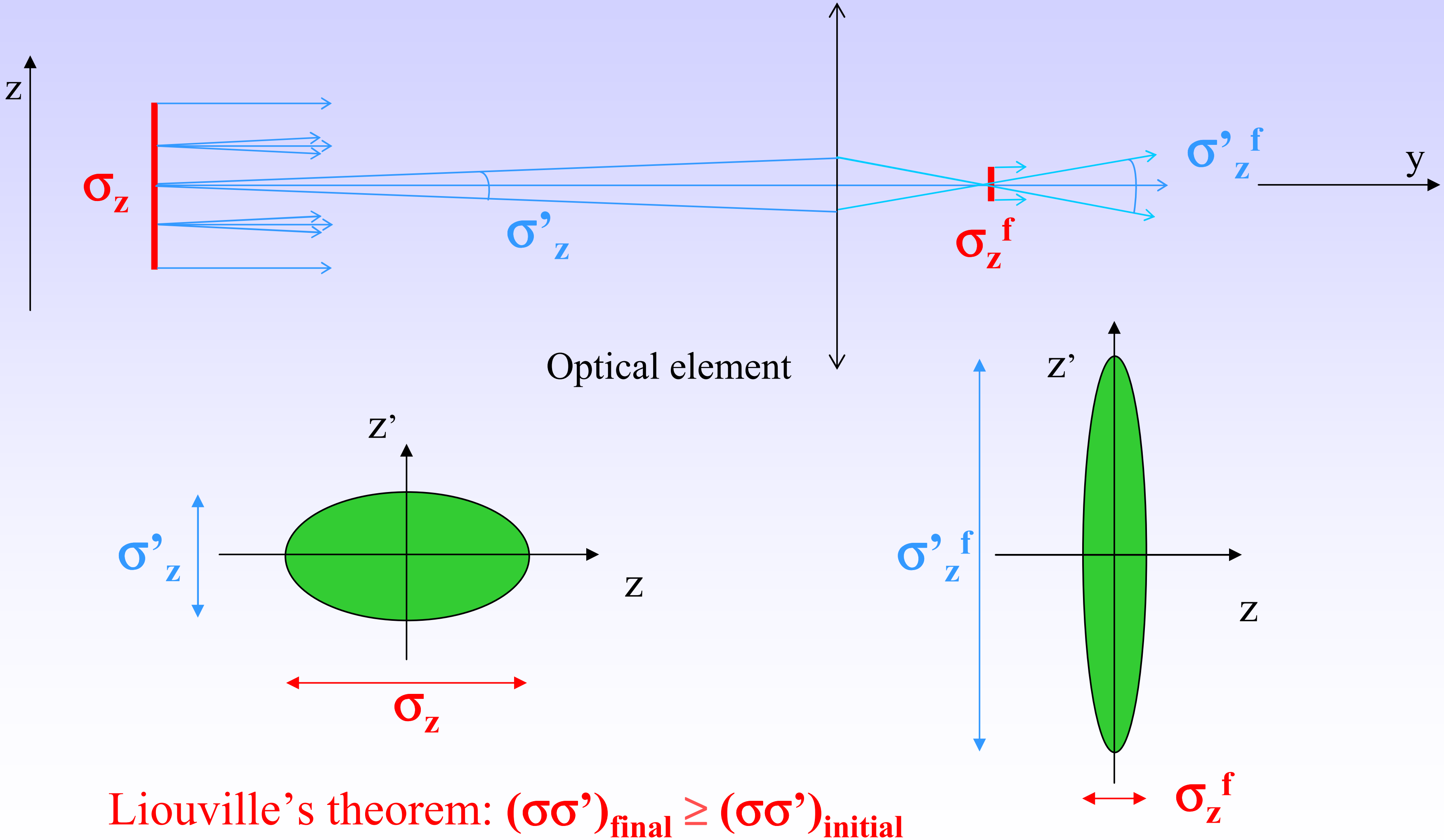
$$Spectral\ Brightness = \frac{photon\ flux}{I}\frac{1}{\sigma_x\sigma_z\sigma'_x\sigma'_z BW}$$

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

→ 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.

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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

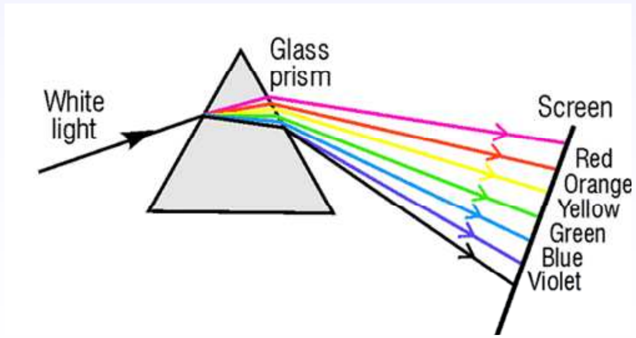
The beamline (2)

Not a simple pipe!

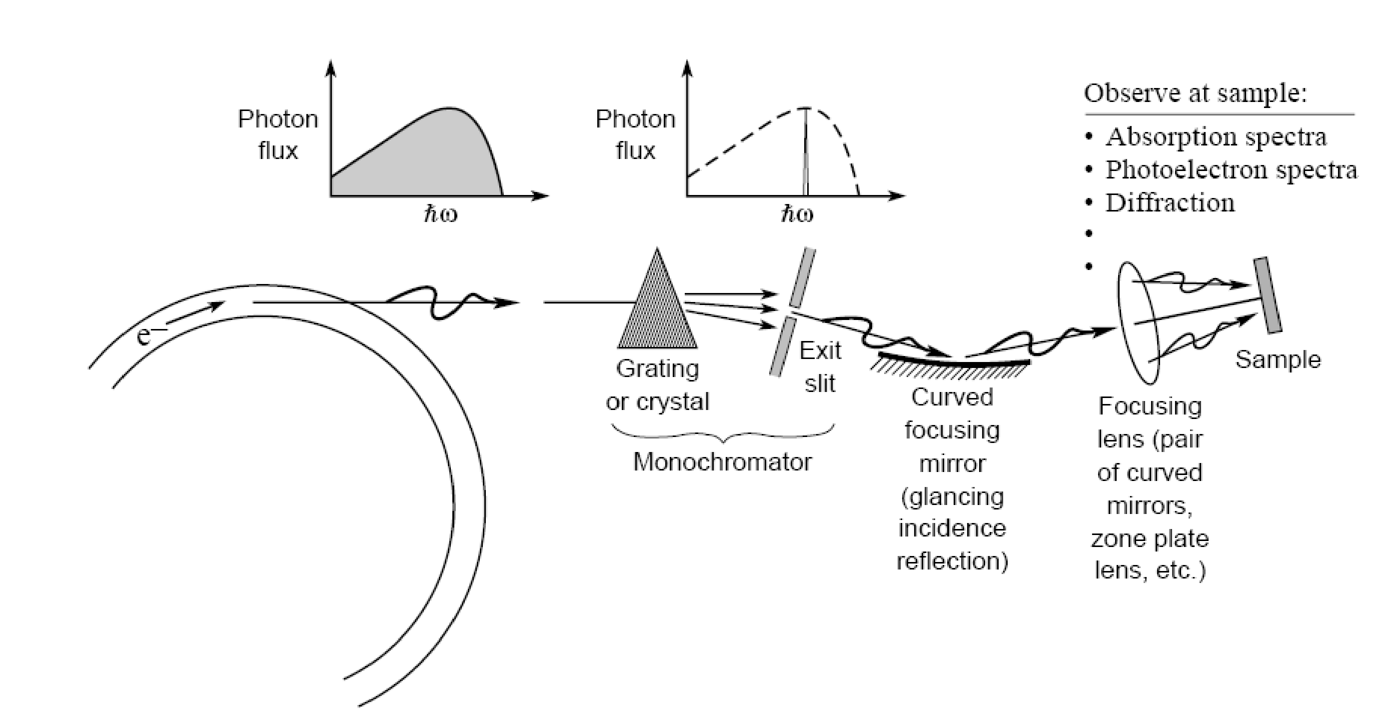
Basic optical elements:

• mirrors, to deflect, focus and filter the radiation

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

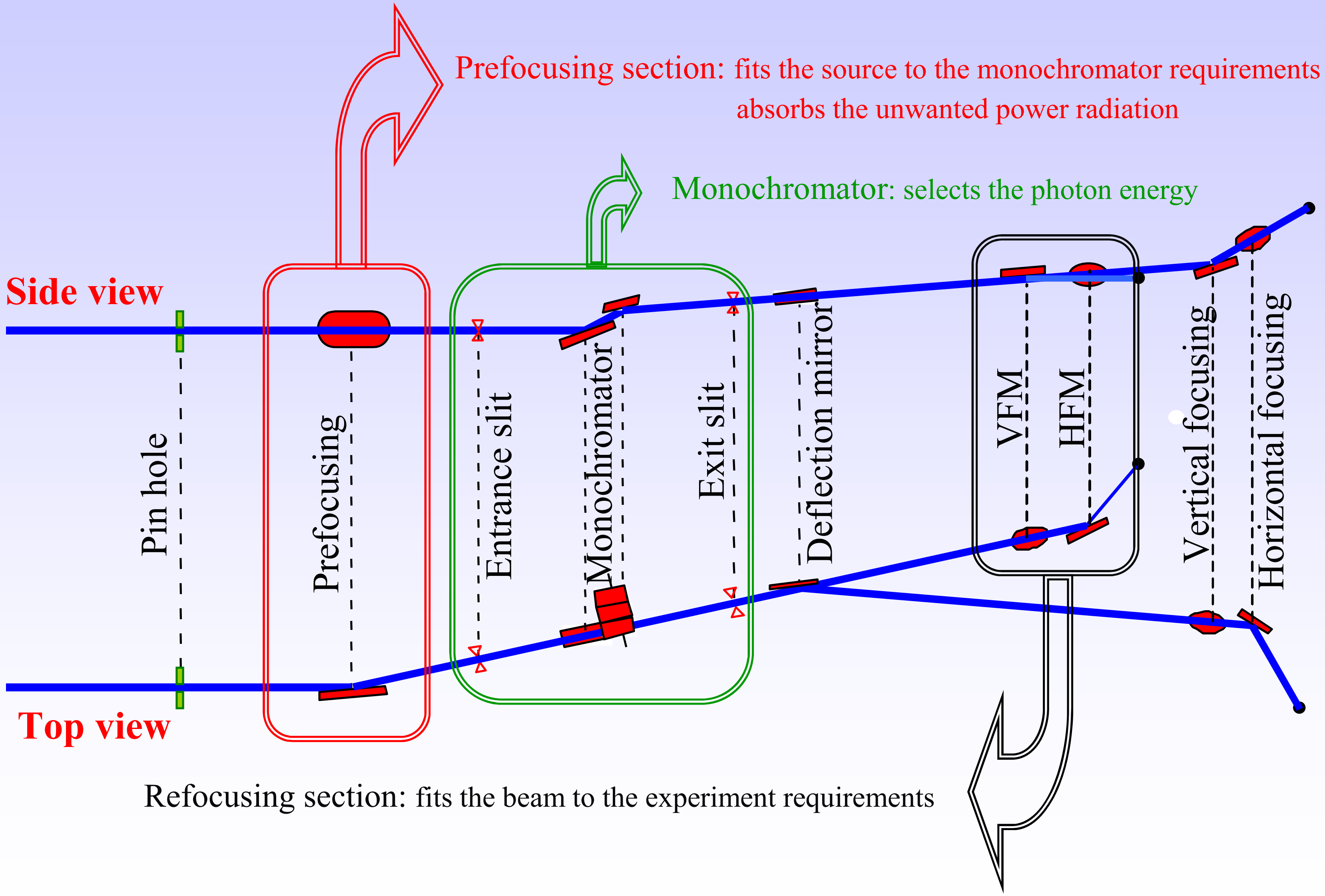


Beamline structure



from D.Attwood

Beamline structure: example



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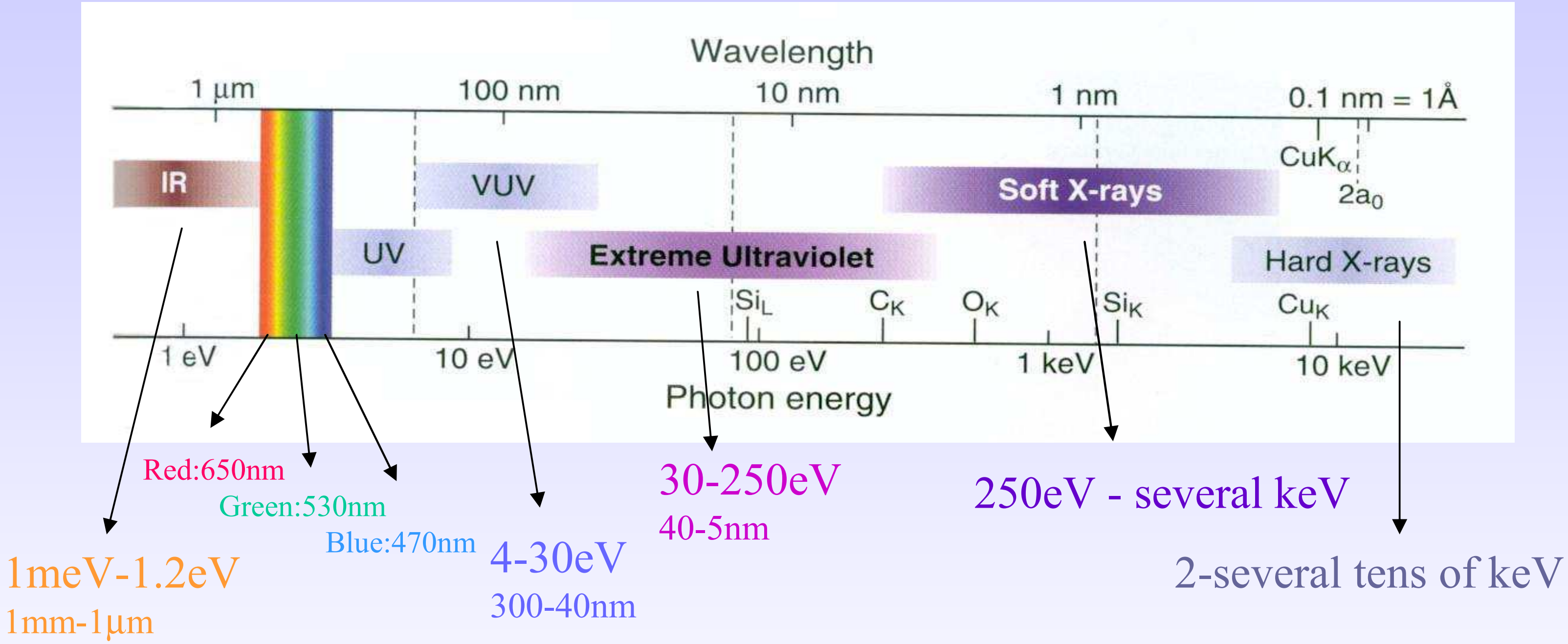
VUV, EUV and soft x-rays



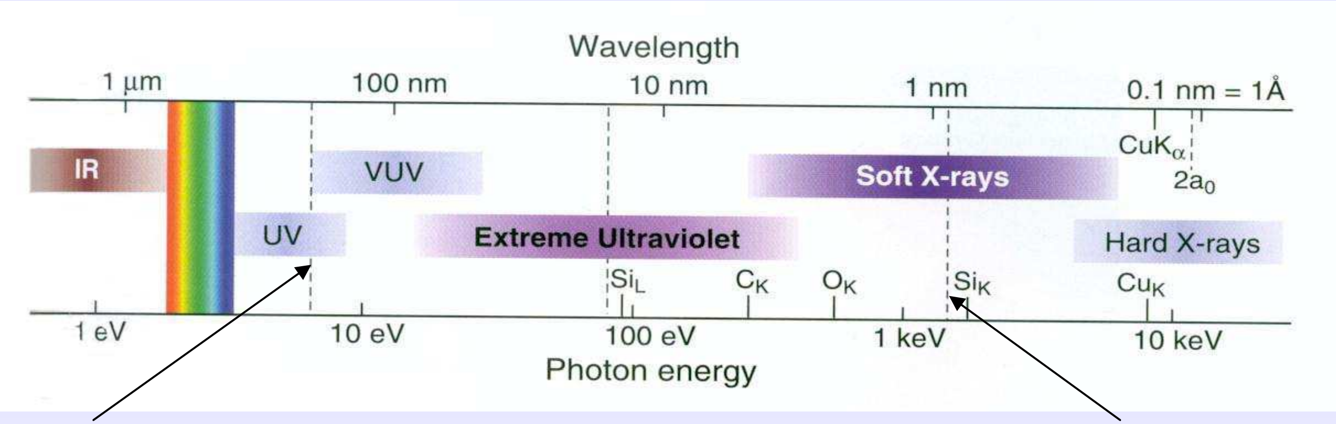
These regions are very interesting because are characterized by the presence of the absorption edges of most low and intermediate Z elements

→ 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

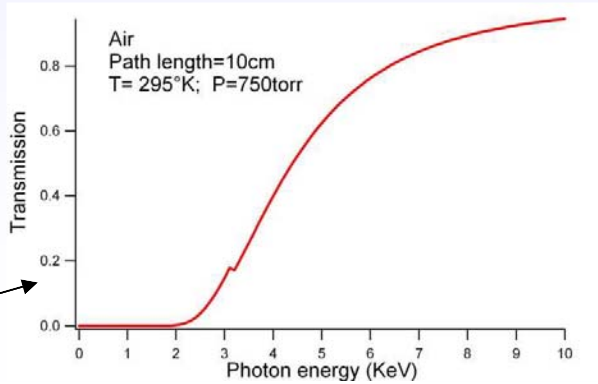
→ No windows

→ The entire optical system must be kept under UH Vacuum

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

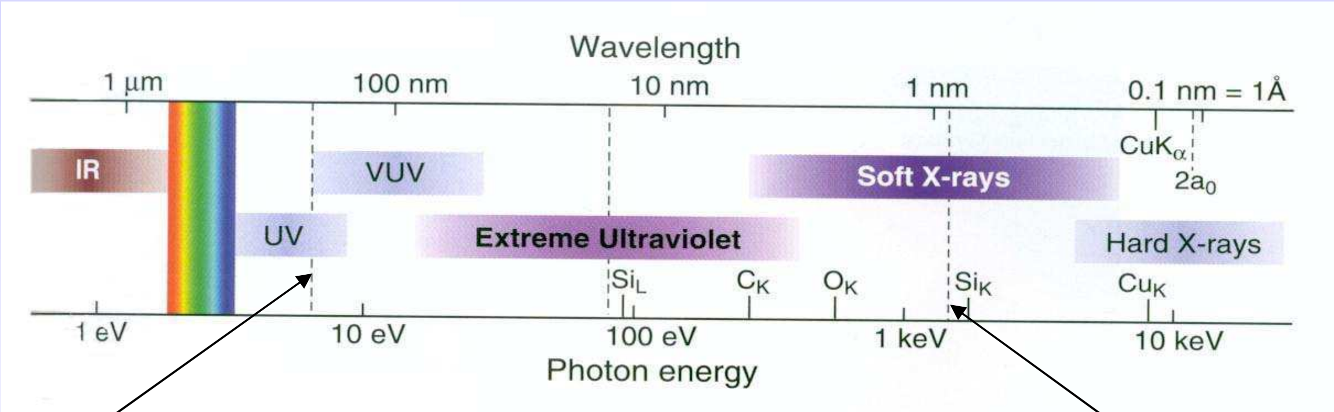
- Not to disturb the storage ring and the experiment
- To avoid photon absorption in air
- To protect optical surfaces from contamination (especially from carbon)

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

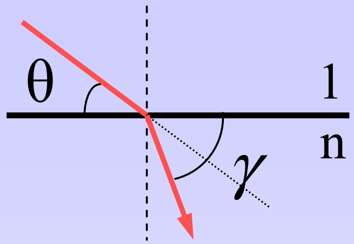
→ The only optical elements which can work in the VUV, EUV and soft x-rays regions are mirrors and diffraction gratings, used in total external reflection at grazing incidence angles

Exceptions: multilayer coated mirrors, zone plates

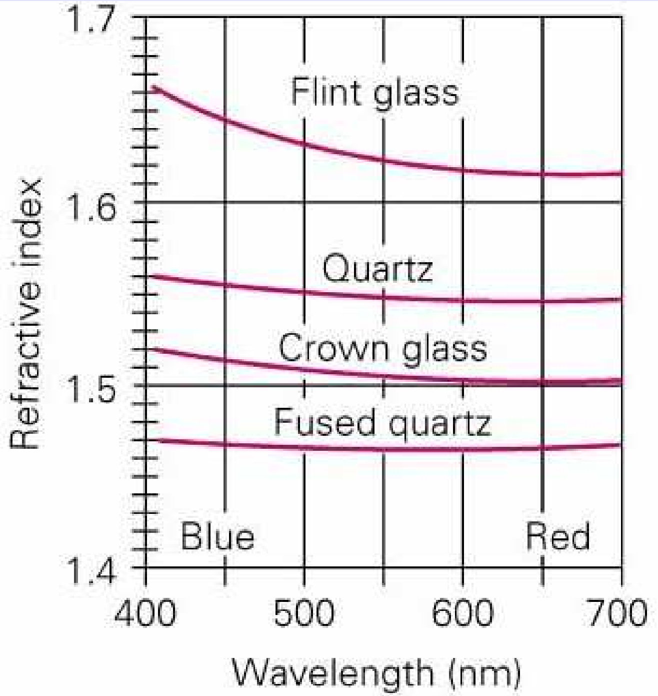
Snell's law, visible light

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

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



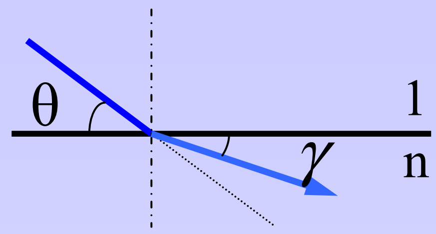
$\mathbf{n > 1 \rightarrow \gamma > \theta}$



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 $n = n_2/n_1$

$n < 1$ → $\gamma < \theta$

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

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

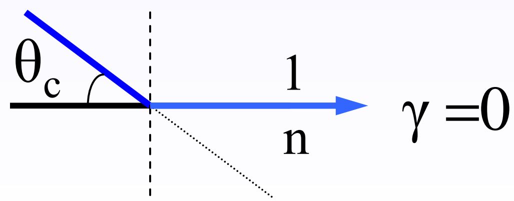
Typical values:
$\delta \approx 10^{-2}$ for 250 eV (5 nm)
$\delta \approx 10^{-4}$ for 2.5 keV (0.5 nm)

→ 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: $\cos\theta_c = n$

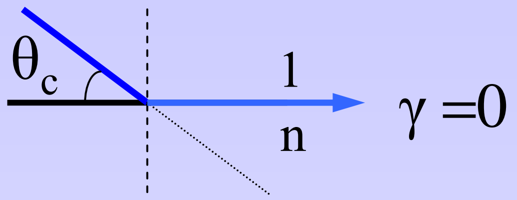
$$1 - \frac{\vartheta_c^2}{2} = 1 - \delta \quad \rightarrow \quad \boxed{\theta_c = \sqrt{2\delta}}$$



$n < 1$

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.

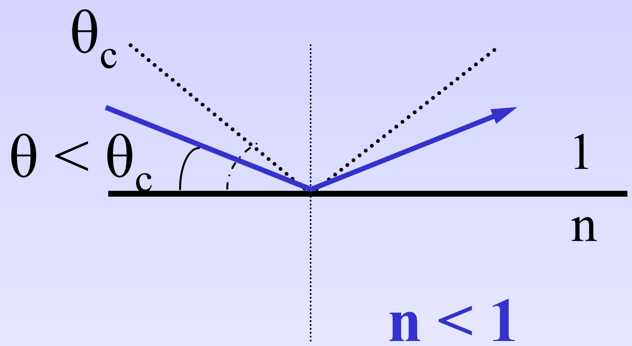
Gold (Z=79):
600 eV → θc ≈ 7.4°
1200 eV → θc ≈ 3.7°
5 keV → θc ≈ 0.9°

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

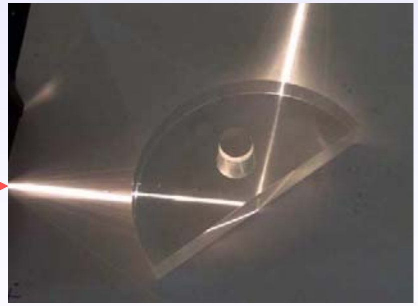
Carbon (Z=6):
100 eV → θc ≈ 250 mrad (14°)

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

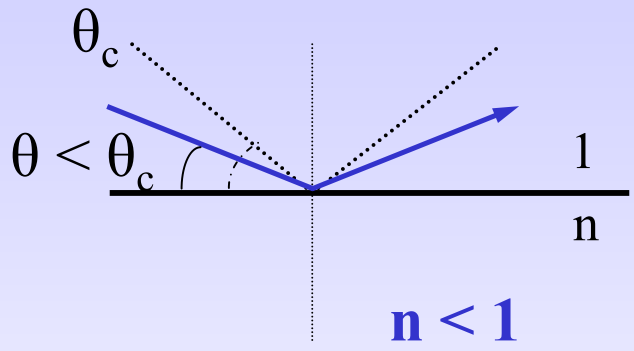
Nearly total external reflection

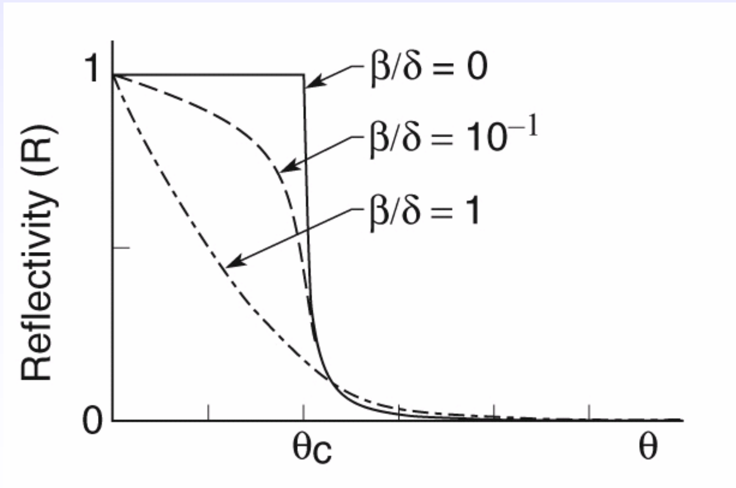
This model of total reflection is incomplete because it doesn't include the effect of the imaginary part of the refraction index.

refractive index=1-δ+iβ

The radiation penetrates into the material 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
→ nearly total reflection





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

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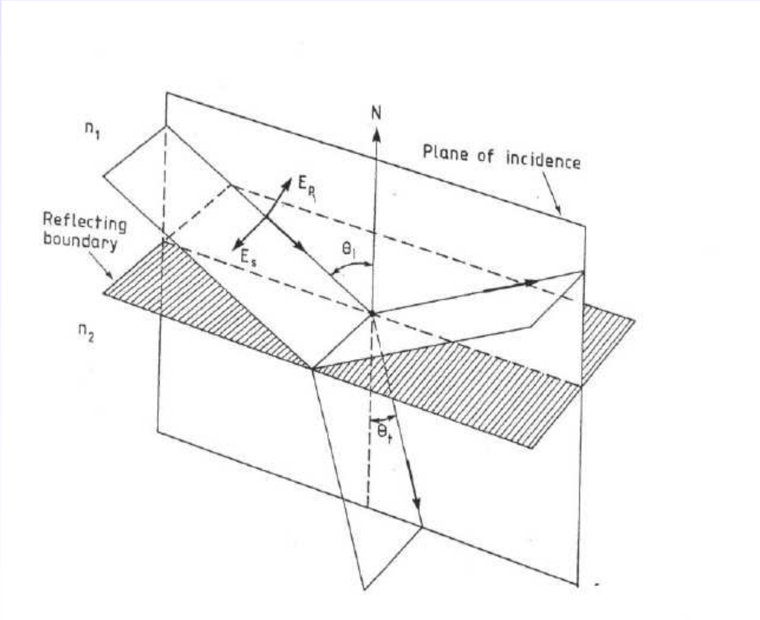
Reflection coefficients (1)

How can the expression of the reflectivity be derived?
R= ratio of reflected and incident intensity

Boundary conditions at the mirror surface:

• The components of $\vec{E}$ and $\vec{H}$ parallel to interface must be continuous

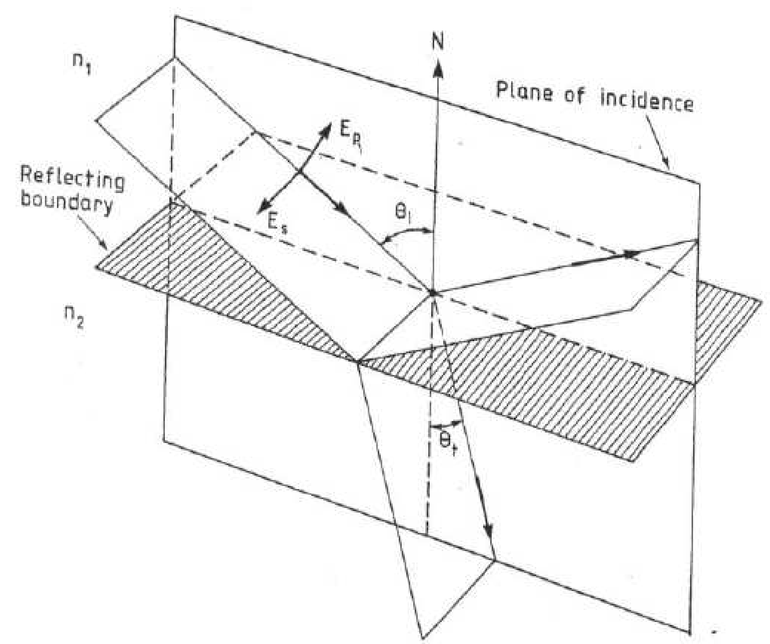
• The components of $\vec{D}$ and $\vec{B}$ perpendicular to interface must be continuous



• The resulting R is a function of the polarization of the incident radiation

s and p polarization

Radiation is usually decomposed into 2 geometries:
s polarization: electric field perpendicular to the plane of incidence
p polarization: electric field parallel to the plane of incidence

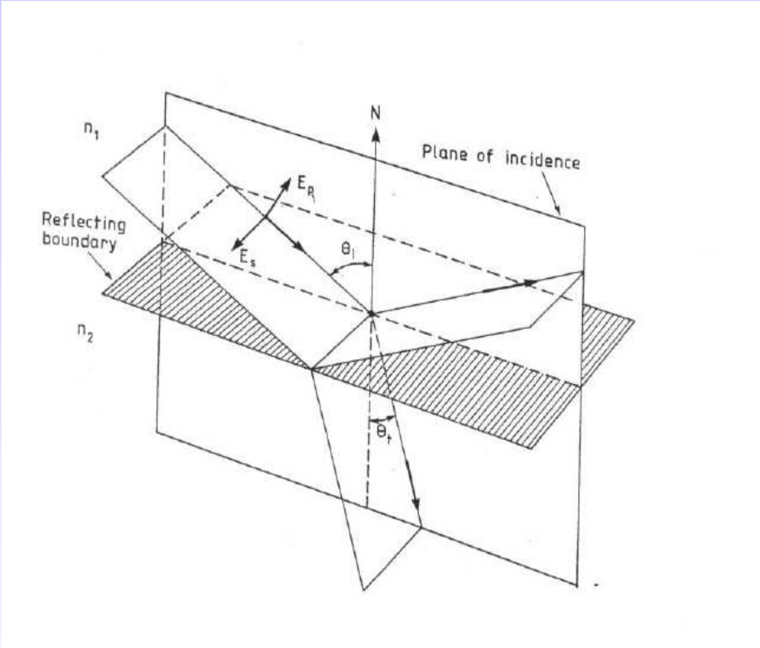


Any incident wave, polarized or not, can be represented in terms of these two polarizations

Reflection coefficients (2)

s polarization:

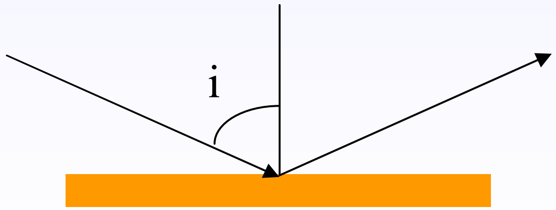
$$R_s = \frac{|\cos i - \sqrt{n^2 - \sin^2 i}\,|^2}{|\cos i + \sqrt{n^2 - \sin^2 i}\,|^2}$$



p polarization:

$$R_p = \frac{|n^2 \cos i - \sqrt{n^2 - \sin^2 i}\,|^2}{|n^2 \cos i + \sqrt{n^2 - \sin^2 i}\,|^2}$$

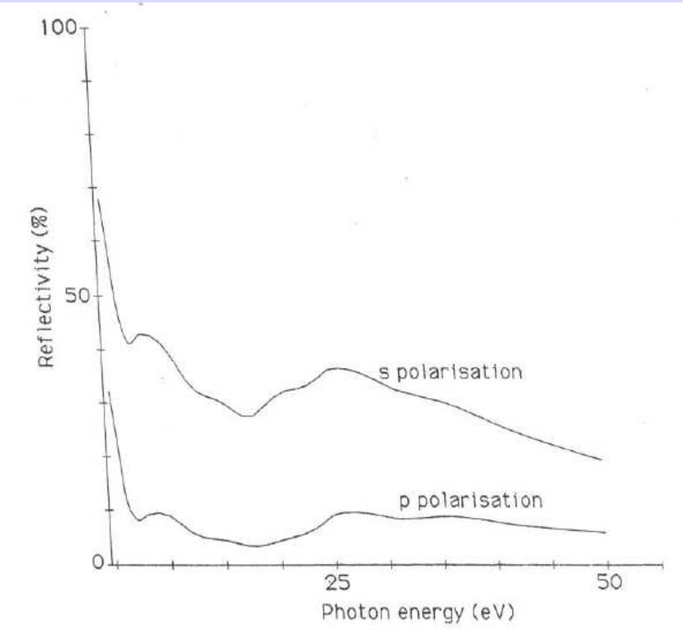
where: n=1-δ+β,
i incidence angle with respect to the normal.



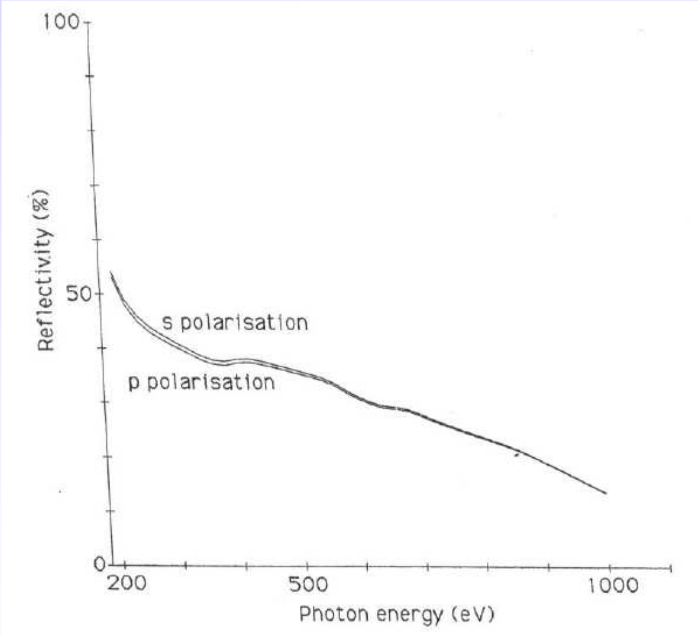
Reflection coefficients (3)

In the VUV region the reflectivity for s polarization is far higher than for p
→ vertical reflection geometry

Rs and Rp converge at small grazing incidence angles



Gold , i=55°



Gold , θ=4°

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

Reflection coefficients (4)

For **normal incidence** (i=0), in the case of x-rays $\delta<<1$, $\beta<<1$:

$$R_{i=0} \cong \frac{\delta^2 + \beta^2}{4}$$

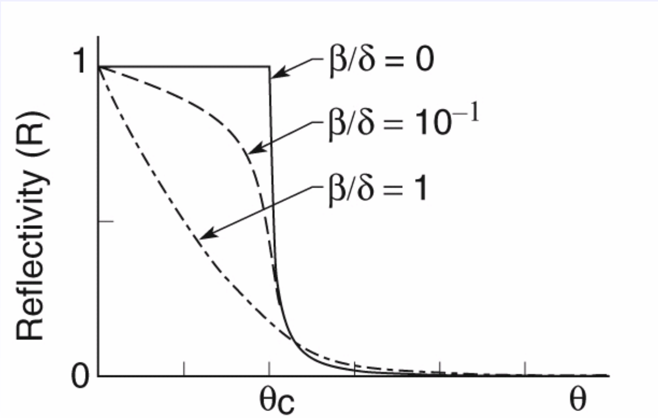
Example:
Nickel @300 eV (4.13 nm), δ=0.0124, β=0.00538 → $R_{i=0}=4.6 * 10^{-5}$

At small **grazing incidence** angle θ:

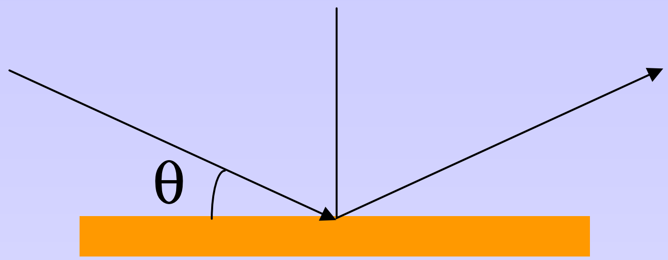
$$R_{s,\theta} = \frac{(\theta - A)^2 + B^2}{(\theta + A)^2 + B^2} \qquad (\theta<<1)$$

$$A=\sqrt{\frac{(a^2+b^2)^{1/2}+a}{2}} \qquad B=\sqrt{\frac{(a^2+b^2)^{1/2}-a}{2}}$$

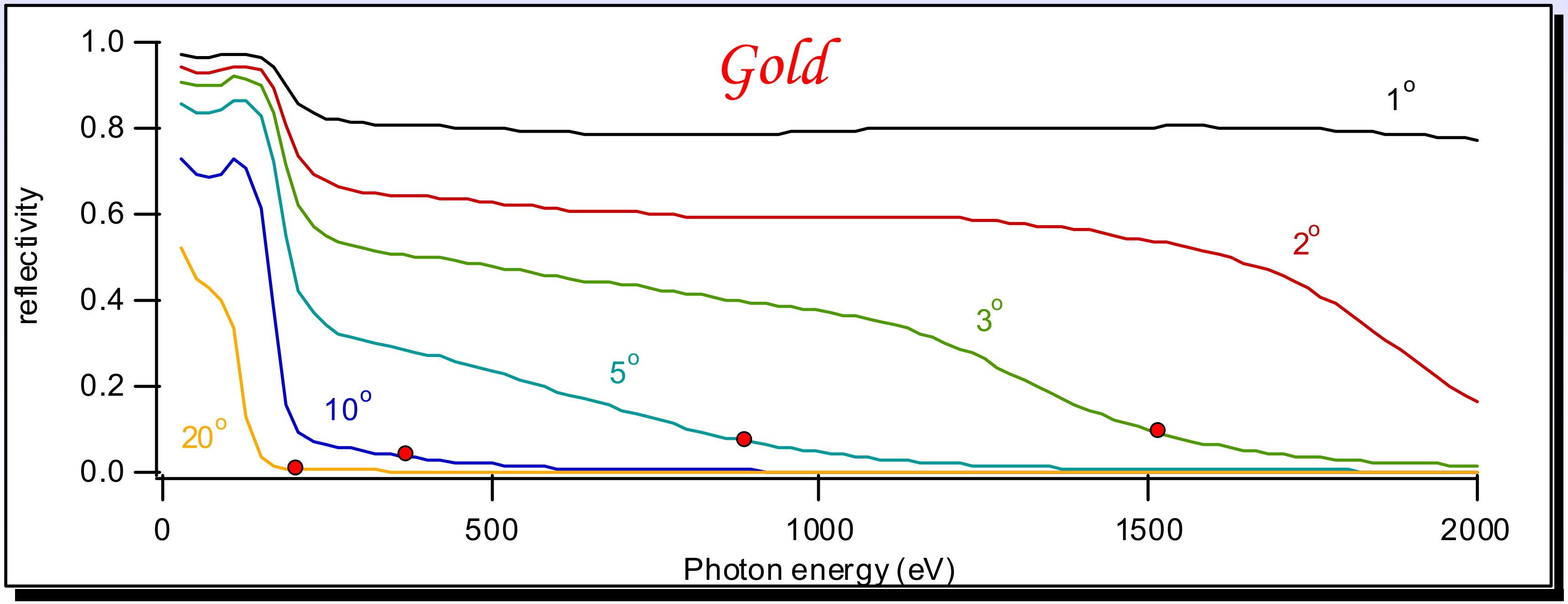
$$a=\theta^2-2\delta \qquad b=2\beta$$



Mirror reflectivity (1)

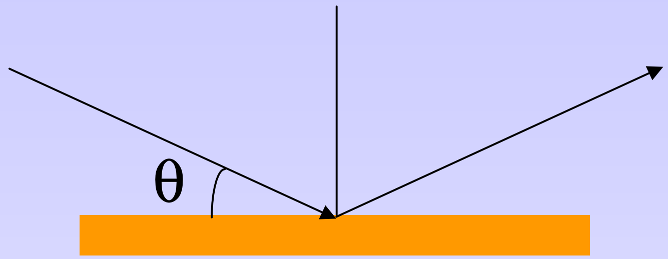


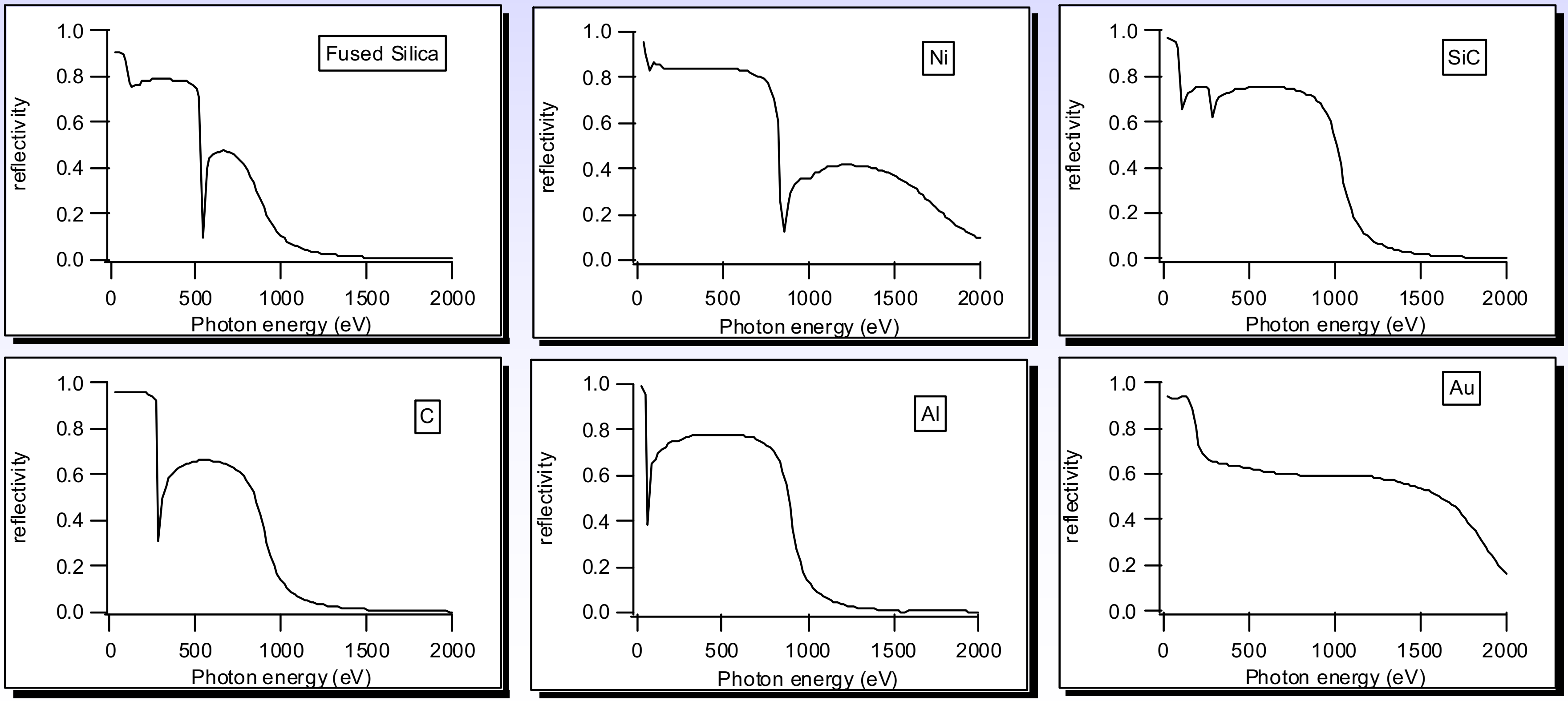
Reflectivity drops down fast with the increasing of the grazing incidence angle
→ only reflective optics at grazing incidence angles
(typically 1°-2° for soft x-rays, few mrad for hard x-rays, 1 mrad= 0.057°)



Mirror reflectivity (2)

$\theta = 2^o$





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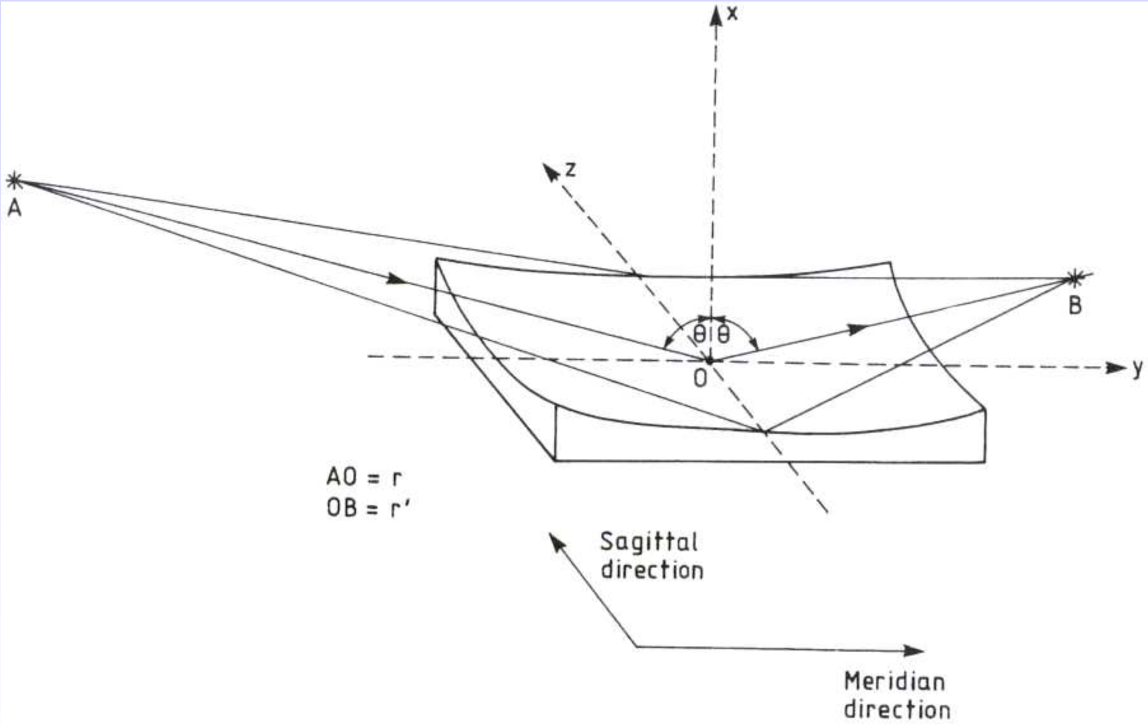
Focusing properties of mirrors

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.

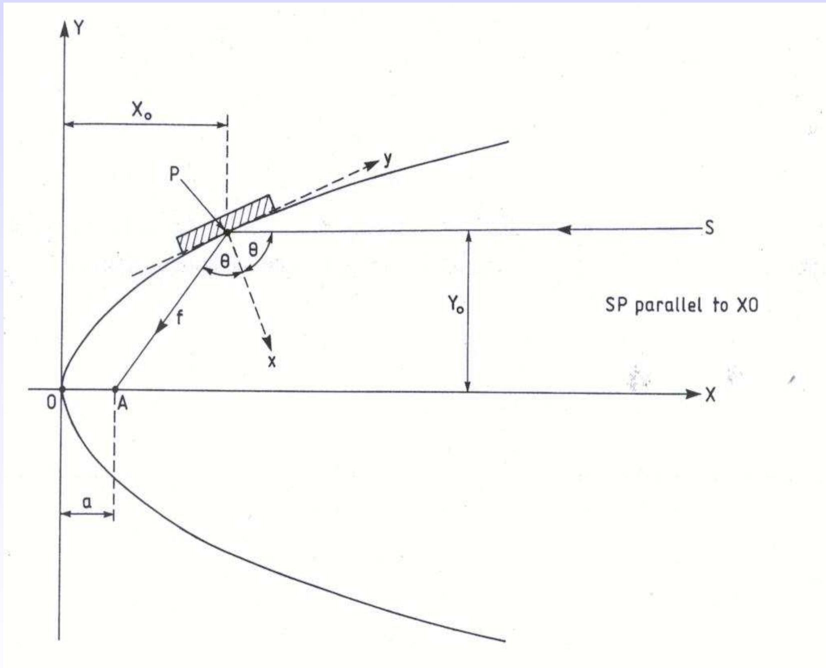
Line equation: $Y^2 = 4aX$

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

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

Position of the pole P:

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



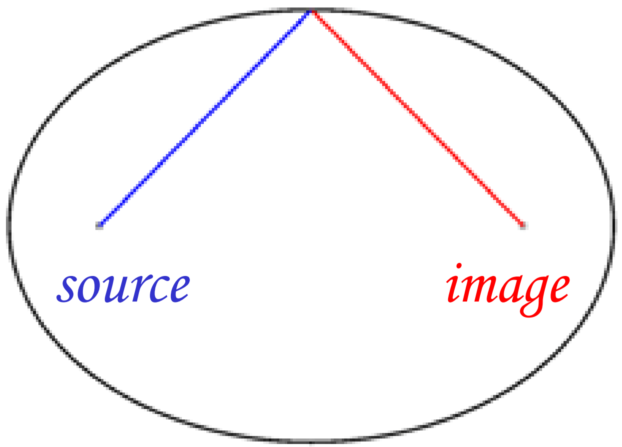
Paraboloid equation:

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

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

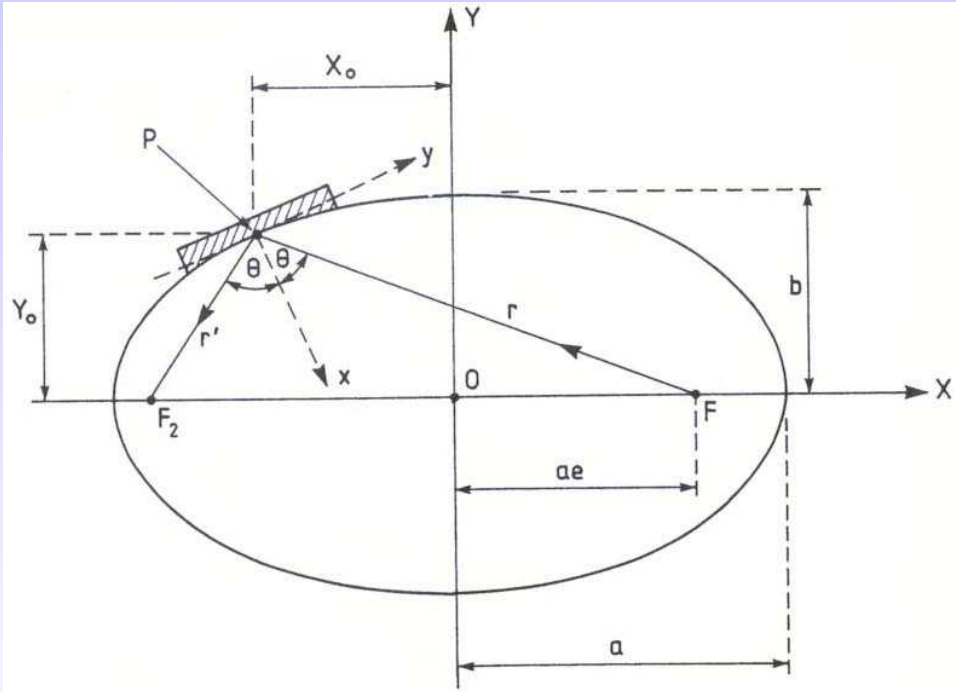
Line equation: $$\frac{X^2}{a^2}+\frac{Y^2}{b^2}=1$$

Ellipsoid equation:

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

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

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



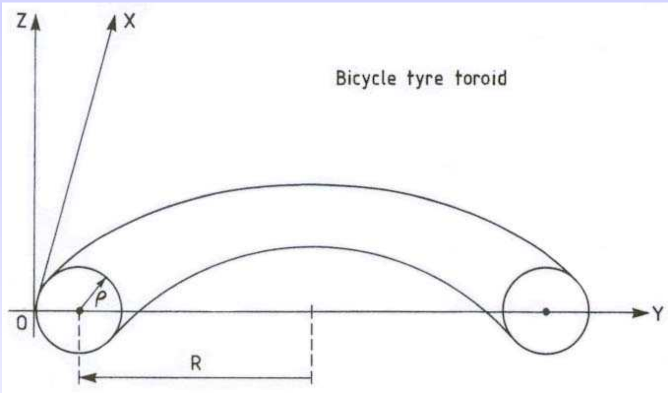
Rays from one focus F_1 will always be perfectly focused to the second focus F_2.

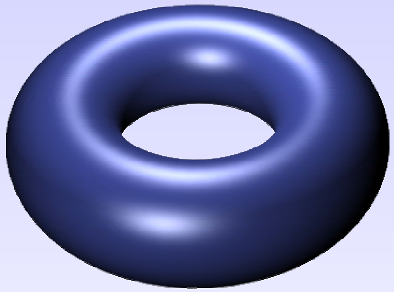
$$x^2\left(\frac{\sin^2\vartheta}{b^2}+\frac{1}{a^2}\right)+y^2\left(\frac{\cos^2\vartheta}{b^2}\right)+\frac{z^2}{b^2}-x\left(\frac{4f\cos\vartheta}{b^2}\right)-xy\left[\frac{2\sin\vartheta\sqrt{e^2-\sin^2\vartheta}}{b^2}\right]=0$$

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

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

Toroid (1)

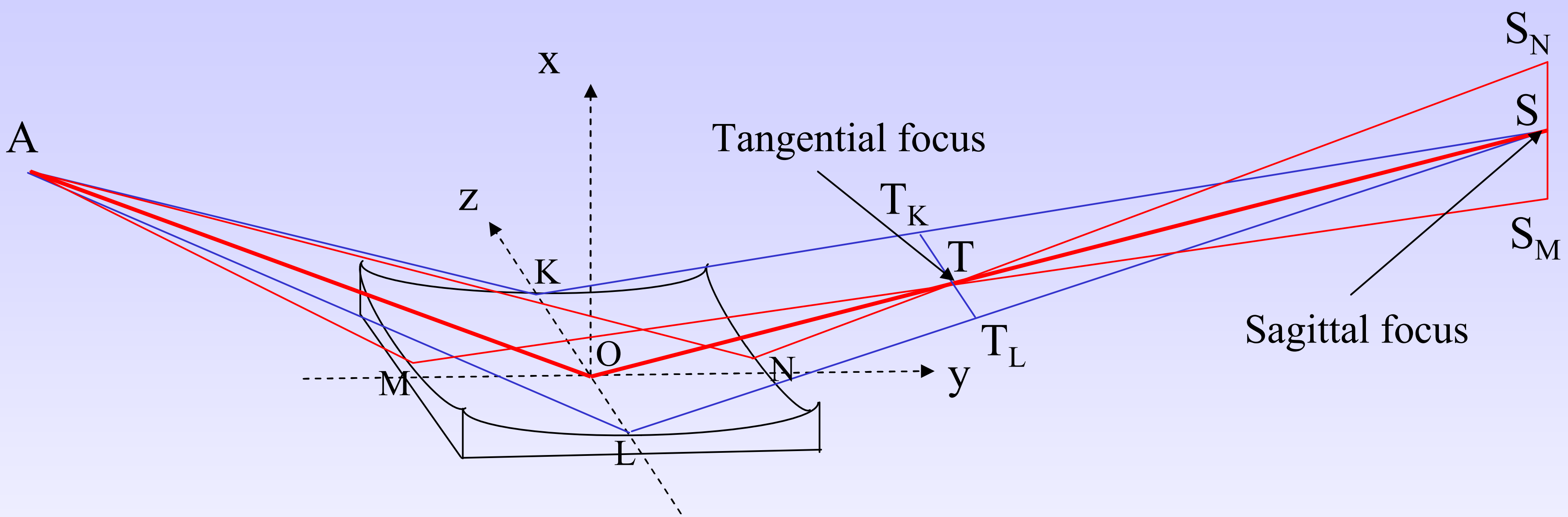




$$x^2 + y^2 + z^2 = 2Rx - 2R(R-\rho) + 2(R-\rho)\sqrt{(R-x)^2 + y^2}$$

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 line images: one in the tangential focal plane and one in the sagittal focal plane

Tangential focus T:

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

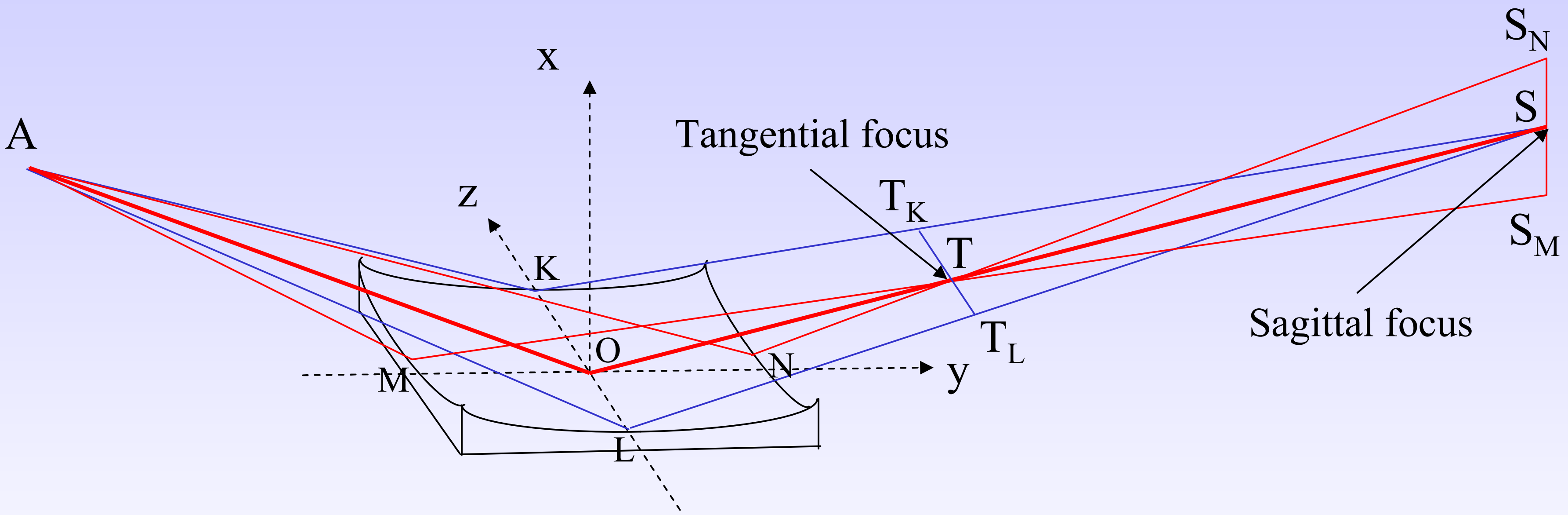
Sagittal focus S:

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

Stigmatic image:

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

Spherical mirror

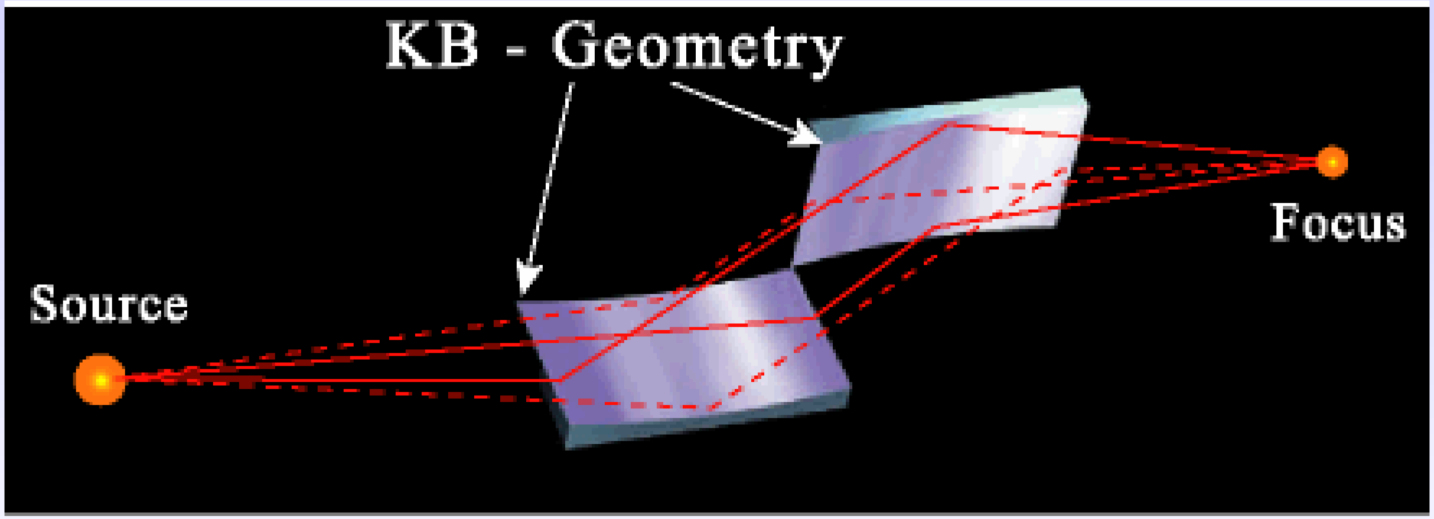


For ρ=R → spherical mirror :

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.

Outline

- SL properties, spectral brightness
- x-ray beamline: tasks, structure, main optical elements
- VUV, EUV and soft x-rays characteristics, properties of reflection
- x-rays mirrors reflectivity
- x-rays mirrors focusing properties
- x-rays mirrors defects

Mirrors defects

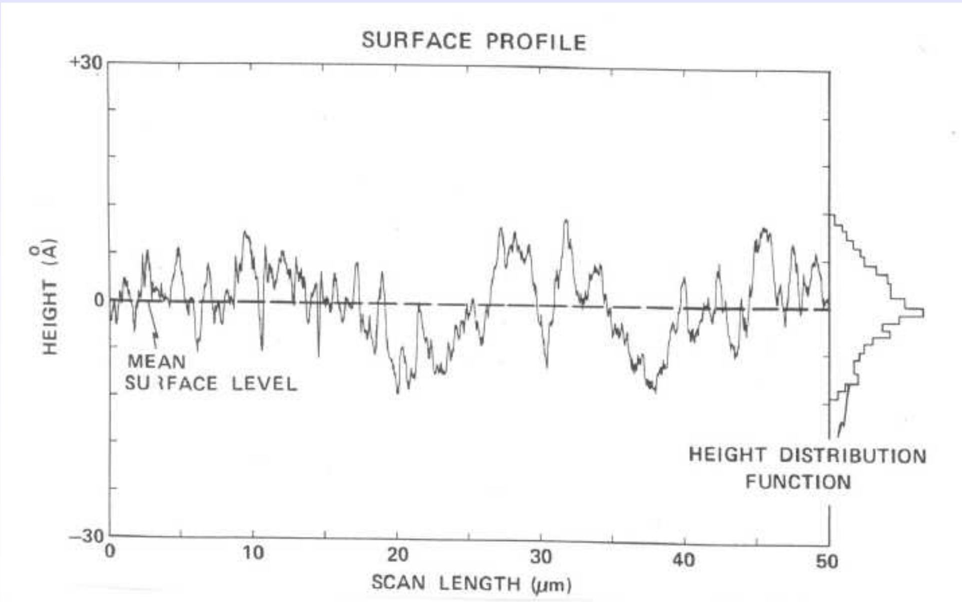
Manufacturing imperfections on a mirror surface:

Microroughness	spatial period <1 mm
Slope errors	spatial period >1 mm

Microroughness (1)

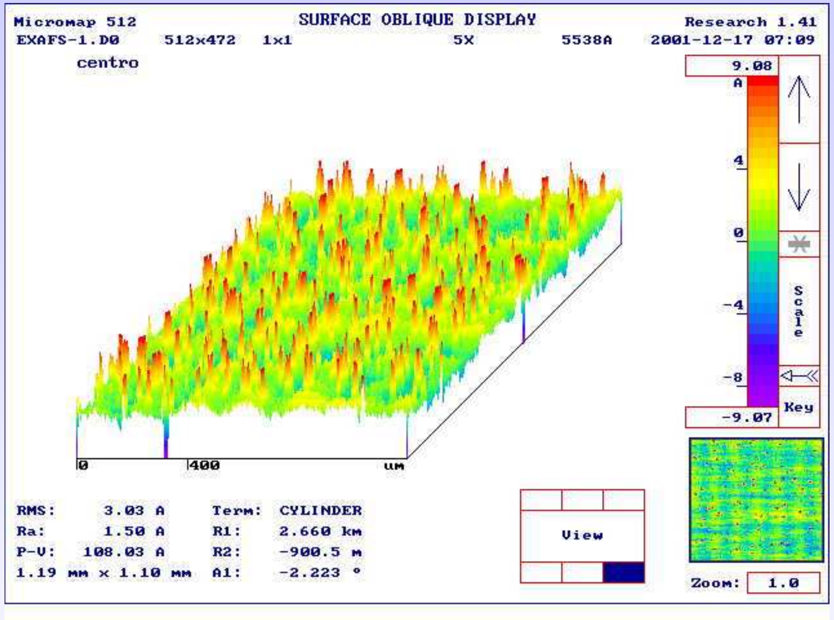
• **spatial period <1 mm**

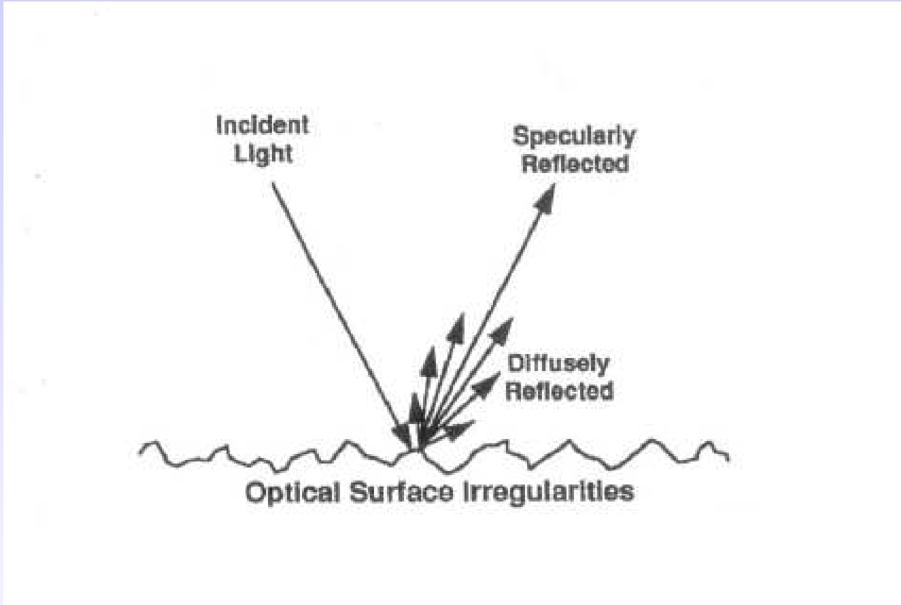
• characterized by the rms value of the surface height measured with respect to the mean surface level. (1-5 Å)



$$\sigma = \sqrt{\frac{1}{n}\sum_{x=0}^{n}\left[s(x) - \overline{s(x)}\right]^2}$$

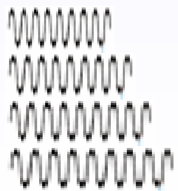
Microroughness (2)



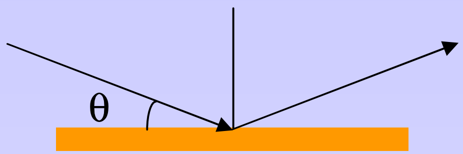


• produces a diffuse background: light is scattered at random directions

• superposition of diffraction gratings,
each diffracting the light in different directions

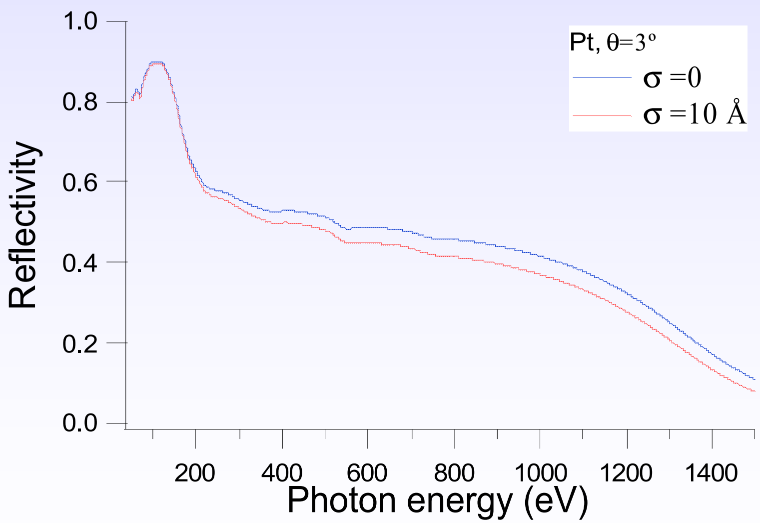


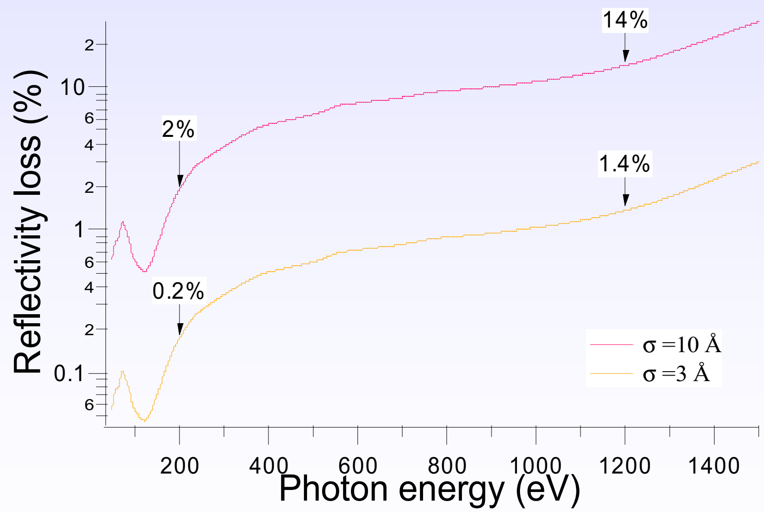
Microroughness (3)



→ the reflectivity decreases: $$R = R_0 e^{-\left(\frac{4\pi\sigma\sin\vartheta}{\lambda}\right)^2}$$

R is the attenuated reflectivity, R_0 is the reflectivity of the ideal smooth surface

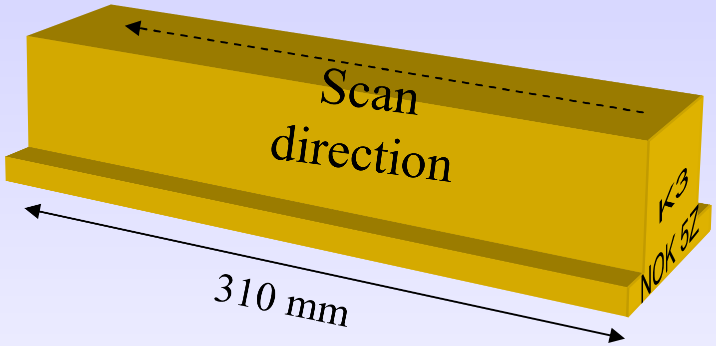


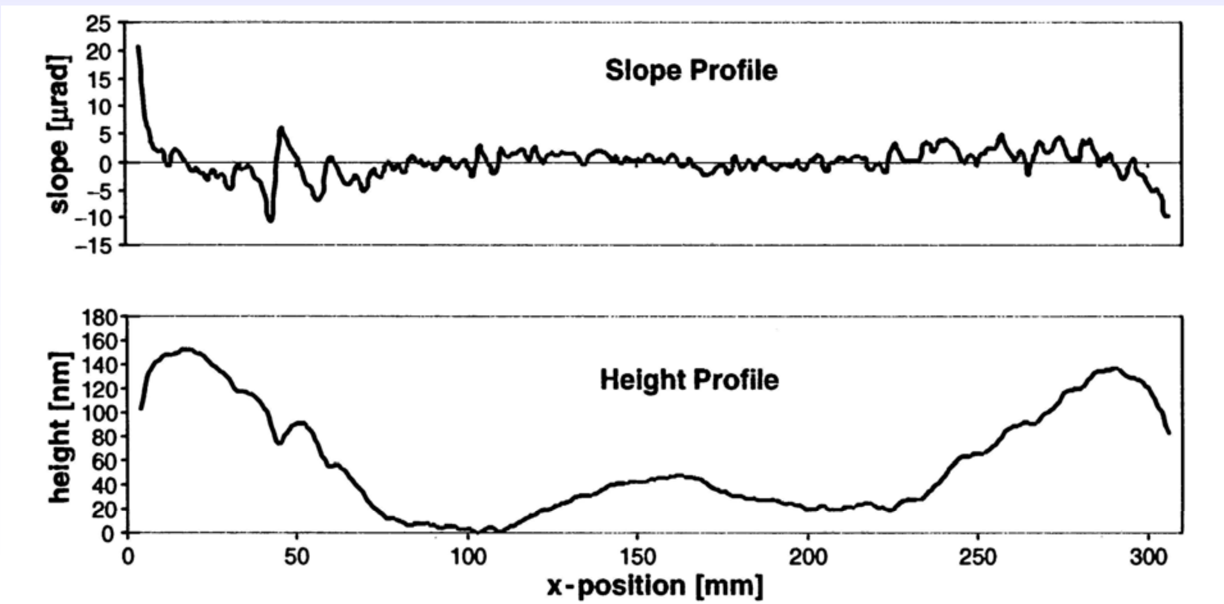


Slope errors (1)

Slope errors: deviations from the the ideal profile of the mirror with **spatial period > 1 mm**

They are characterized by the rms value of the derivative of the error profile (0.5-5 μrad)





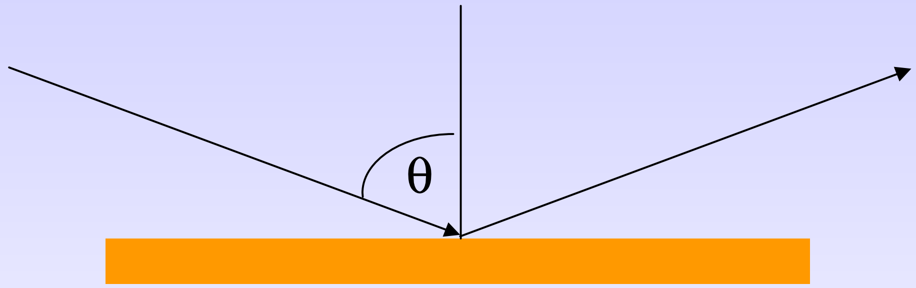
$$\delta(x) = \frac{dy}{dx}$$

$$y(x)$$

Slope errors (2)

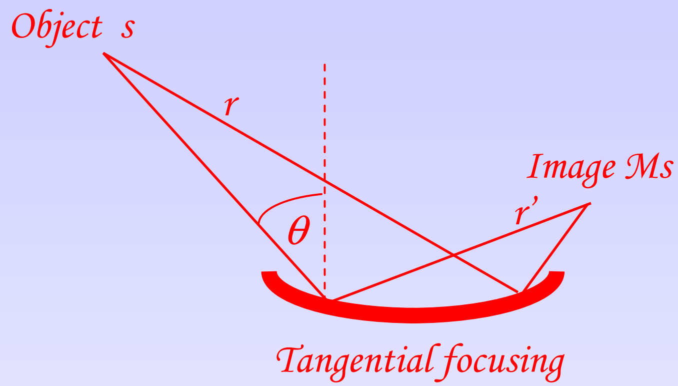
Slope errors enlarge the image formed by specular reflected beam

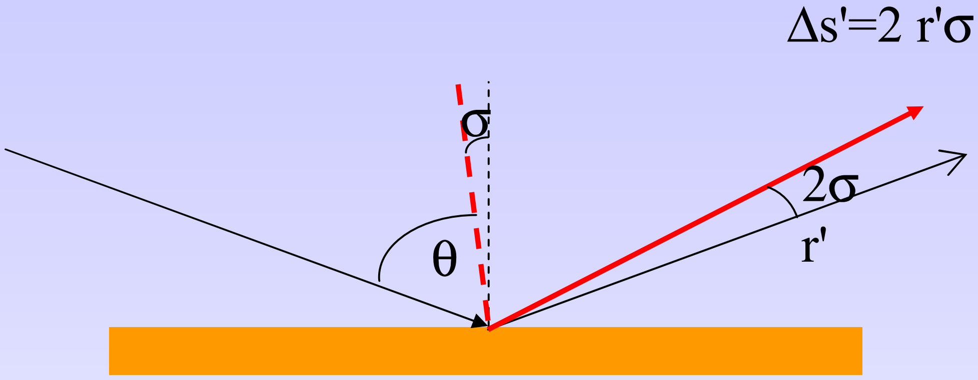
When a ray strikes the surface of a mirror at an incidence angle it is reflected at the same angle:

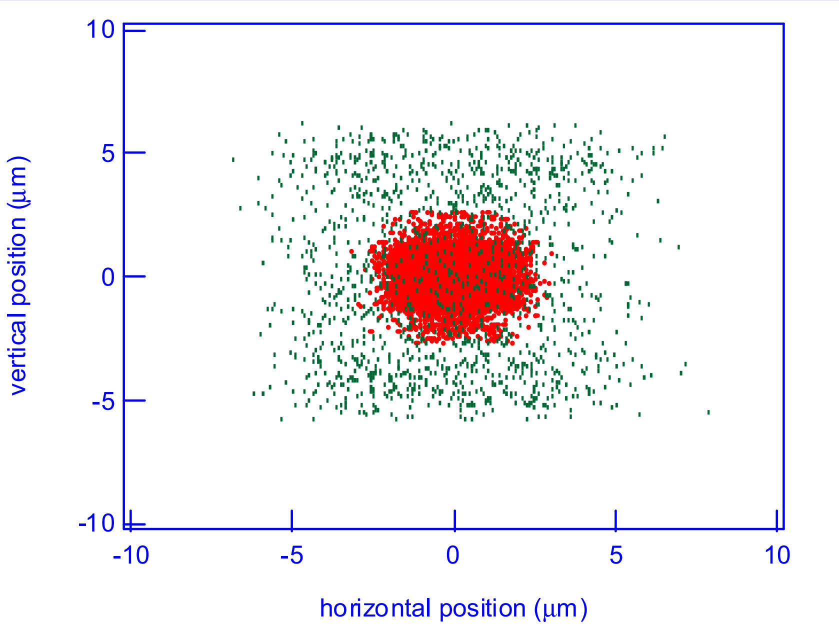


Slope errors locally rotate the direction of the normal to the optical surface
→ rotate the direction of the reflected beam

Meridional slope errors

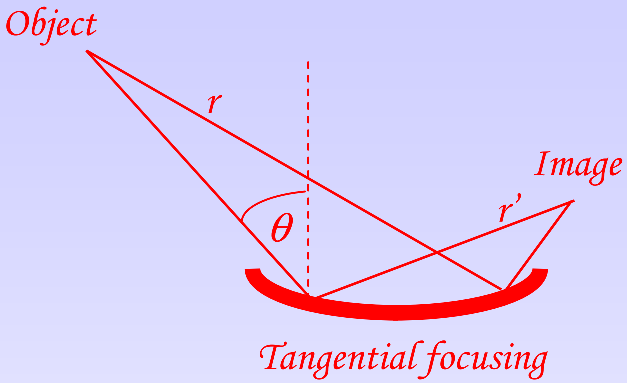


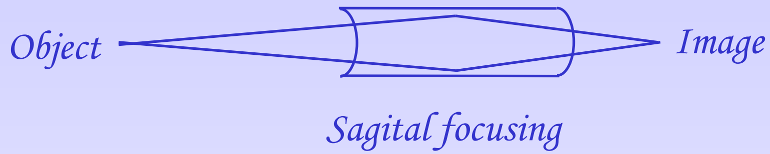


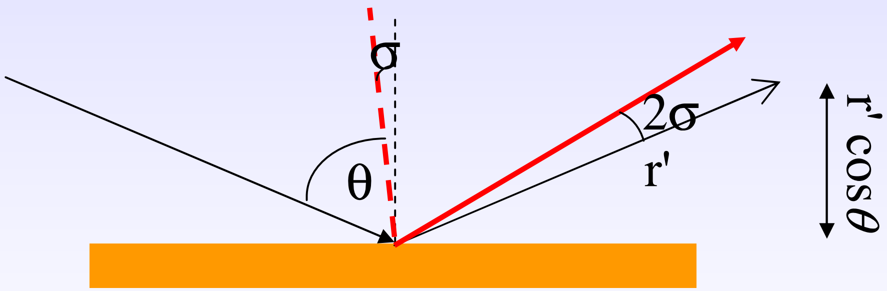


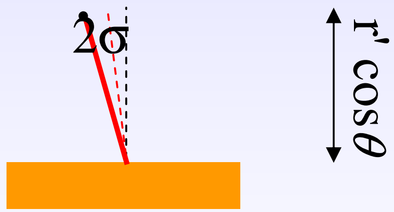
$$s' = \sqrt{(Ms)^2 + (2\, r'\sigma)^2}$$

Meridional and sagittal slope errors









$\Delta s_t' = 2\ r'\sigma$

$\Delta s'_s = 2\ r' \cos\theta\,\sigma$

Significant difference in the effect of meridional and sagittal slope errors:

$\theta = 87° \rightarrow \cos\theta = 0.05 \rightarrow \Delta s_t' = 20\ \Delta s'_s$

References (1)

These notes have been taken from:

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

• 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

• T.Matsushita, H.Hashizume, “X-ray Monochromators”, in “Handbook on Synchrotron Radiation”, Vol.1b, E.-E. Koch, Editor, North Holland, 1983, chapter 4

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

• J.Samson and D.Ederer, “Vacuum Ultraviolet Spectroscopy I and II”, Academic Press, San Diego, 1998

• 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