

A diagram illustrating X-ray optics. It shows a series of parallel lines representing X-ray beams entering from the top left. These beams pass through a series of curved mirrors that reflect and focus them towards the right. The background is dark with some faint light patterns.

X-ray Optics

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Synchrotron Radiation & Free Electron Lasers

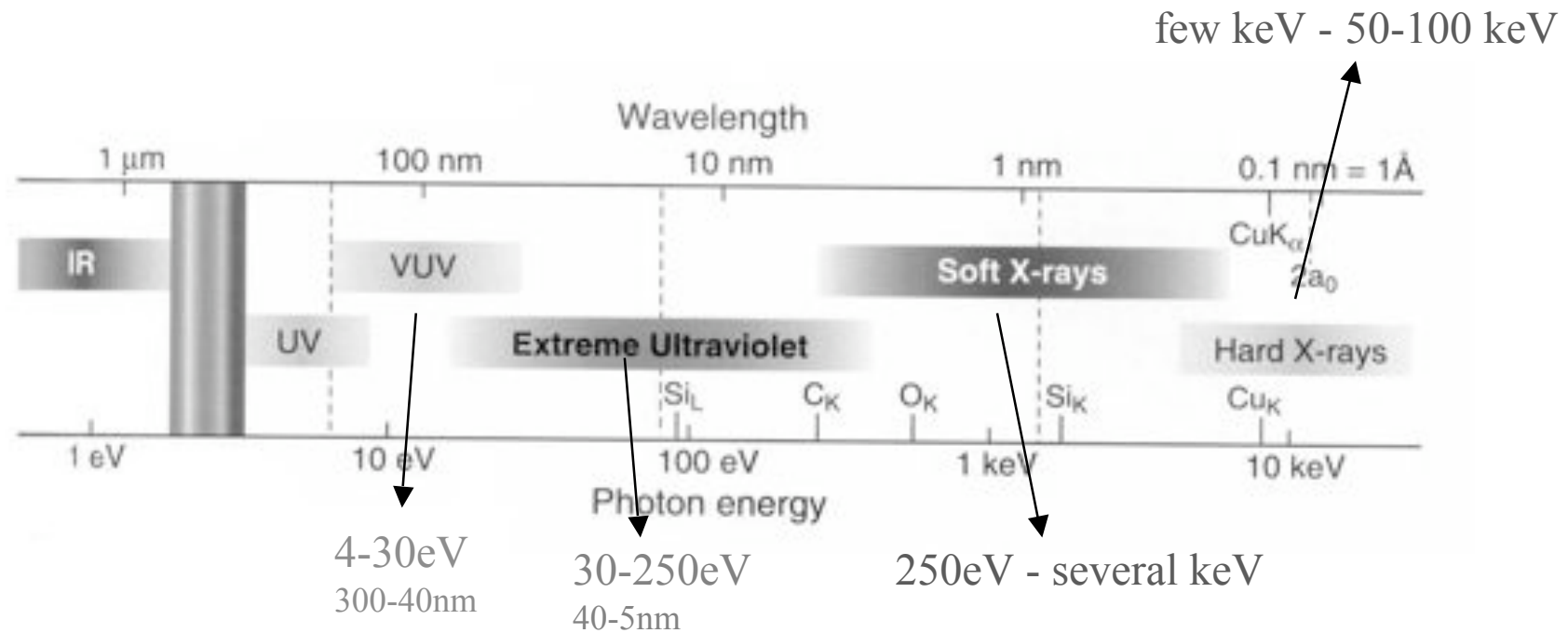
6 - 15 April 2011

Majorana Center for Scientific Culture, Erice, Sicily

Joint US-CERN-
Japan-Russia
School on Particle
Accelerators

A grayscale aerial photograph of a coastline. The foreground shows a body of water, likely the sea. In the middle ground, there is a prominent, rugged mountain range or coastline. The background shows more distant land and possibly other mountains under a clear sky.

Energy regions



These regions are very interesting because they 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.

Refraction Index

refractive index $\mu = 1 - \delta - i\beta$

$$\delta = (e^2 \lambda^2 / 2\pi m c^2) |N + \sum_H N_H [\lambda / \lambda_H]^2 \ln[\lambda_H^2 / \lambda^2 - 1]|$$

δ (unit decrement) related to the speed in the medium

β related to the absorption

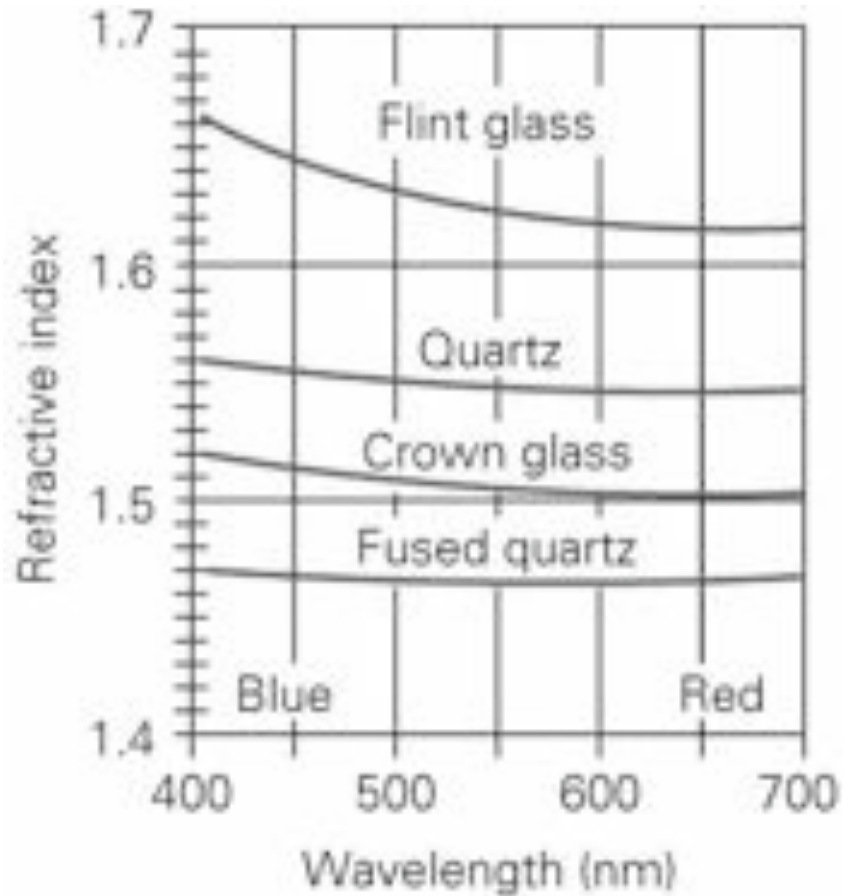
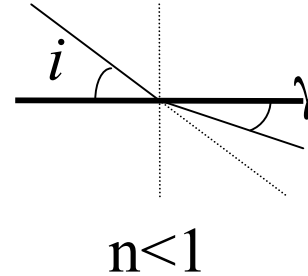
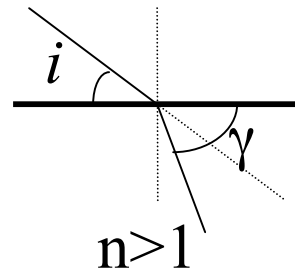
N = electron density (10^{23} - 10^{24} el./cm³)

λ_H = adsorption edge's wavelength

$$\lambda \text{ far from } \lambda_H \Rightarrow \delta = N e^2 \lambda^2 / 2\pi m c^2$$

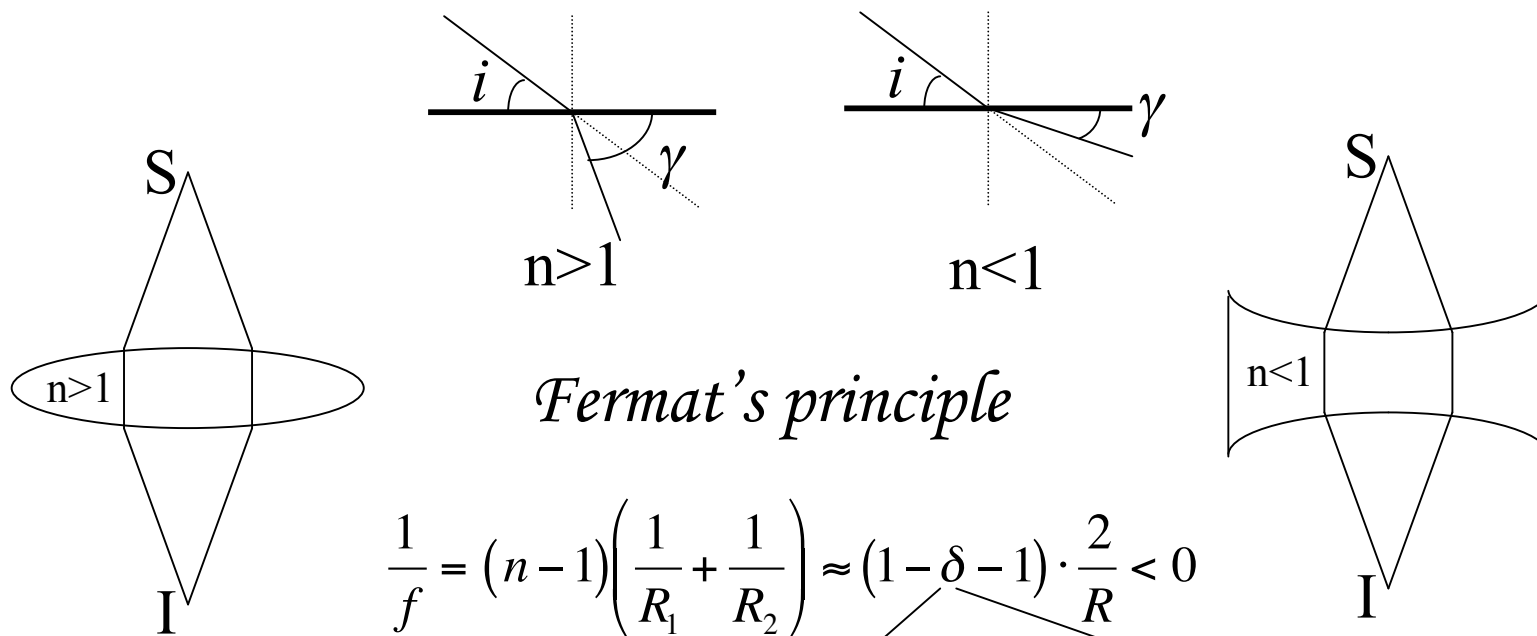
$$\beta = \lambda \mu_1 / 4\pi \quad \mu_1 = \text{linear absorption coefficient}$$

Snell Law



Snell's law: $n_1 \cos \gamma = n_2 \cos i$

Snell Law



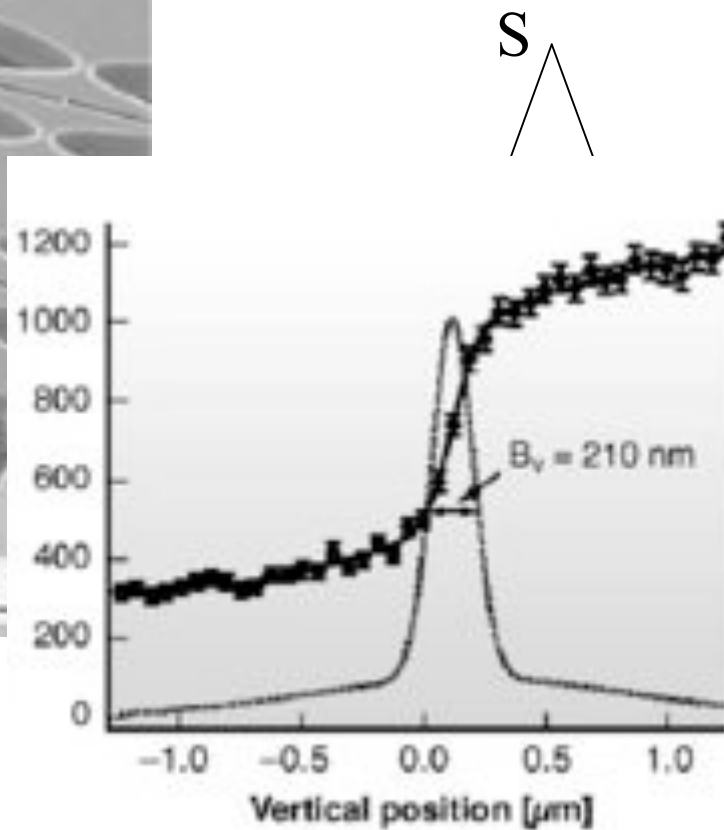
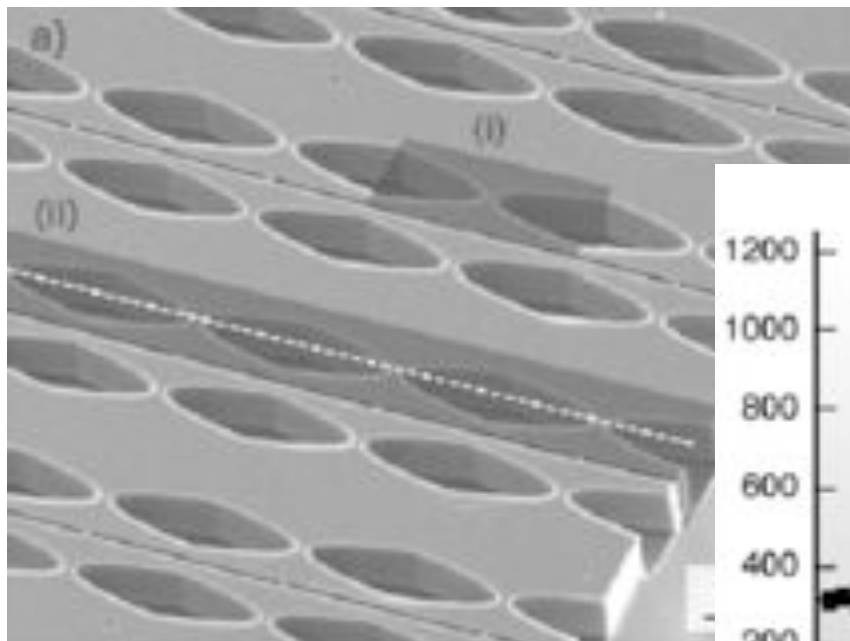
Fermat's principle

$$\frac{1}{f} = (n - 1) \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \approx (1 - \delta - 1) \cdot \frac{2}{R} < 0$$

$$\delta = \frac{Ne^2 \lambda^2}{2\pi mc^2} \approx 10^{-2} - 10^{-4}$$

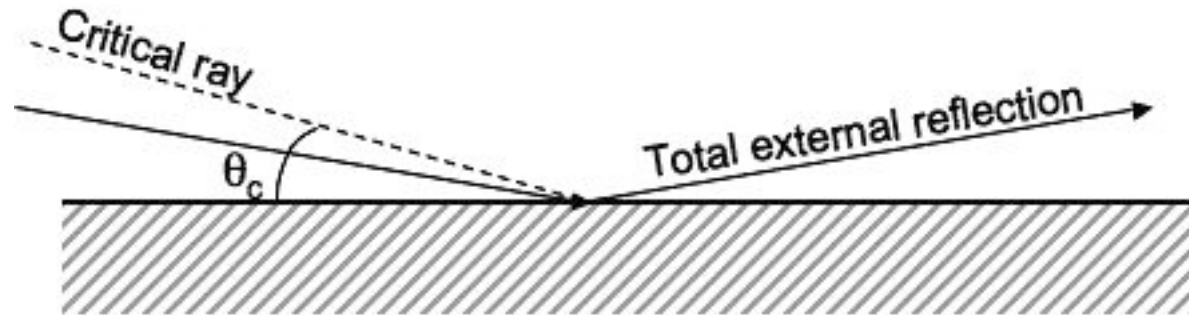
$$\delta \approx 10^{-4} \quad HXR \Rightarrow f \approx 1m \quad \text{if} \quad R \approx 1mm$$

X-ray Lenses



$$\delta \approx 10^{-4} \quad \text{HXR} \Rightarrow f \approx 1\text{m} \quad \text{if} \quad R \approx 1\text{mm}$$

Snell law - Total external reflection



Snell's law: $\cos\gamma = \cos i/n$

$$\gamma = 0 \quad n = \cos i_c$$

i_c critical angle: total external reflection

$$\sin i_c = \lambda (e^2 N / \pi m c^2)^{1/2}$$

$$\lambda_c(\text{min}) = 3.333 \cdot 10^{-13} N^{-1/2} \sin i_c$$

shorter wavelength needs smaller angles of incidence

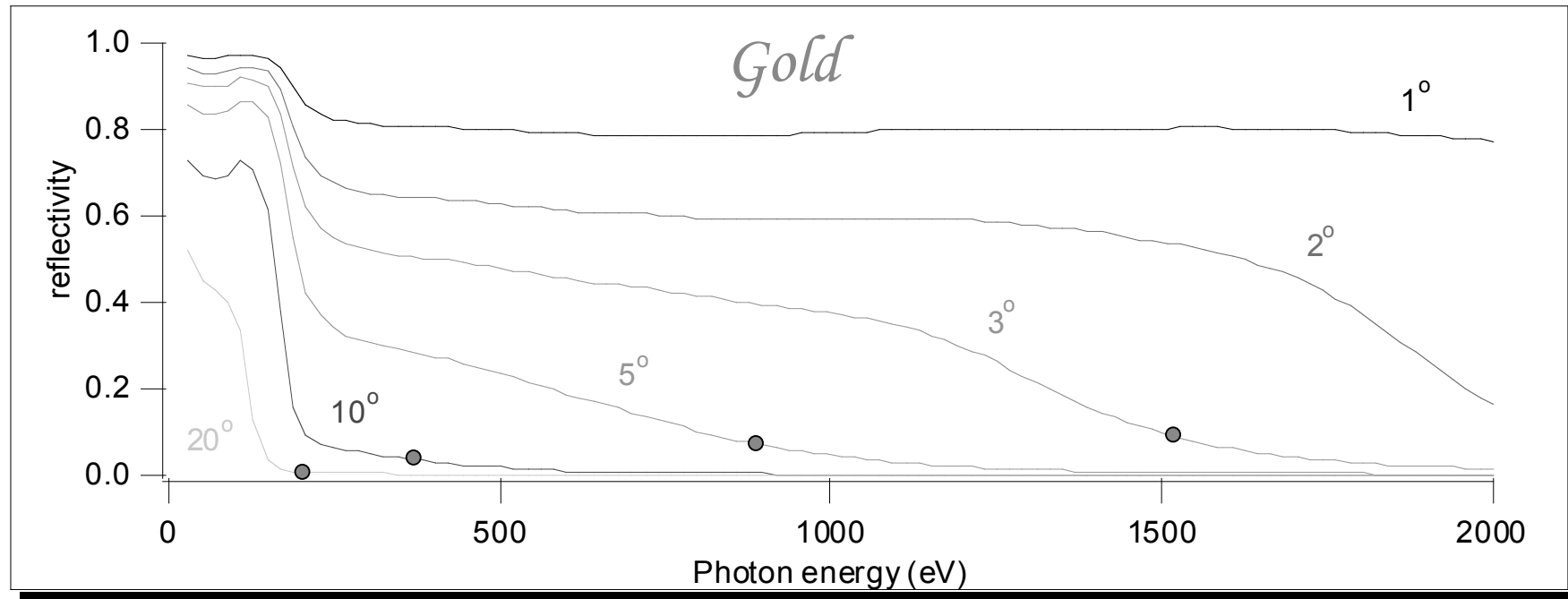
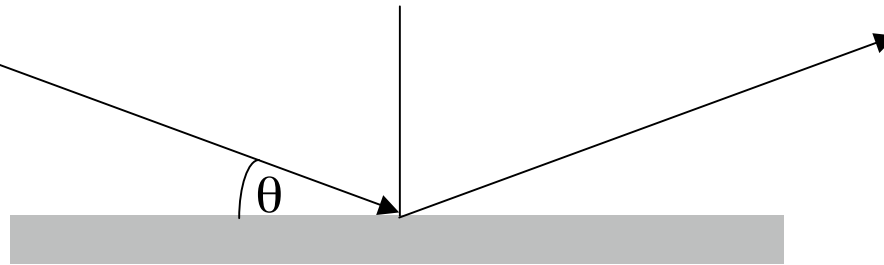
Materials with higher density (i.e. higher atomic weight) have higher reflectivity

Material	Density (g/cm ³)	N (electron/cm ³)	λ_{min} nm
Pentadecane (oil)	0.77	7×10^{22}	$64.1 \sin i$
Glass	2.6	78×10^{22}	$37.9 \sin i$
Aluminum oxide	3.9	115×10^{22}	$31.2 \sin i$
Gold	19.3	466×10^{22}	$15.4 \sin i$

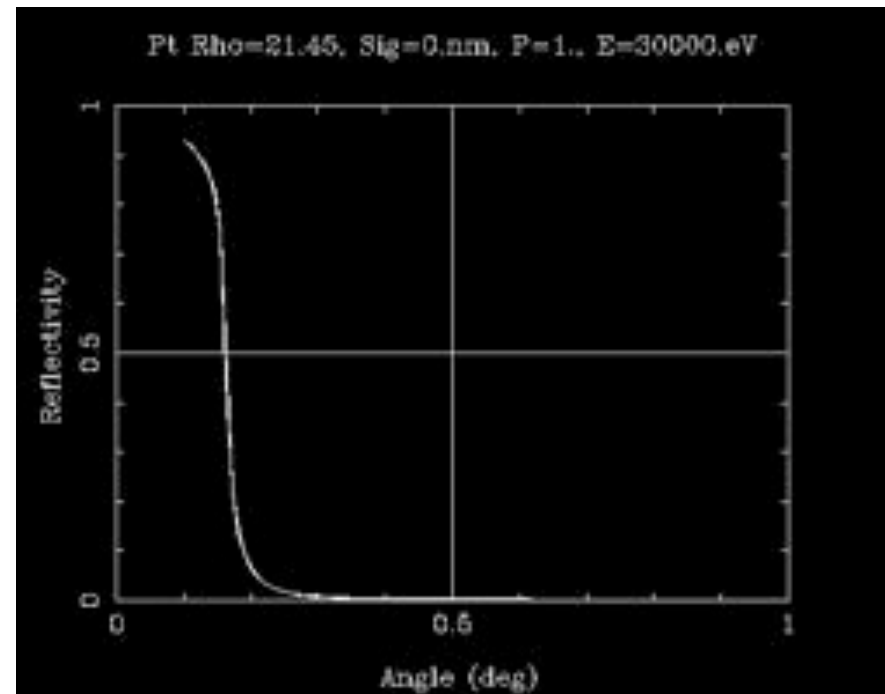
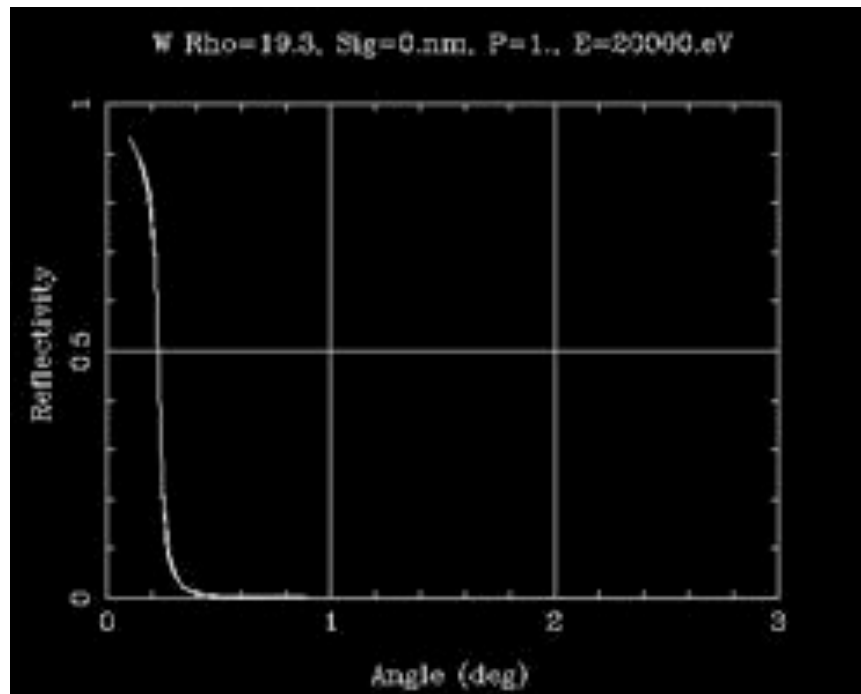
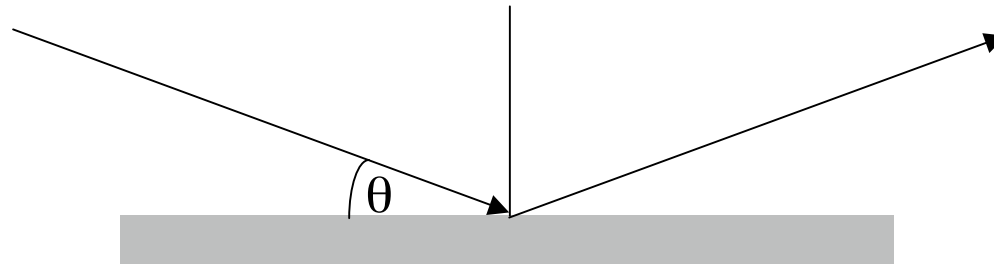
$$i = 5^\circ: \quad \lambda_{\text{min}} \text{glass} = 3.3 \text{ nm} = 375 \text{ eV}$$

$$\lambda_{\text{min}} \text{gold} = 1.34 \text{ nm} = 923 \text{ eV}$$

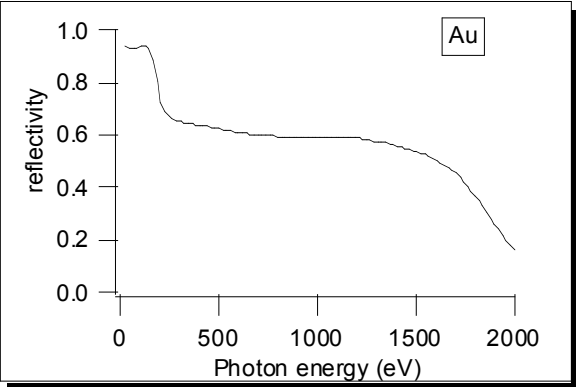
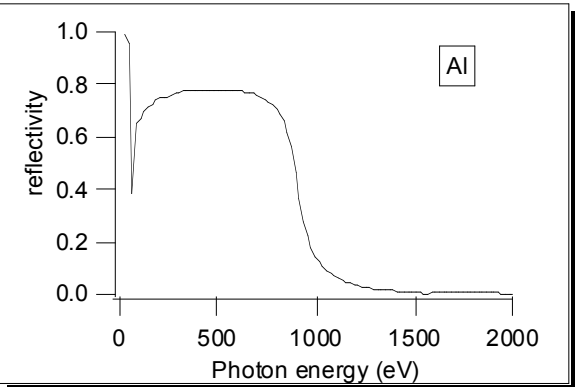
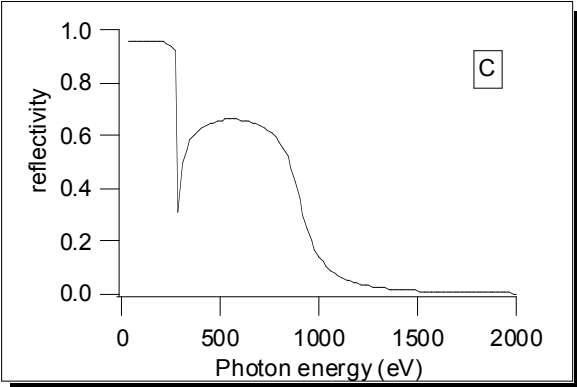
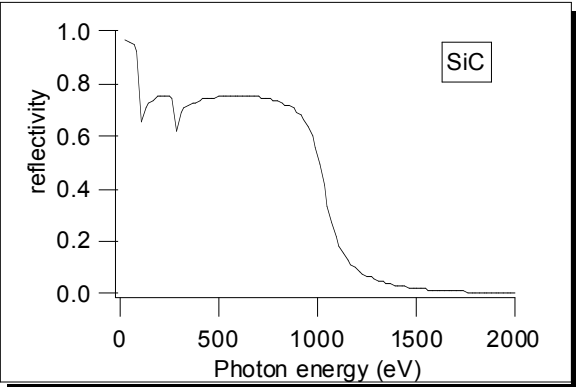
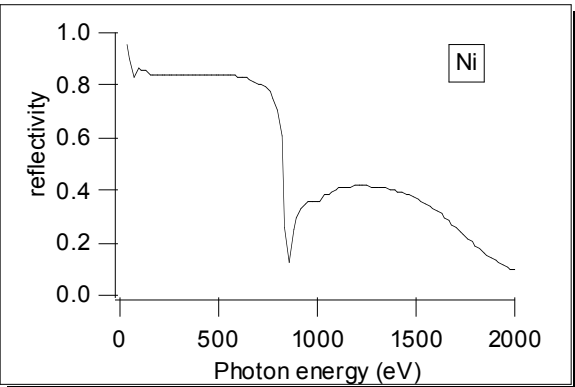
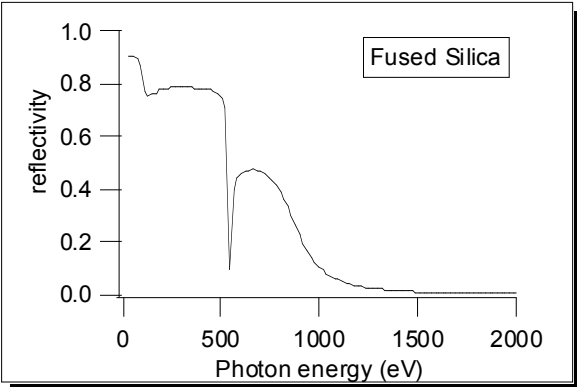
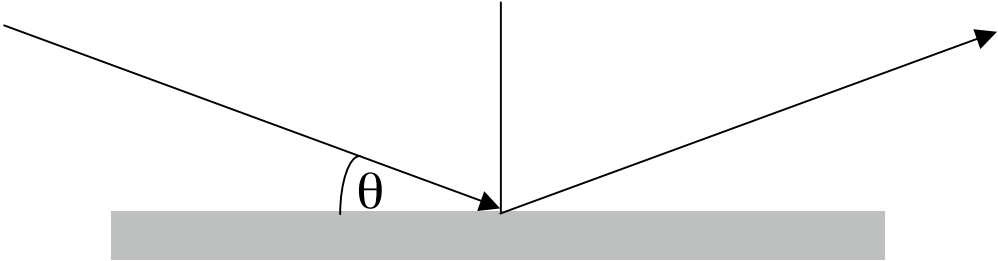
Grazing incidence mirror reflectivity



Hard X-ray reflectivity



Other coatings



Effect of Defects (slope errors)

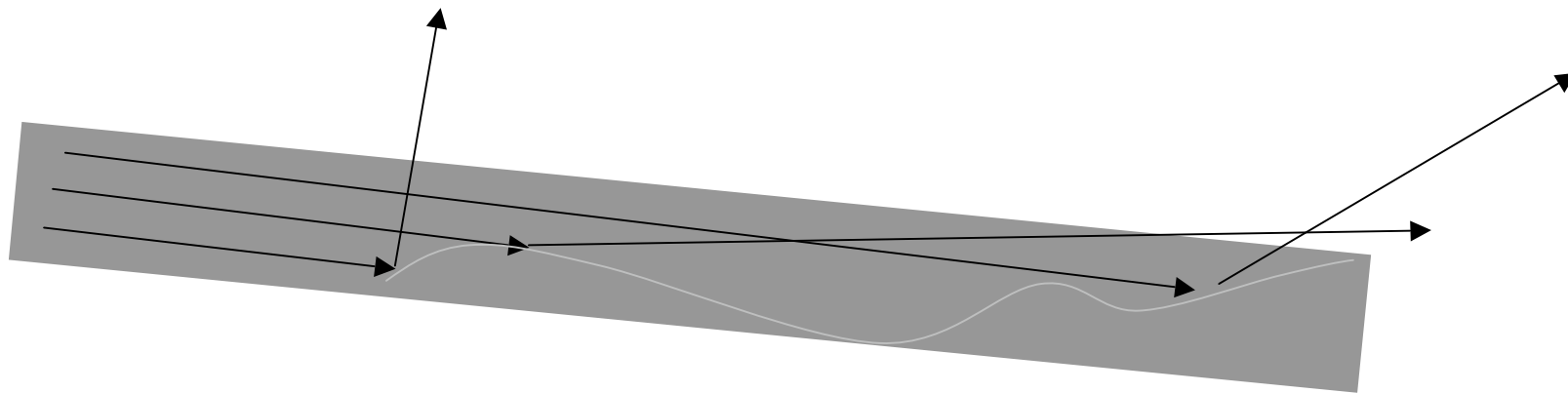
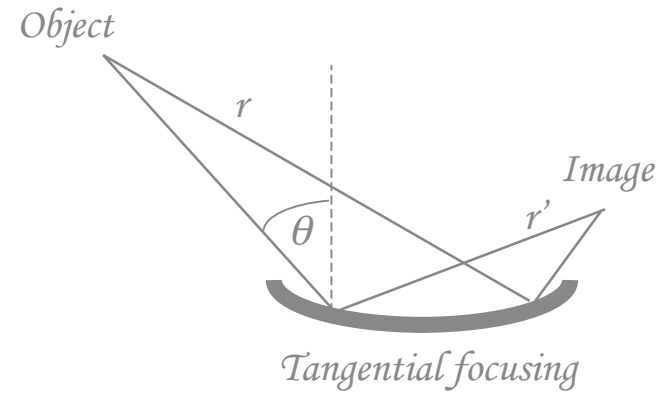
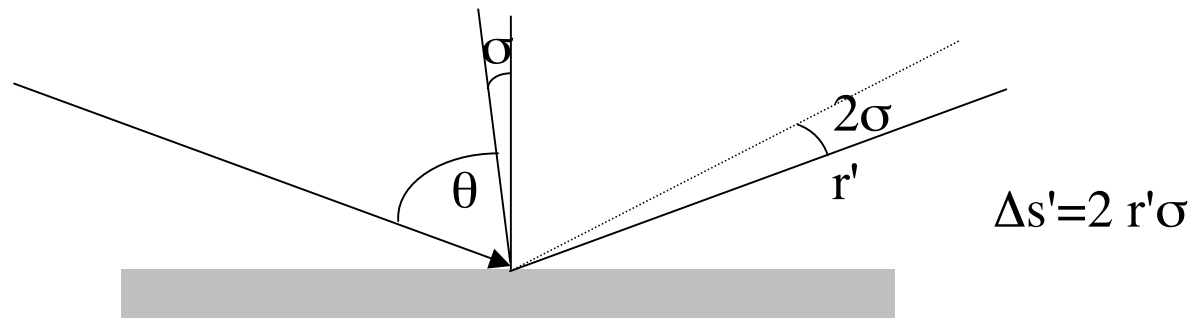
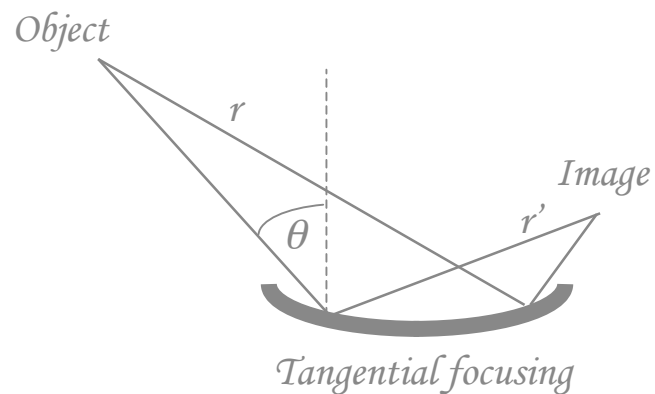
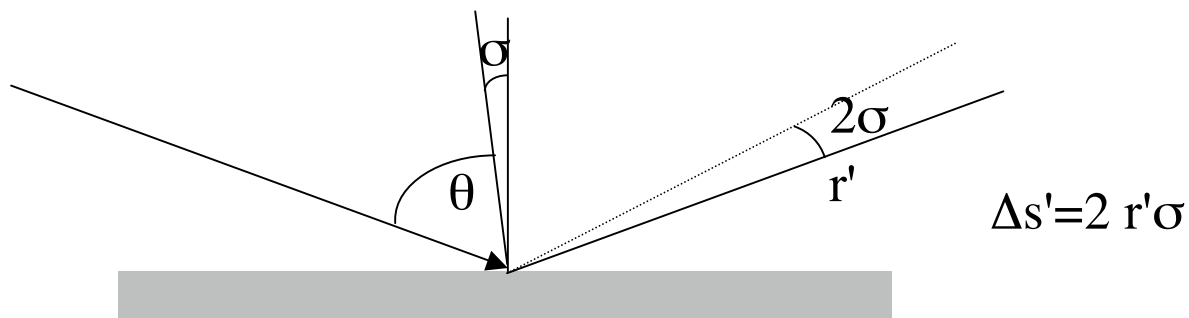


Image (spot) enlargement



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

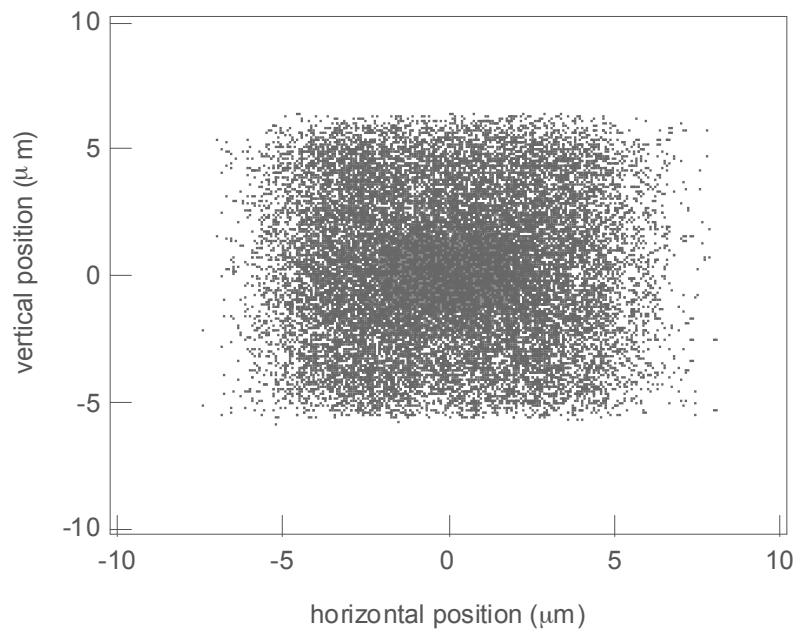


Image (spot) enlargement

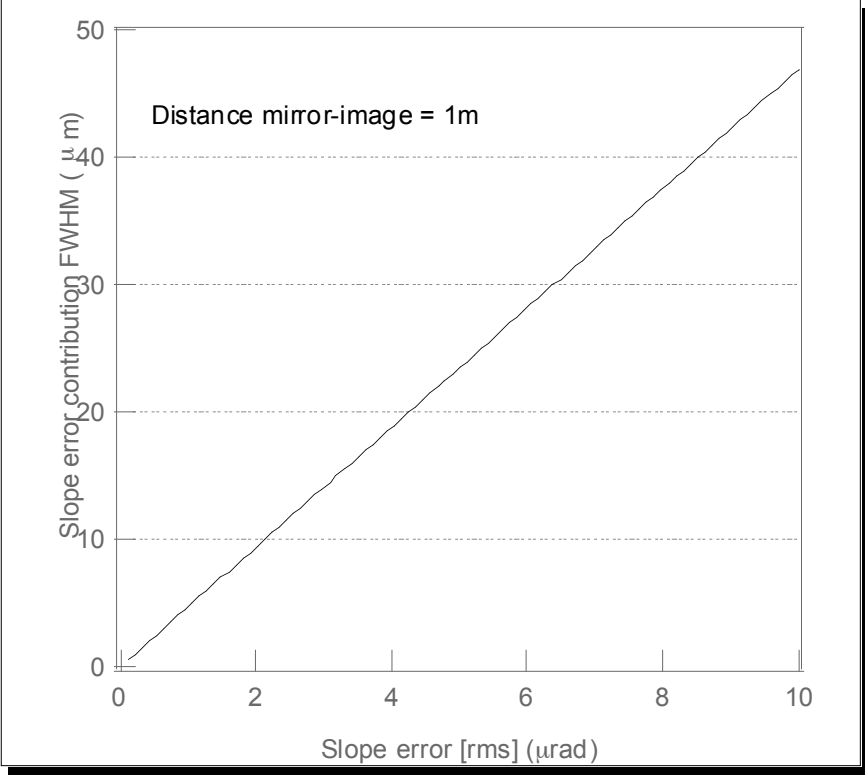
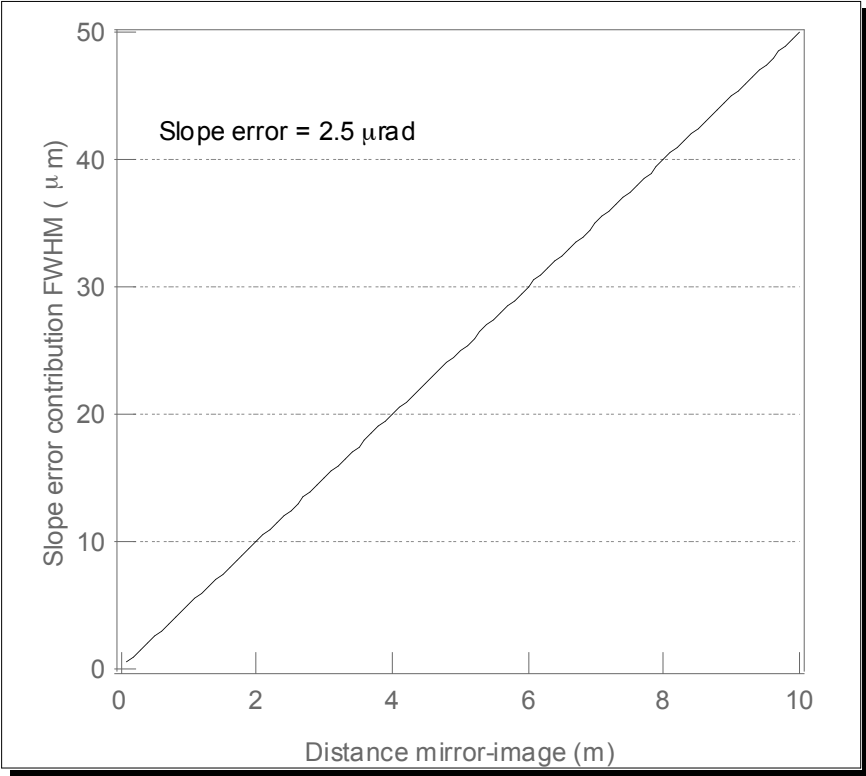
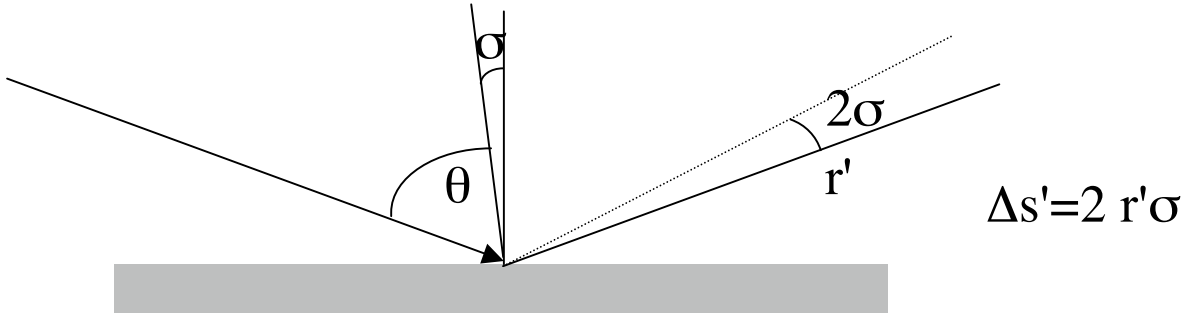
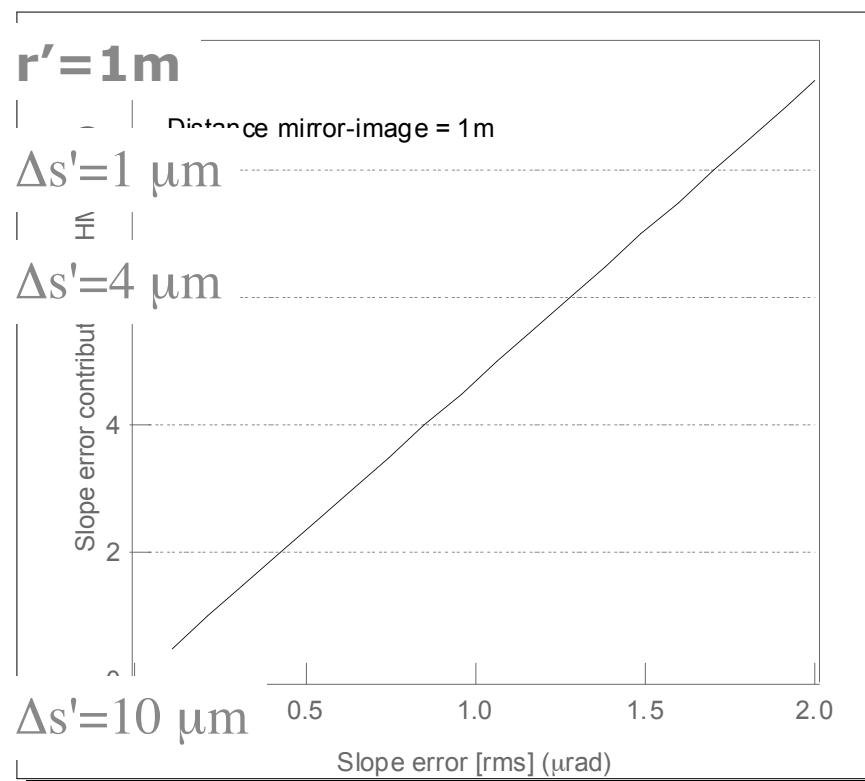


Image (spot) enlargement

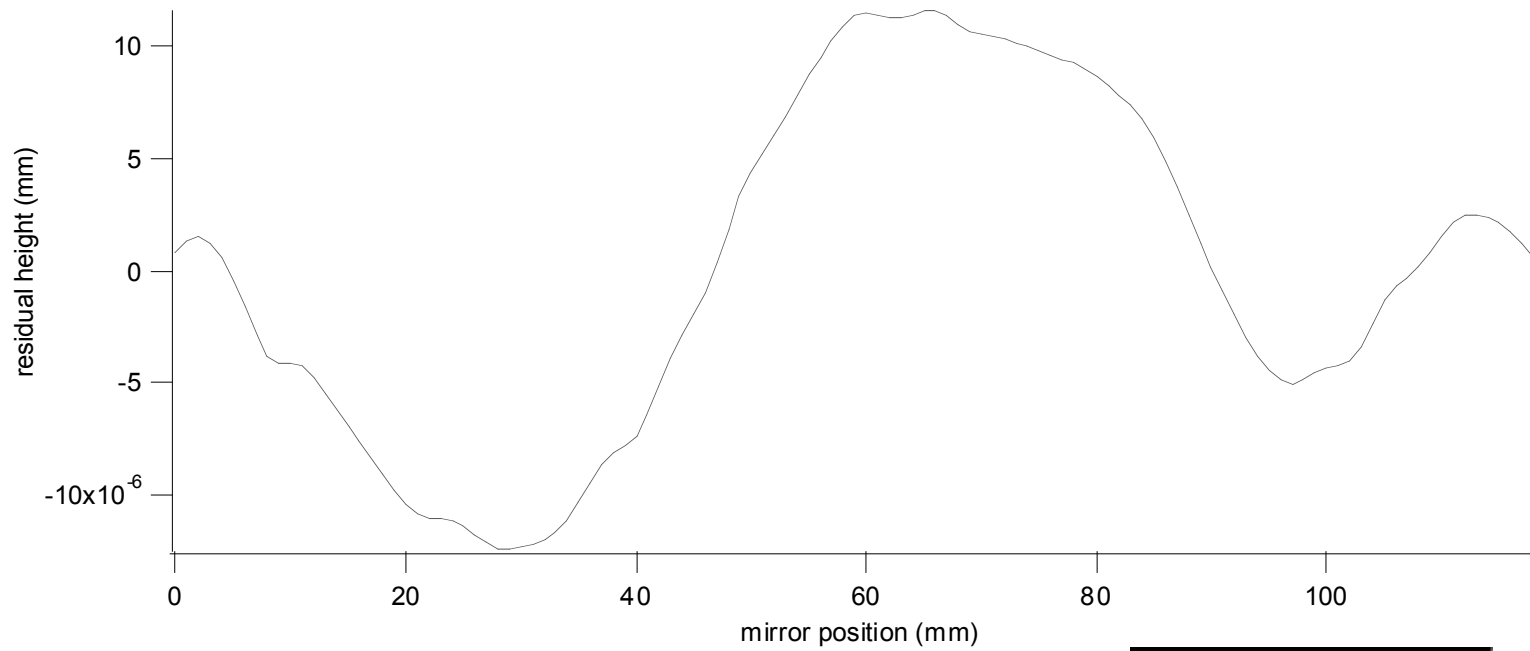
Typical manufacturer capabilities (SESO, ZEISS, Winlight, Jobin Yvon)

Shape	Length	rms errors
Spherical/flat	Up to 500 mm	< 0.5 μrad
Spherical/flat	> 500 mm	1 μrad
Toroidal	Up to 500 mm	$\geq 1 \mu\text{rad}$
Toroidal	> 500 mm	$\geq 1\text{-}2 \mu\text{rad}$
Aspherical	Up to 500 mm	$\geq 1\text{-}2 \mu\text{rad}$
Aspherical	> 500 mm	$\geq 2 \mu\text{rad}$

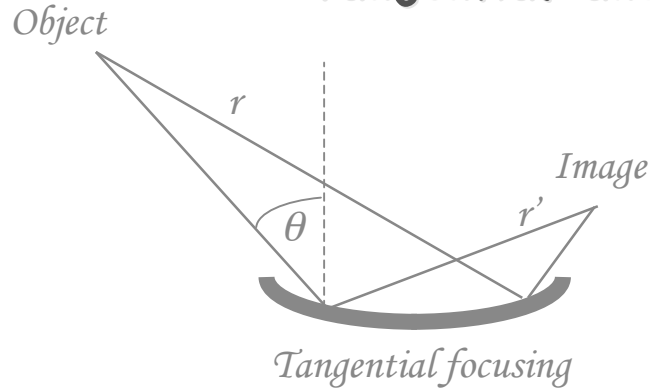


Mirror profile precision

Typical manufacturer capabilities (SESO, ZEISS, Winlight, Jobin Yvon)



Tangential and Sagittal focusing geometries



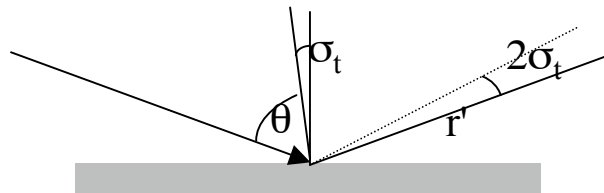
Term F_{20} of the optical path function

$$(1/r + 1/r') \cos \theta / 2 = 1/\mathcal{R} \quad \text{spherical mirror}$$



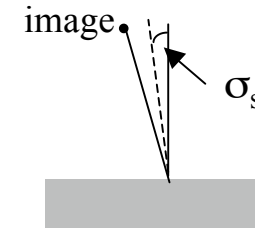
Term F_{02} of the optical path function

$$(1/r + 1/r') / (2 \cos \theta) = 1/\mathcal{R} \quad \text{cylindrical/toroidal mirror}$$

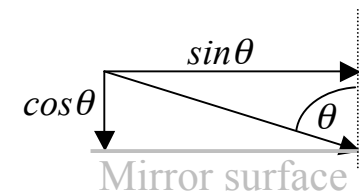


$$\Delta s'_t = 2 r' \sigma_t$$

t

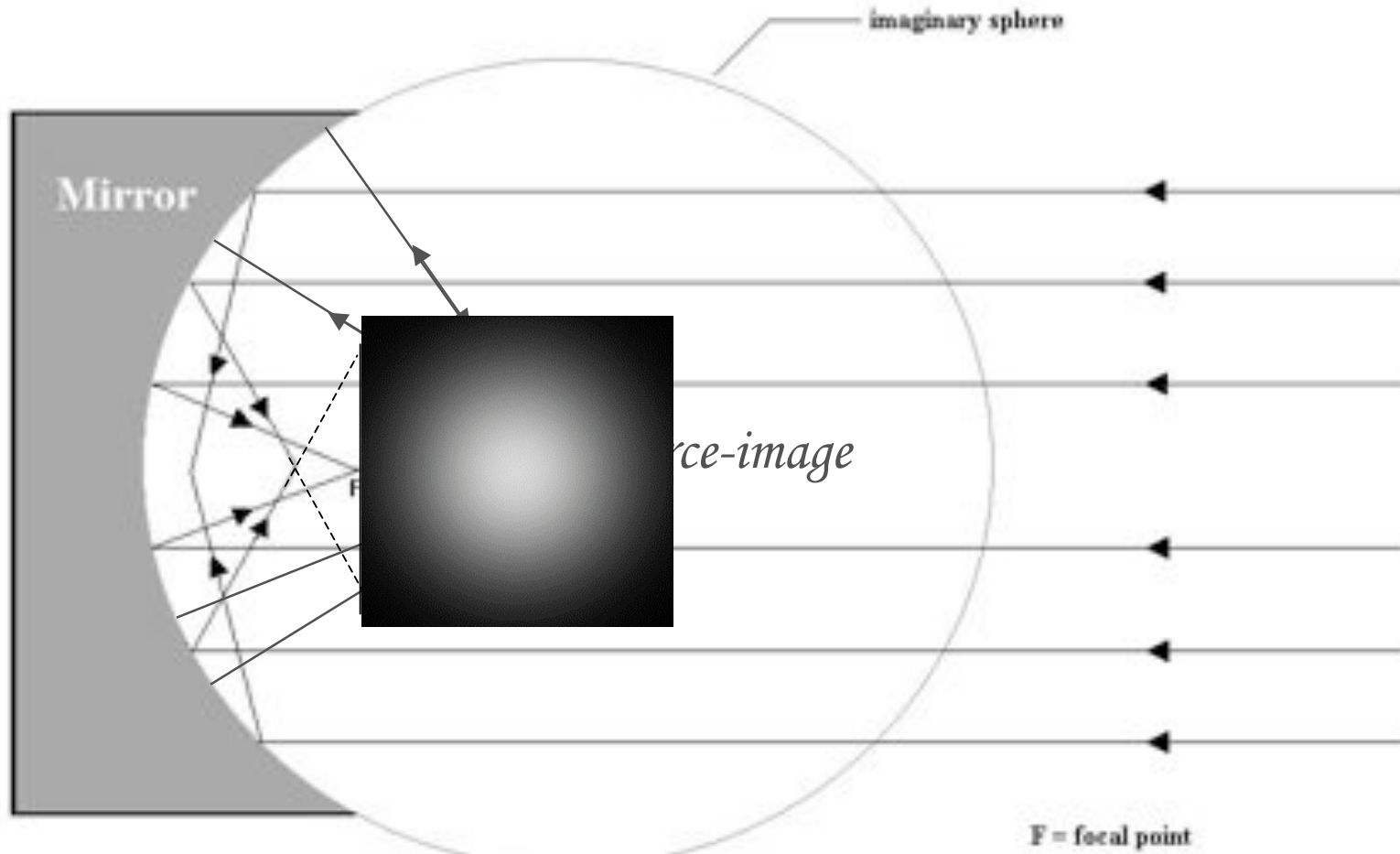


$$\Delta s'_s = 2 r' \cos \theta \sigma_s$$



Aberrations

Solution: work in 1:1 configuration



Spherical mirror suffer of spherical aberration

Deviations from perfect imaging are called aberrations

Torodial mirror

The bicycle tyre toroid is generated by rotating a circle of radius ρ in an arc of radius R . In general, two non-coincident focii are produced: one in the meridional plane and one in the sagittal plane

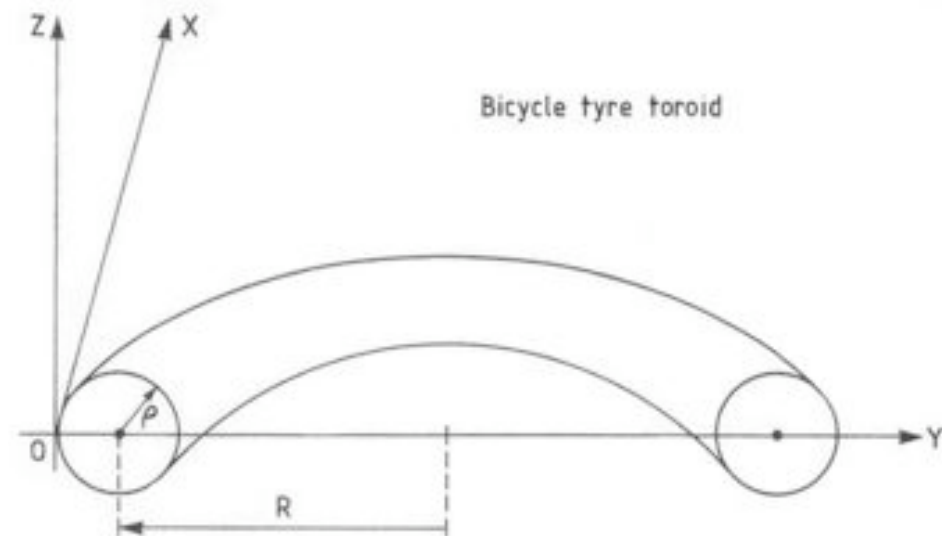
Tangential focus:

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

Sagittal focus:

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

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



Toroidal mirror focal properties

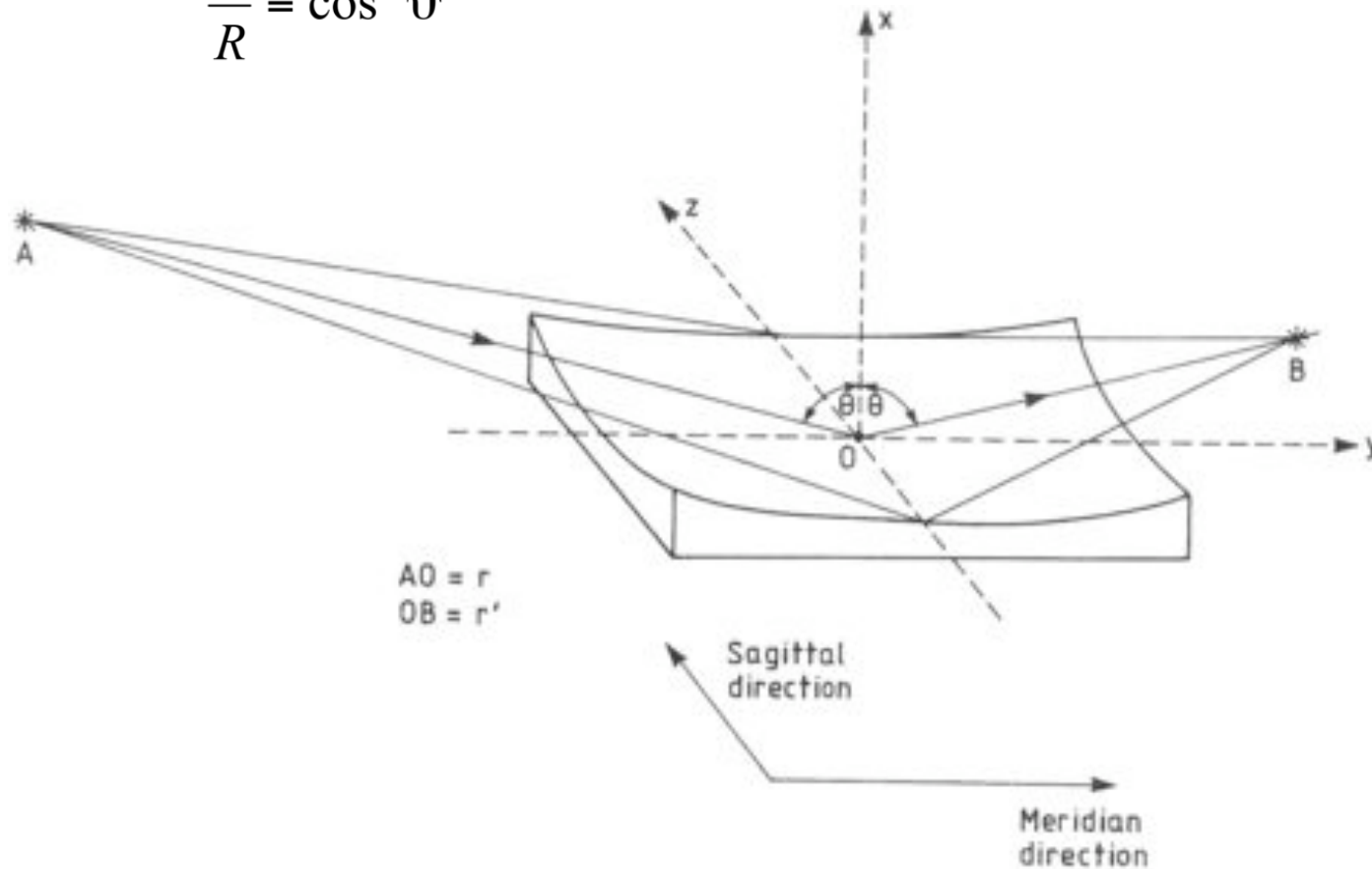
Tangential focus:

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

Sagittal focus:

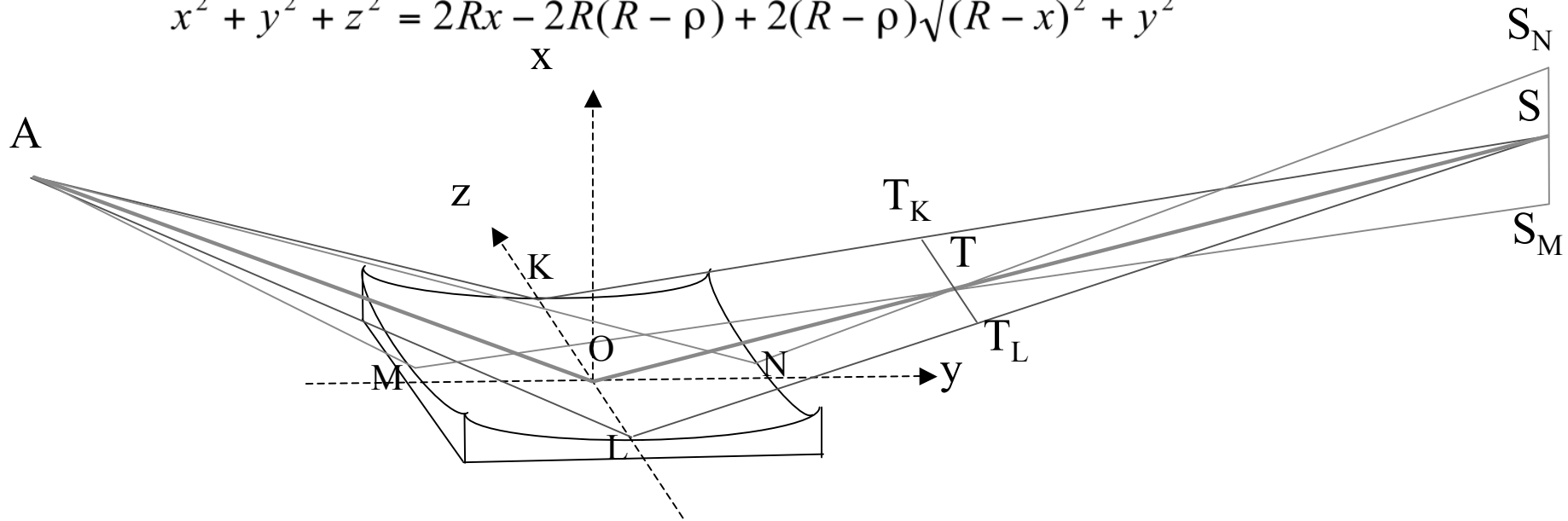
$$\left(\frac{1}{r} + \frac{1}{r'}\right) \frac{1}{2 \cos \vartheta} = \frac{1}{\rho}$$

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



Toroidal mirror focal properties

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

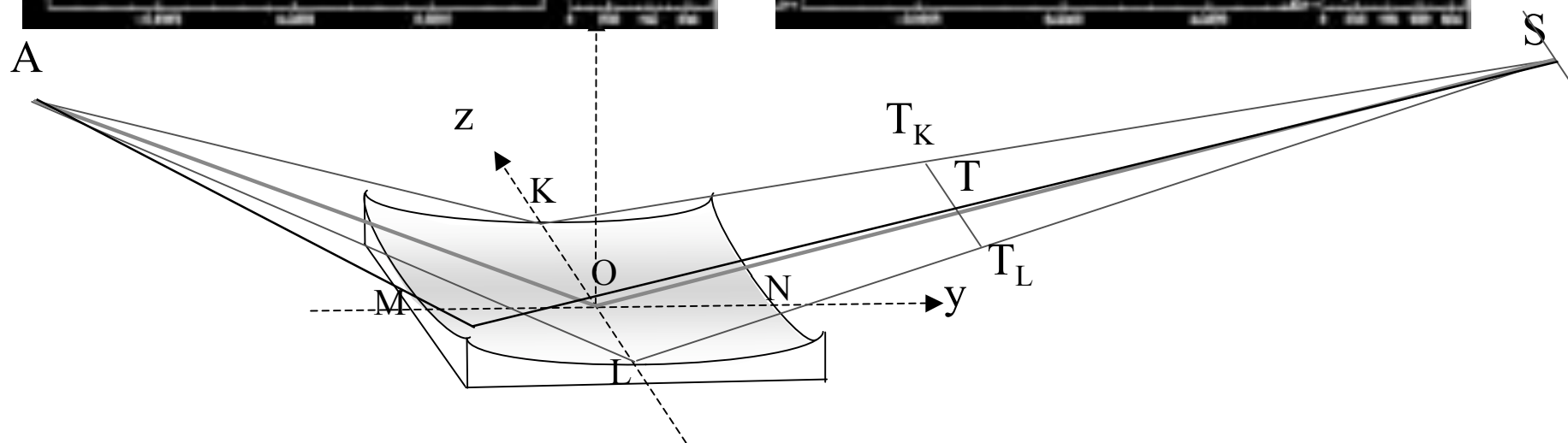
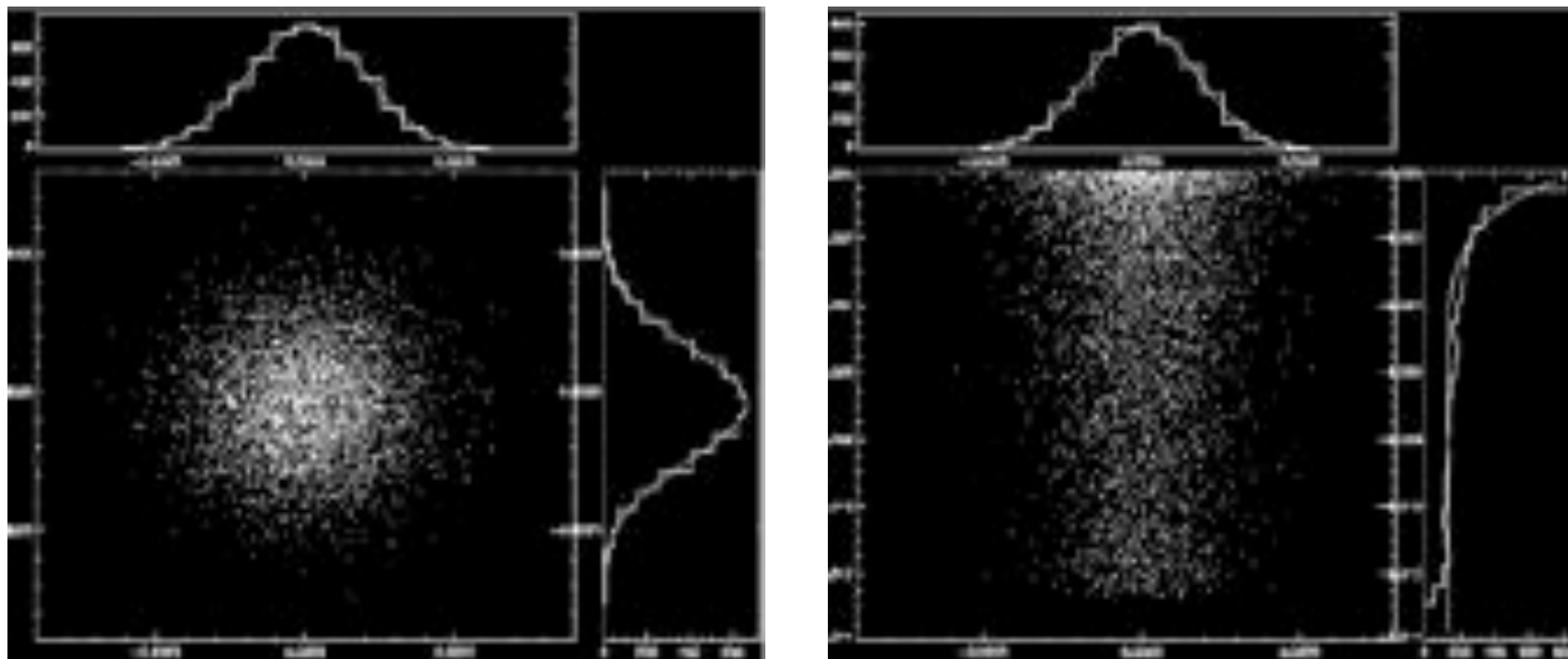


For $\rho=R \rightarrow$ spherical mirror

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 focusses in the sagittal direction.

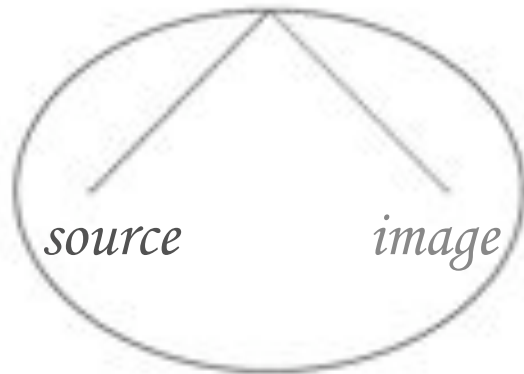
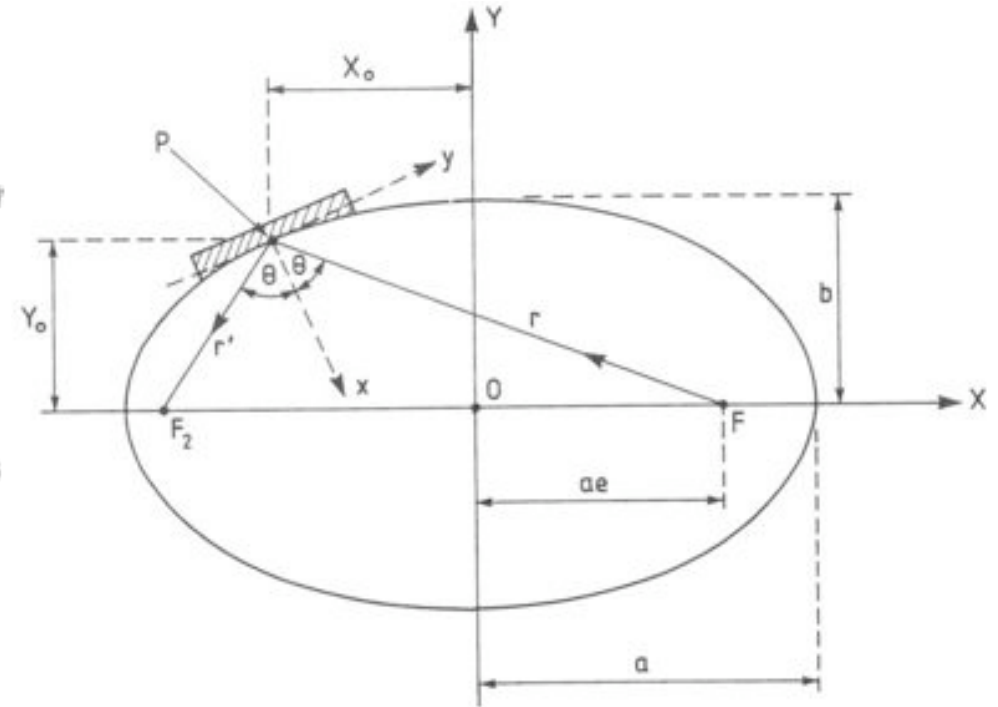
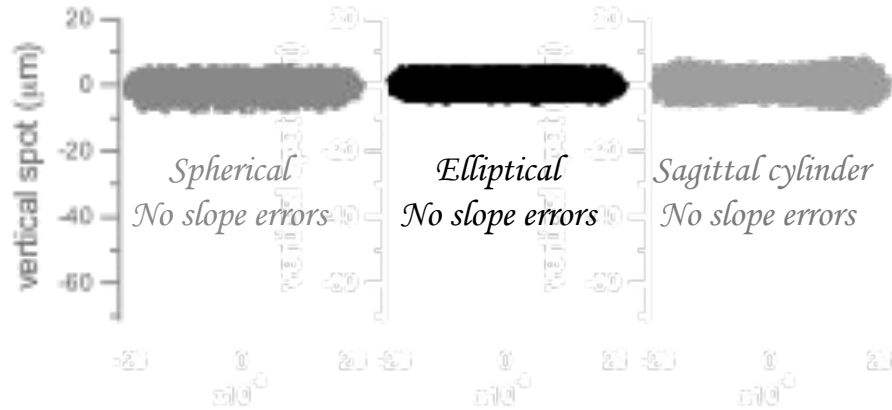
Toroidal mirror Tangential and Sagittal focus



Other focusing geometries

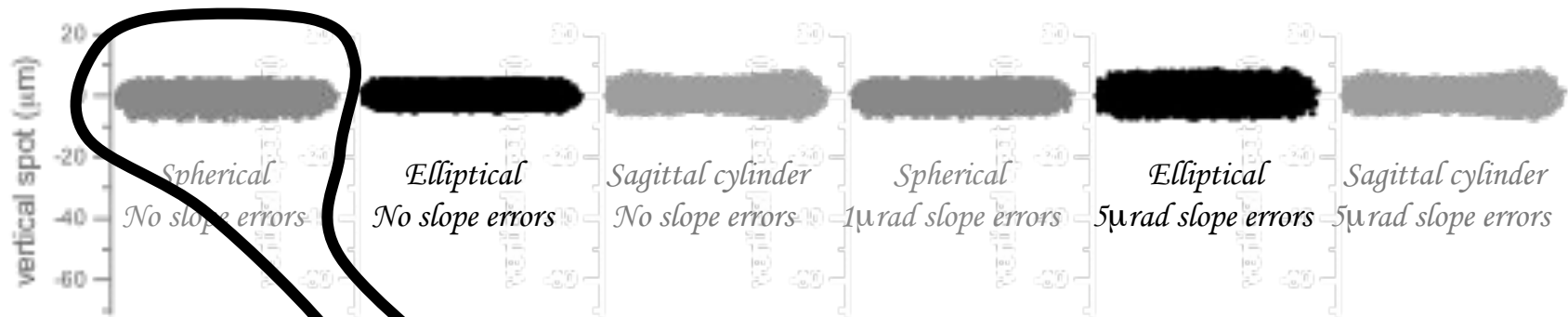
source $80 \mu\text{m}$ vertical; $r=4000 \text{ mm}$ $r'=400 \text{ mm}$ (10:1) $\theta=88^\circ$

Beam divergence $100 \times 100 \mu\text{rad}$

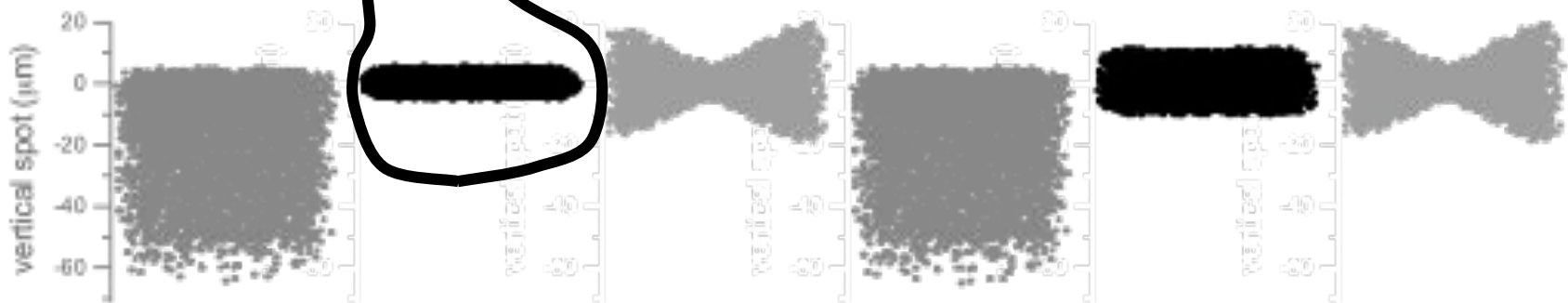


In search of the perfect focusing geometry

Beam divergence $100 \times 100 \mu\text{rad}$



Beam divergence $500 \times 500 \mu\text{rad}$



Spherical mirrors are good for small demagnification and/or small divergence
Elliptical mirrors are better for very large demagnifications and larger divergence but..

the slope errors have to be small

Toroidal / parabolic mirrors are perfect if the induced aberration are acceptable

Paraboloids

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

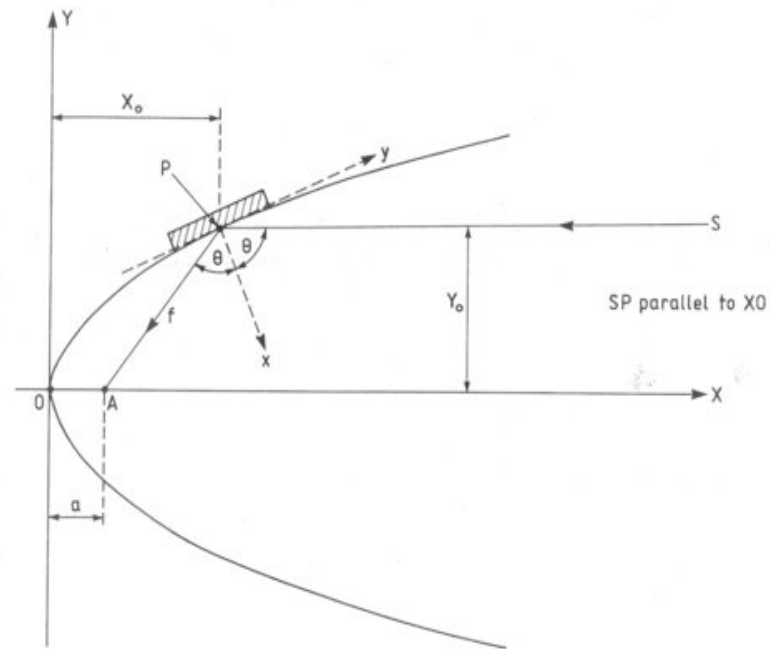
Position of the pole P:

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

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

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

D. Cocco *X-Ray optics*, Erice, 6-15 April 2011

Other mirror defect - Roughness

Slope errors = every deviation from the ideal surface with period larger than $\sim 1,2$ mm

Typical definition is μrad or arcsec rms.

*Alternative definition is $\lambda/10$ or $\lambda/20$ and so on... P-V or rms
used for normal incidence mirror or "poorer" quality mirrors*

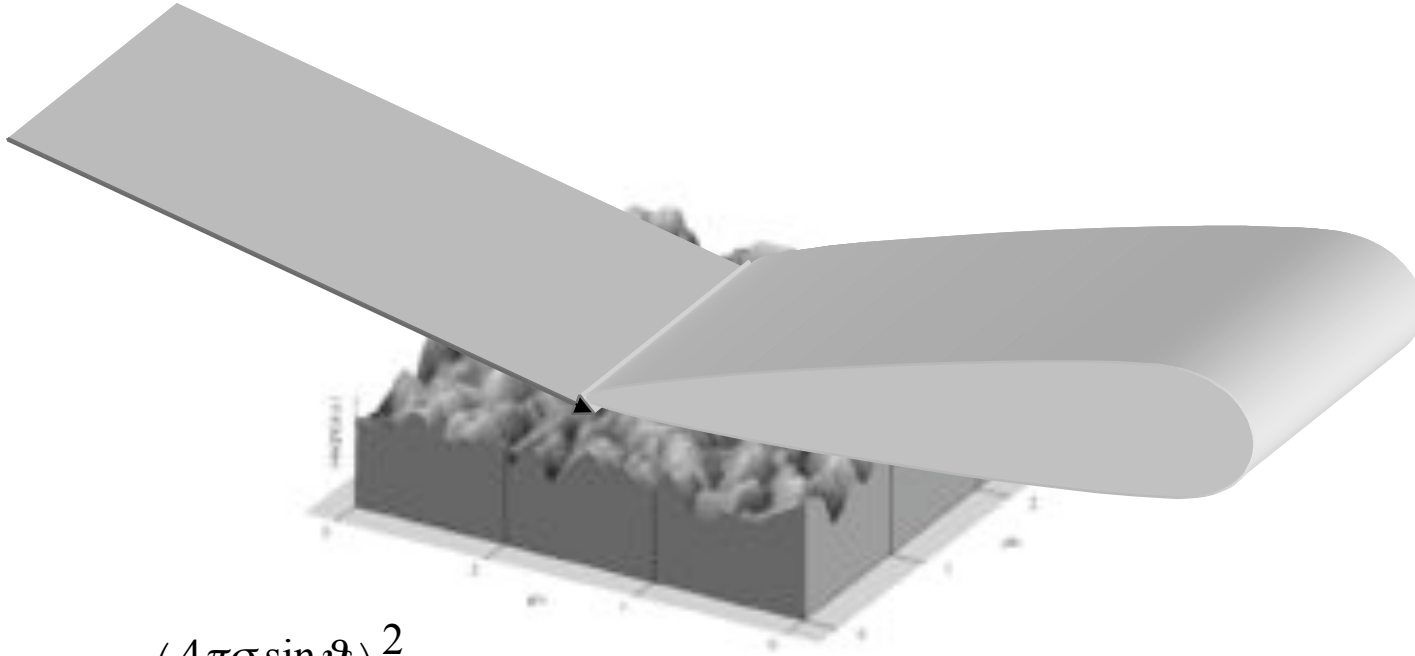
Roughness = every deviation from the ideal surface with period smaller than $\sim 0.5-1$ mm

Typical definition is \AA rms.

*Alternative definition is surface quality 20-10 or 10-5 (scratch-dig)
used for normal incidence mirror or "poorer" quality mirrors*

*A dig is nearly equal in terms of its length and width. A scratch could be much longer than width
20-10 means 20/1000 of mm max scratch width 10/100 mm max dig dimension*

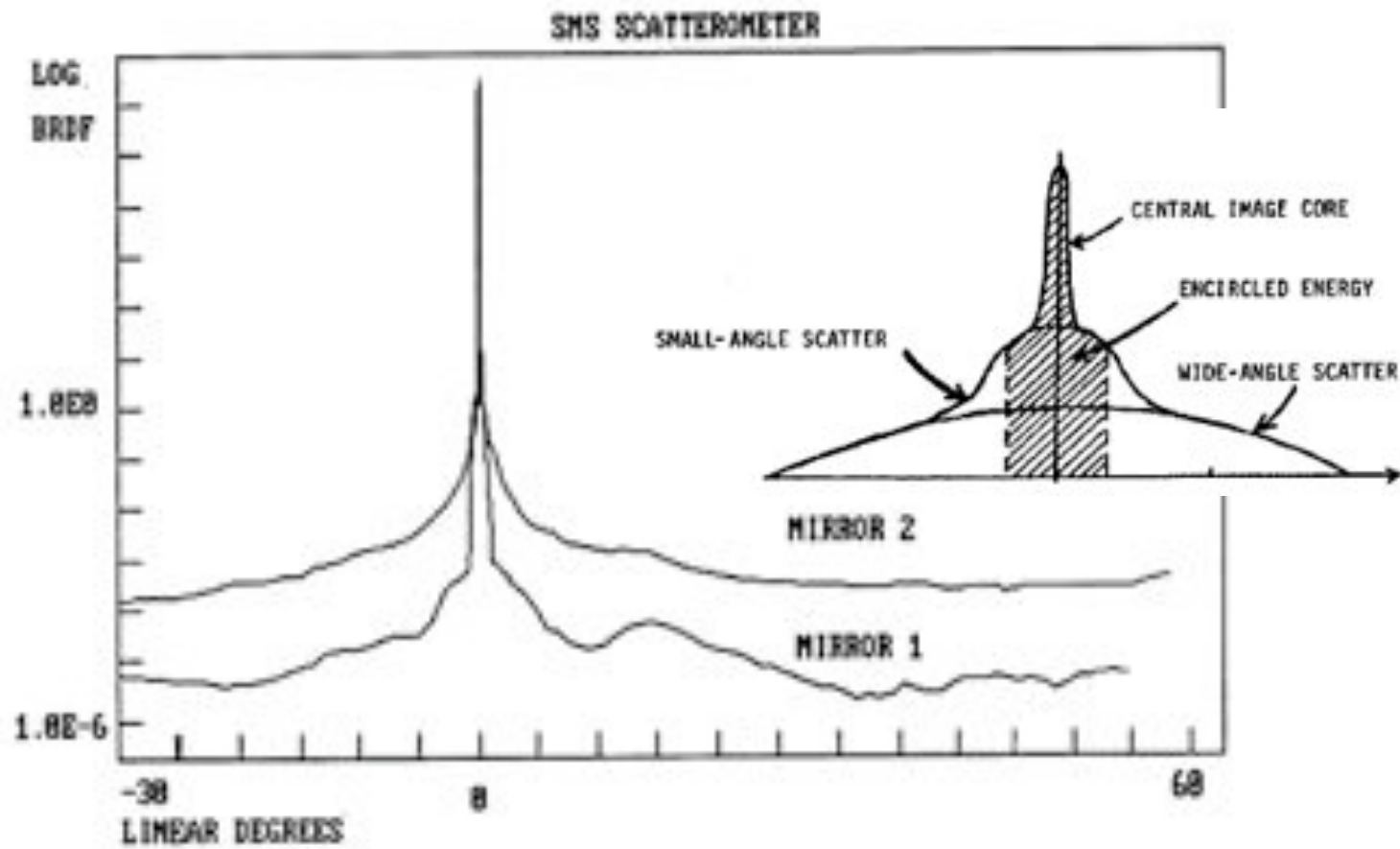
Roughness



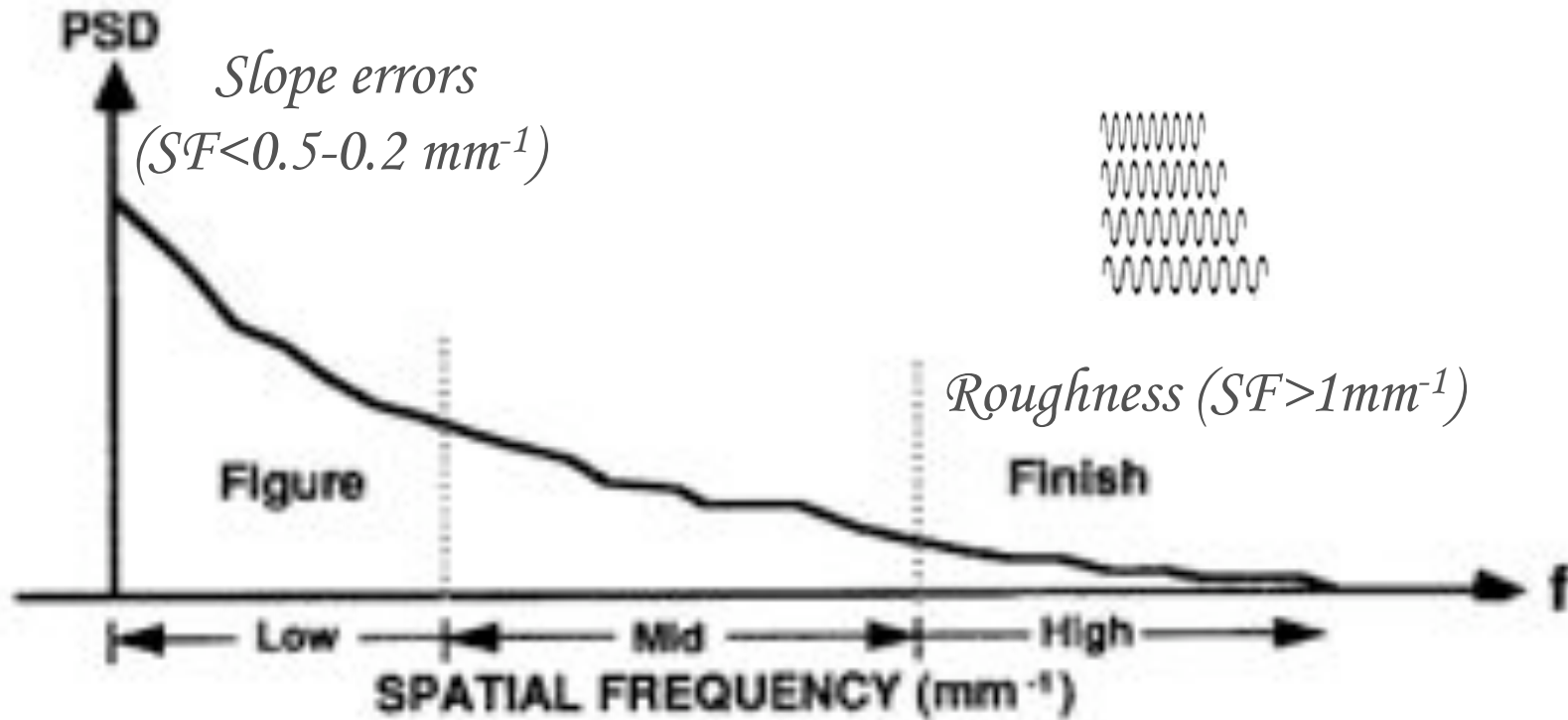
$$I = I_0 e^{-\left(\frac{4\pi\sigma \sin \vartheta}{\lambda}\right)^2}$$

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

Roughness



Power spectral density



Roughness



Mode: PSI
Mag: 20.5 X

3-Dimensional Display

Date: 01/24/97
Time: 14:11:49

Surface Statistics:

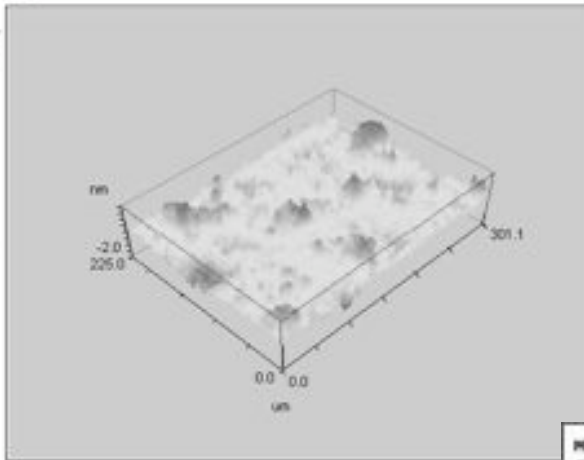
Ra: 0.34 nm
Rq: 0.43 nm
Rz: 3.09 nm
Rt: 3.50 nm

Set-up Parameters:

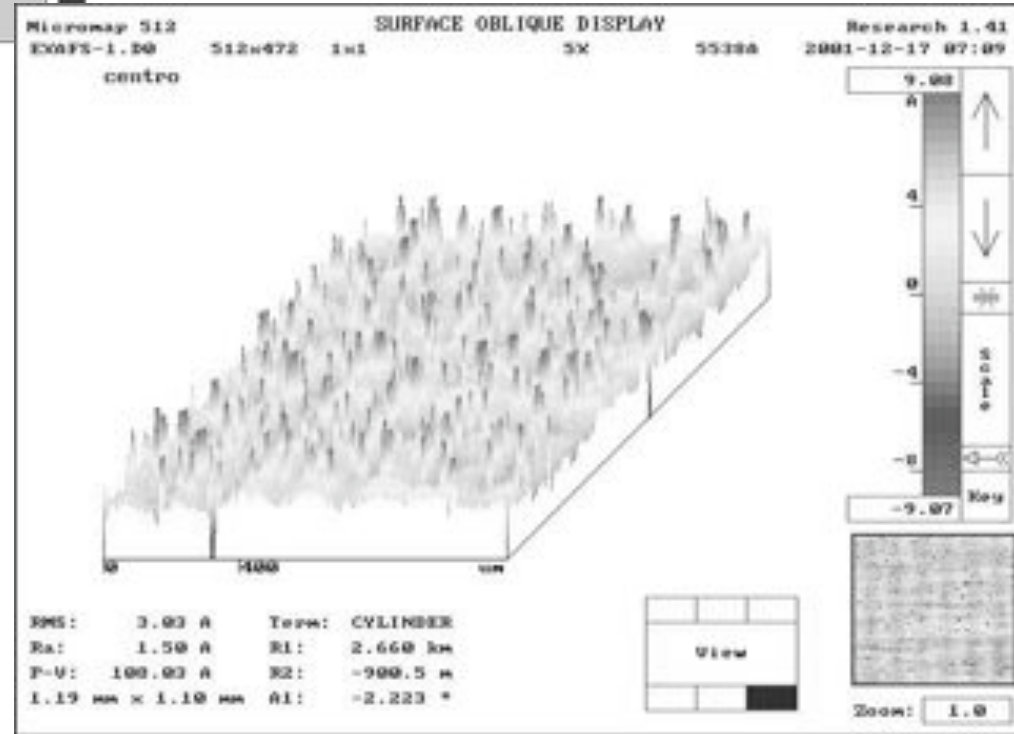
Size: 368 X 236
Sampling: 820.31 nm

Processed Options:

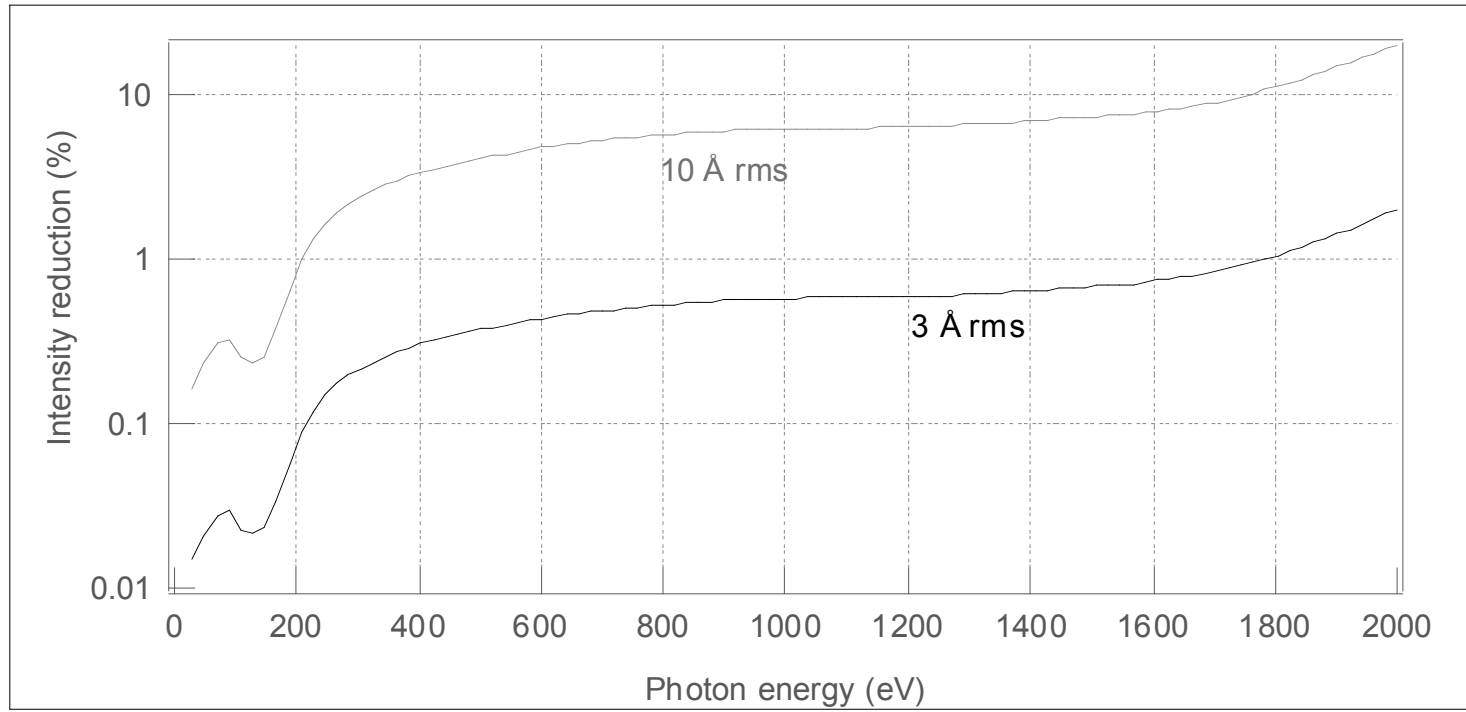
Terms Removed:
Cylinder & Tub
Filtering:
None



Title: 011797_S135
Note: Spot [Center]



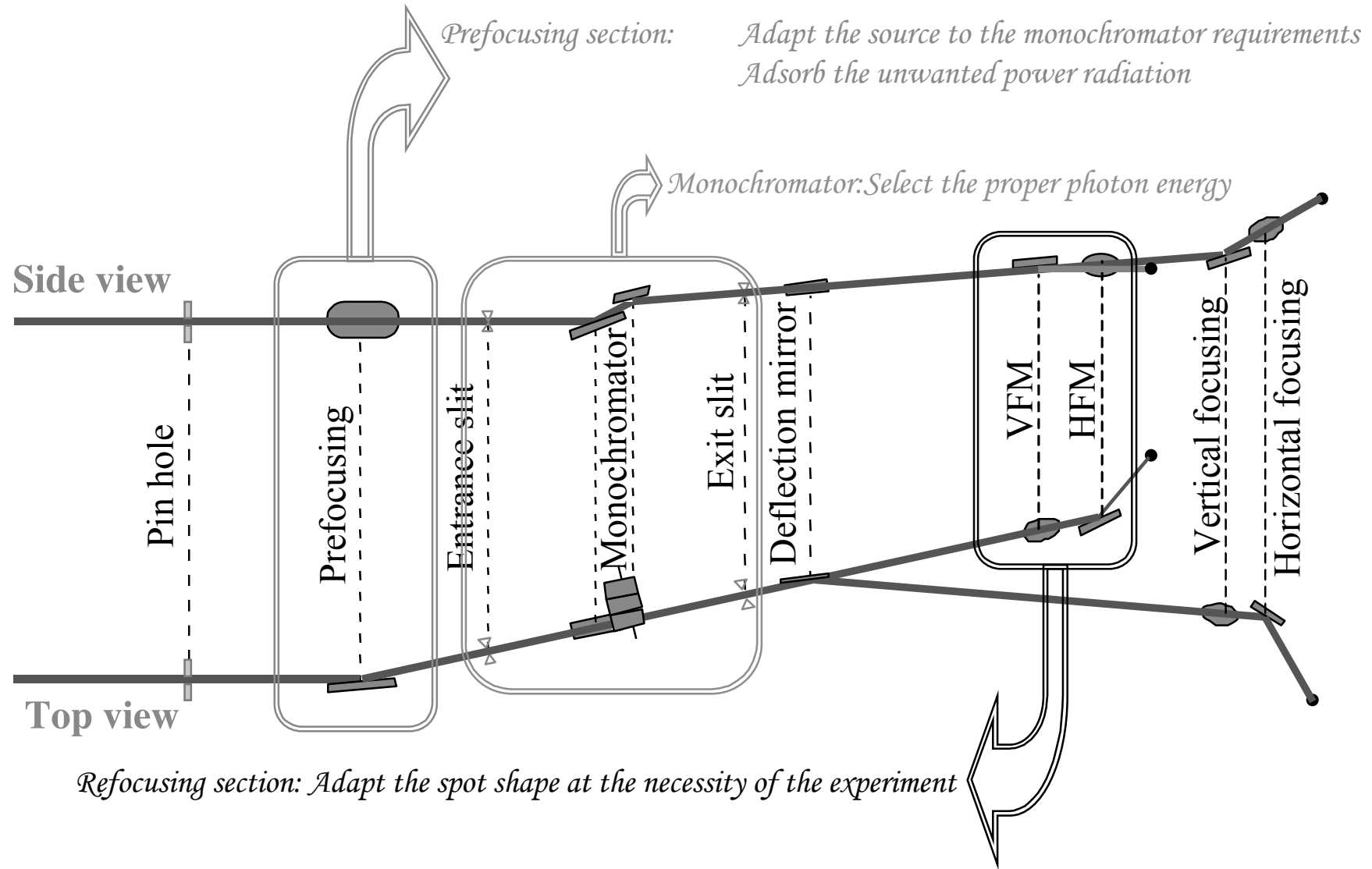
Flux reduction



Shape	Spherical/Flat	Toroidal/aspherical
Roughness (Å)	3 standard 1 best	5 standard 3 best (1-2 if very lucky)

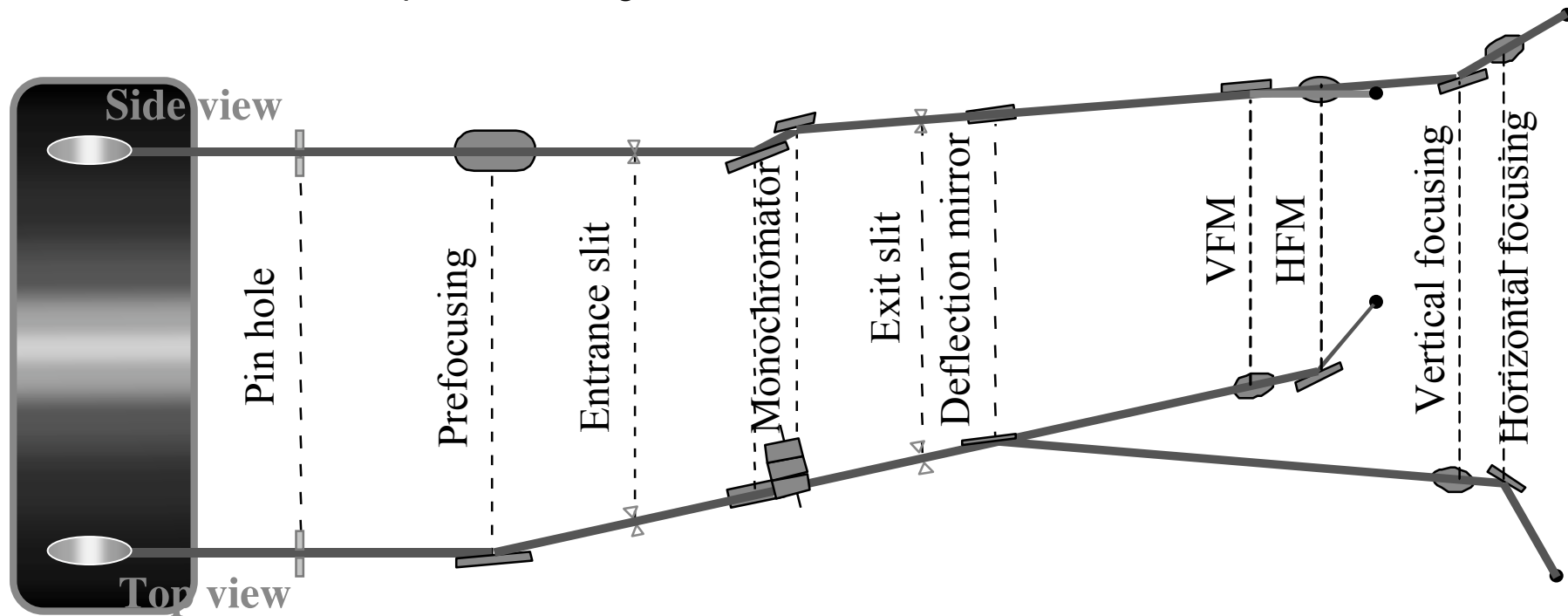
$$I = I_0 e^{-\left(\frac{4\pi\sigma \sin \vartheta}{\lambda}\right)^2}$$

Synchrotron Radiation Beamlines

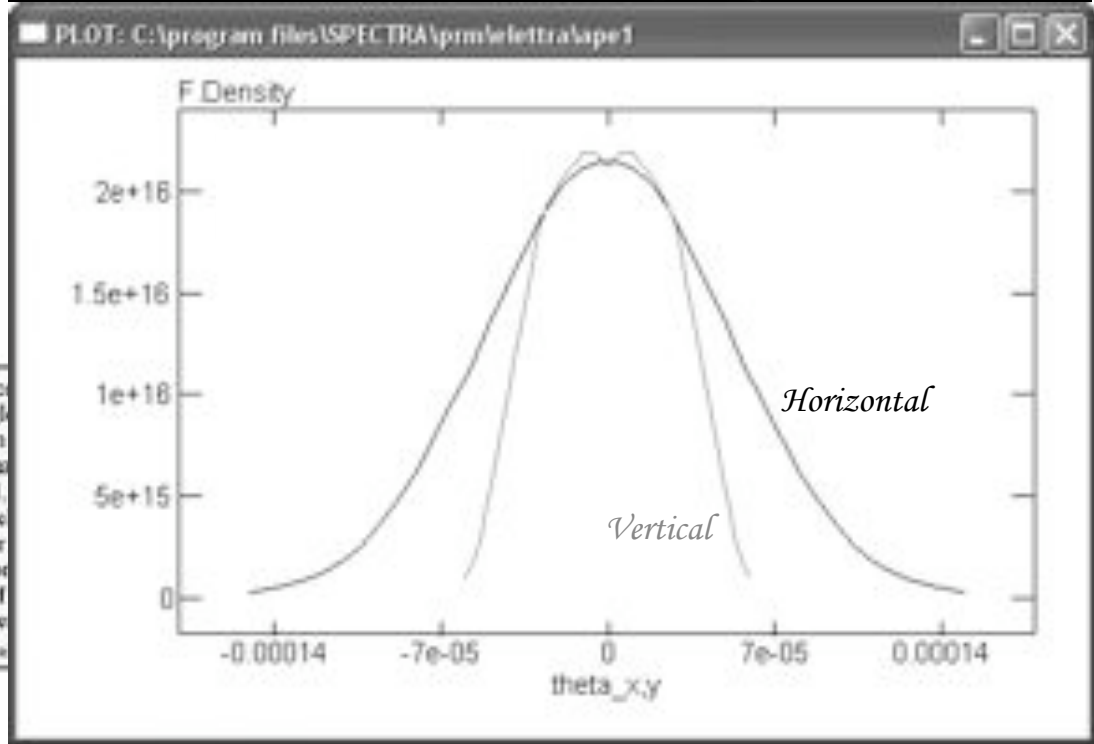
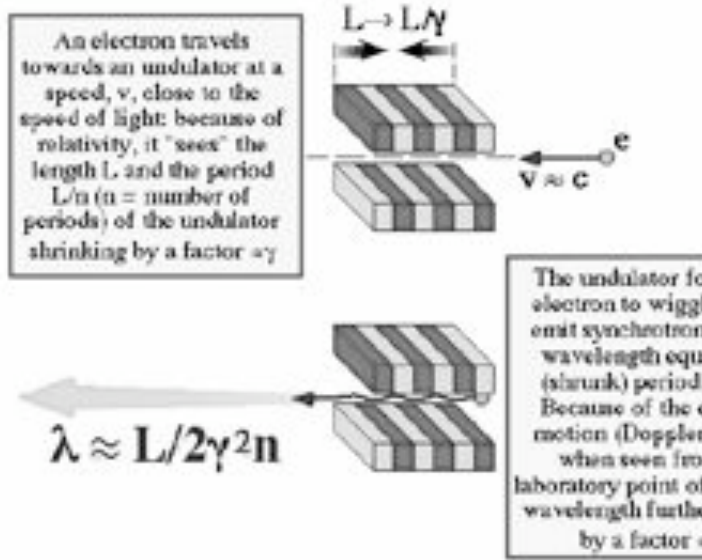
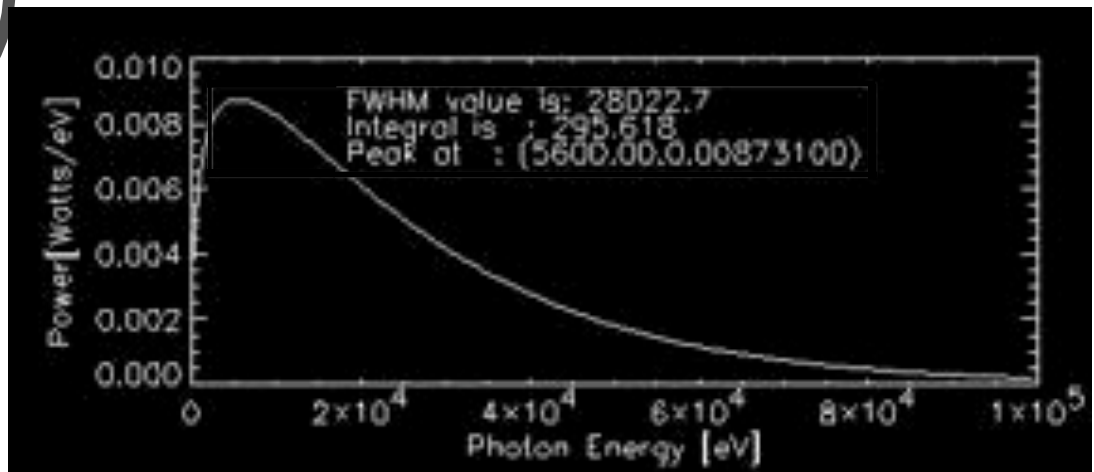
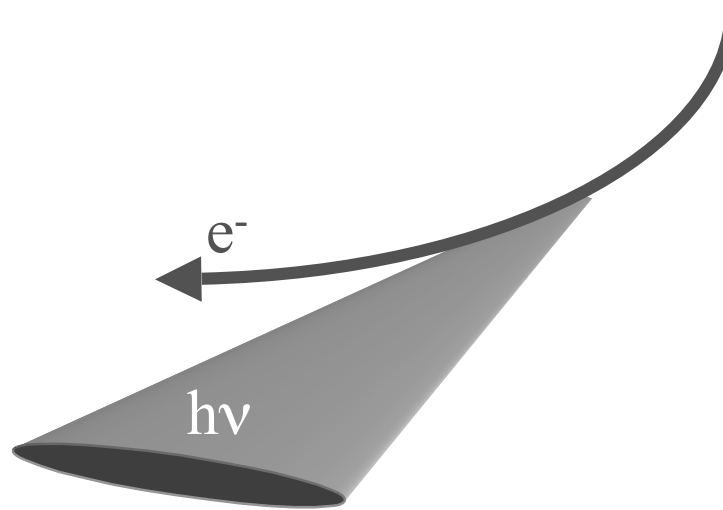


Synchrotron Radiation Beamlines

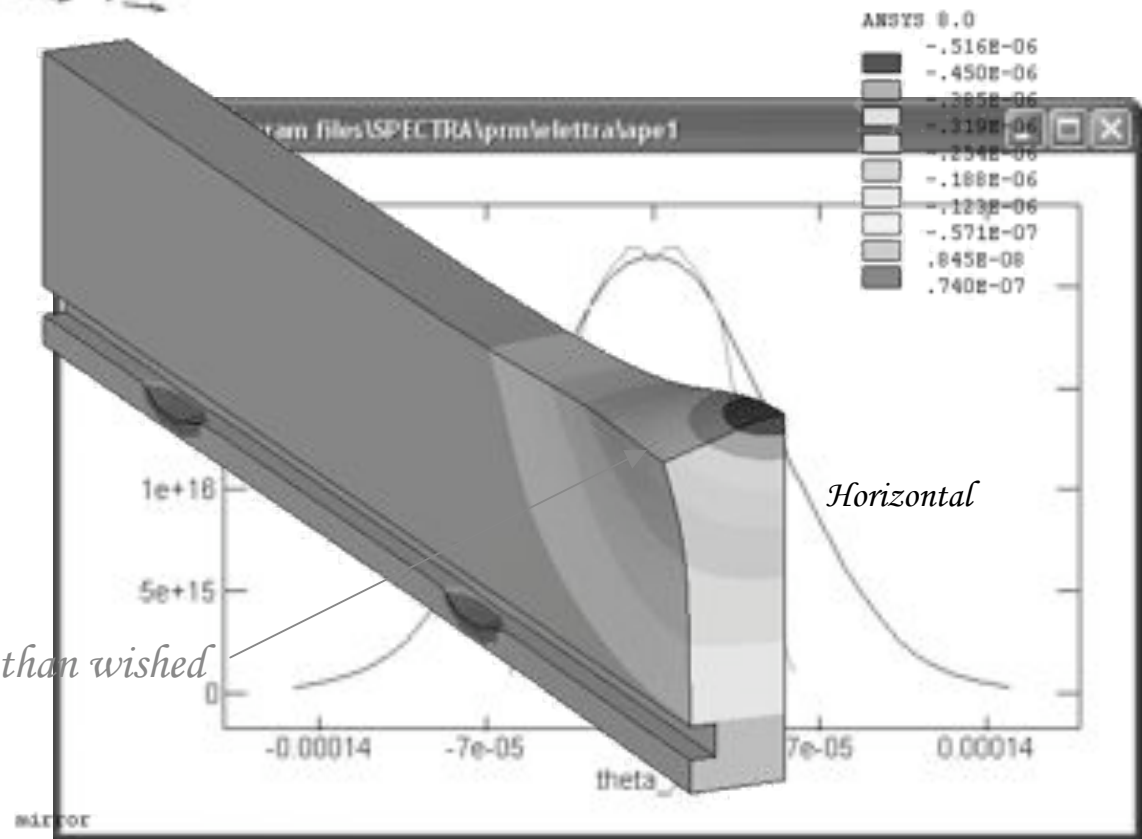
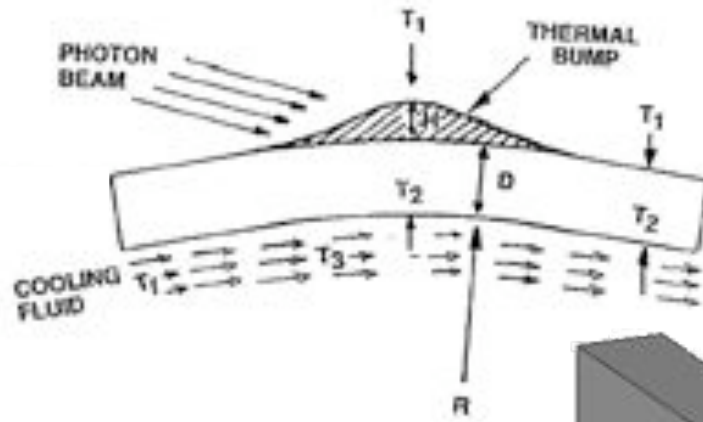
There are several reasons to choose a mirror substrate, one is the power arriving on it



SR sources



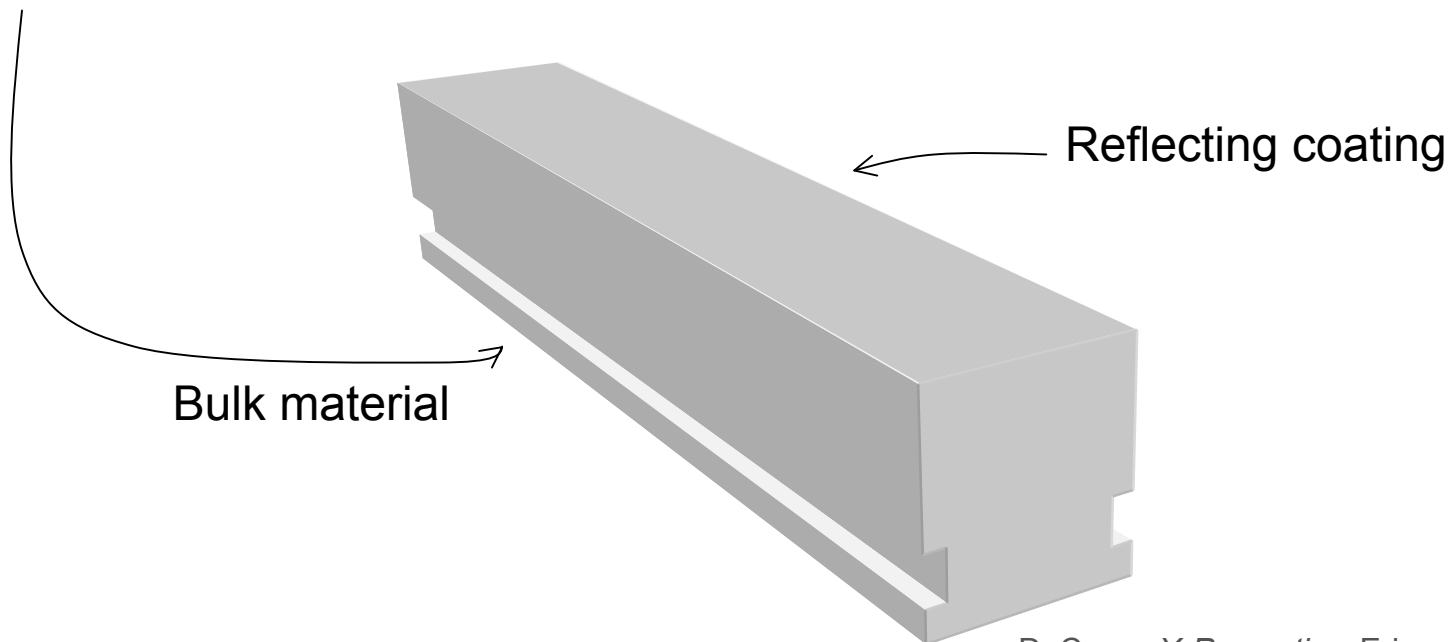
Thermal deformations



$400W \rightarrow 1\mu m$; 10 to 100 time larger than wished

Properties of typical mirror materials

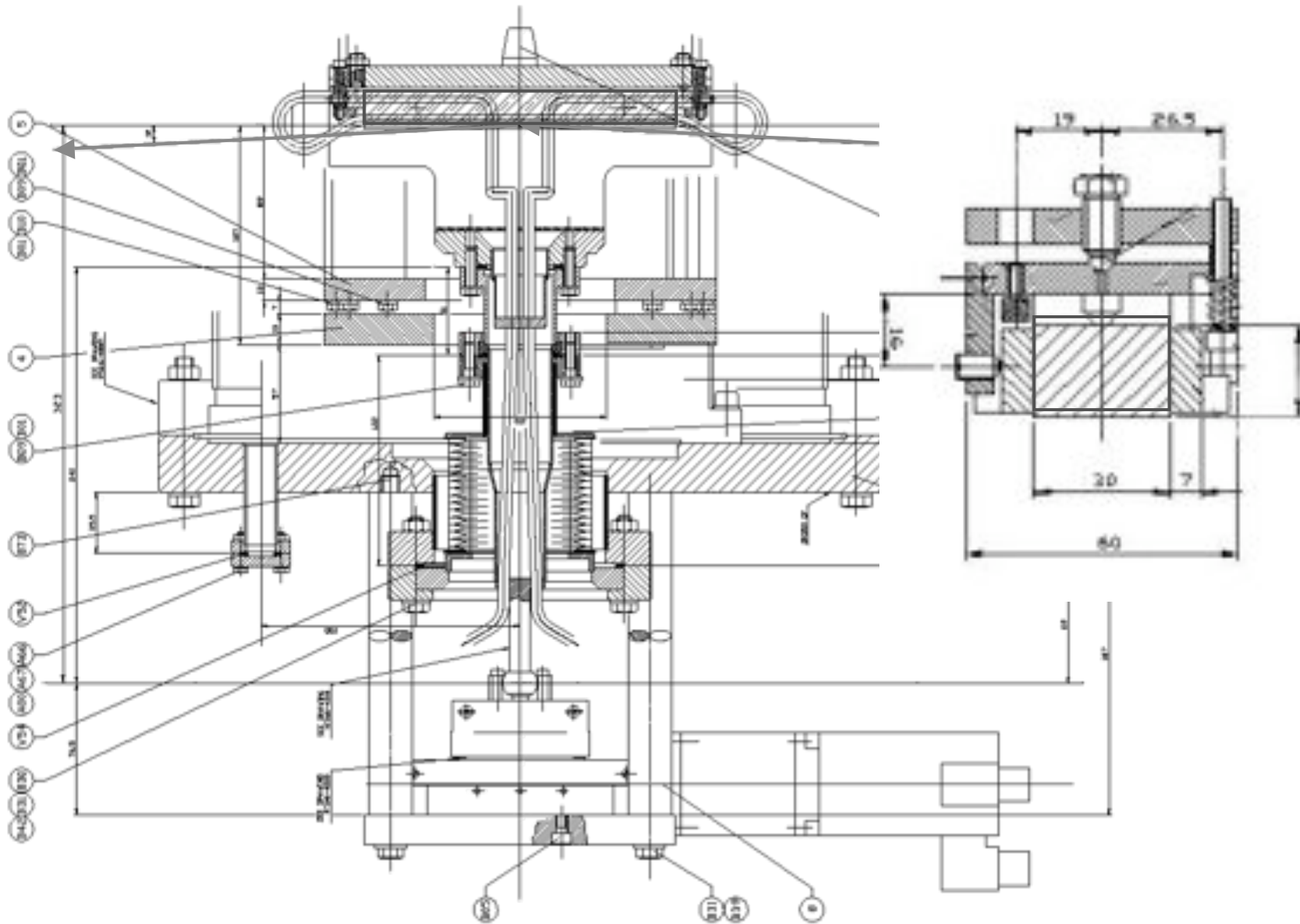
	Density	Young's modulus	Thermal expansion	Thermal conductivity	Figure of merit
	gm/cc	GPa	(α) ppm/ $^{\circ}$ C	(k) W/m/ $^{\circ}$ C	k/ α
Fused silica	2.19	73	0.50	1.4	2.8
Zerodur	2.53	92	0.05	1.60	32
Silicon	2.33	131	2.60	156	60
SiC CVD	3.21	461	2.40	198	82
Aluminum	2.70	68	22.5	167	7.42
Copper	8.94	117	16.5	391	23.7
Glidcop	8.84	130	16.6	365	22
Molybdenum	10.22	324.8	4.80	142	29.6



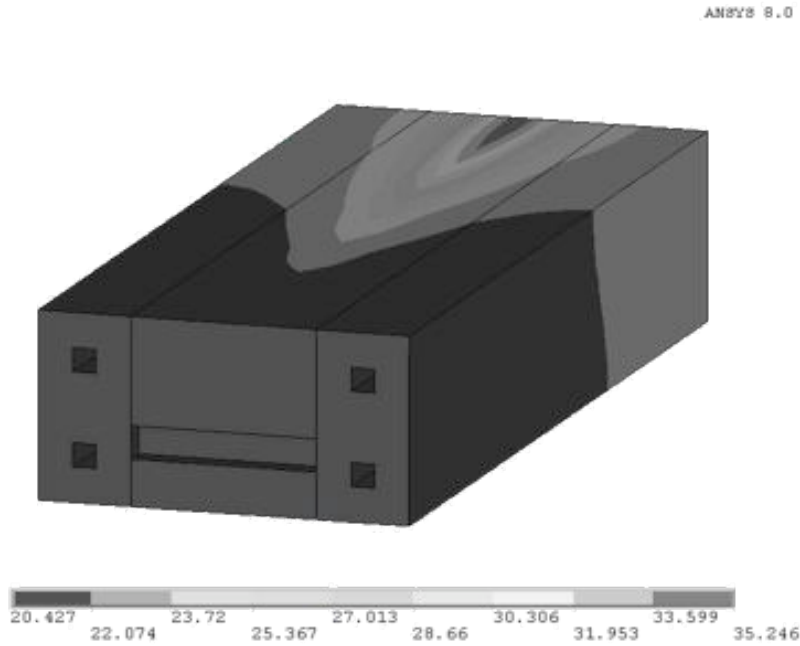
Silicon bulk mirrors



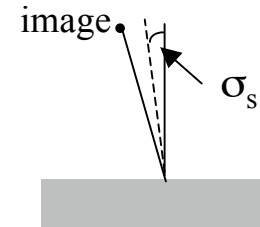
Direct side cooling



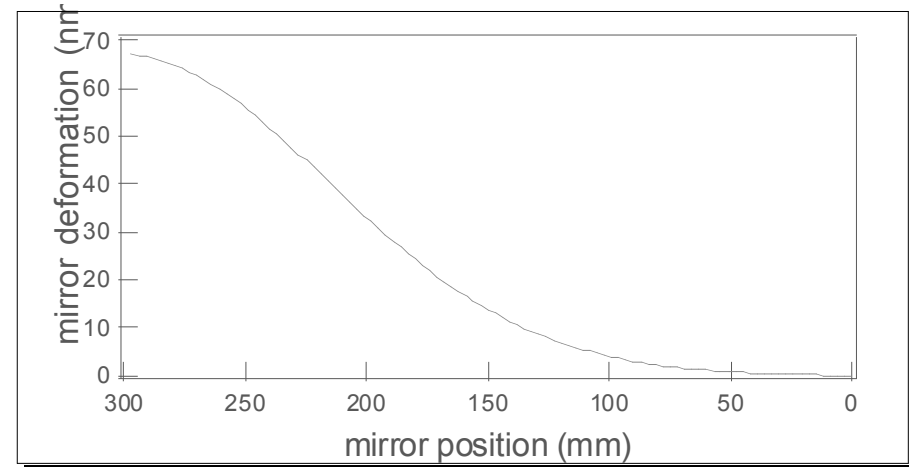
Direct side cooling



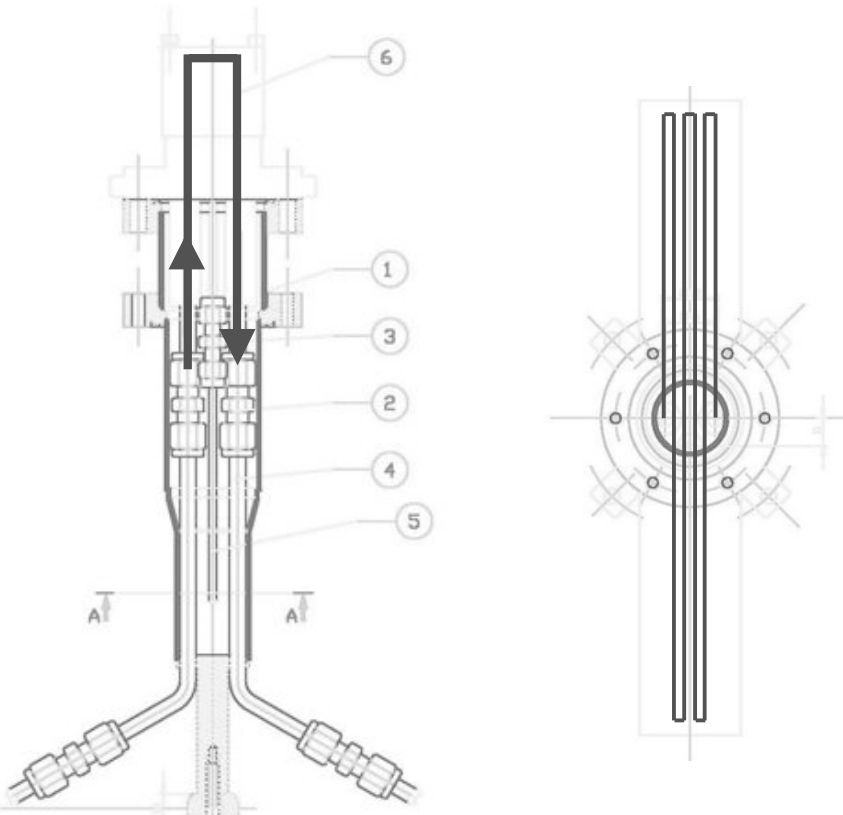
1st mirror sagittally oriented



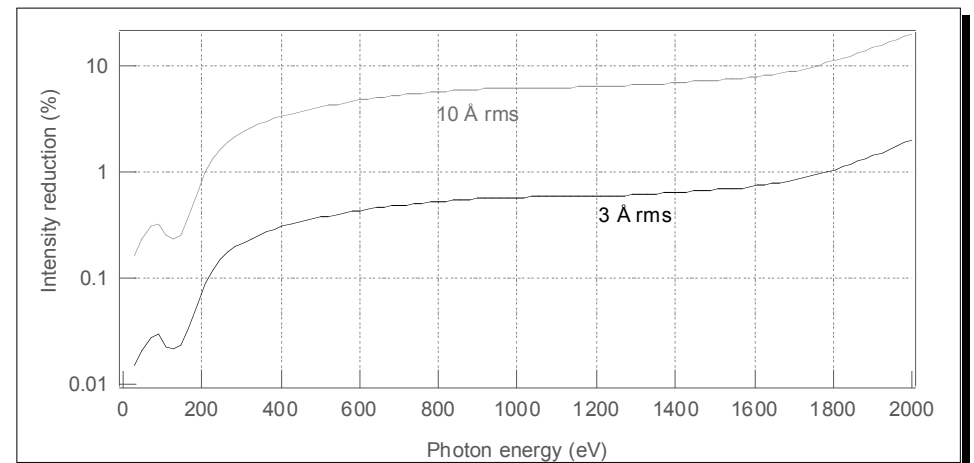
$$\Delta s'_s = 2 r' \cos \theta \sigma_s$$



Internally cooled mirrors



Shape	Spherical/Flat
Roughness (Å)	3 standard 1 best
Glass/Silicon	
Roughness (Å)	5 standard 2-3
Metallic	best



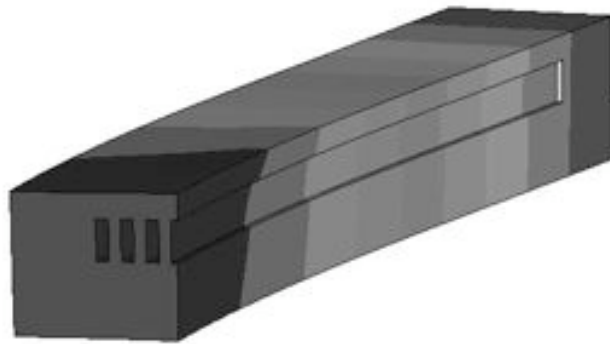
Internally cooled mirrors (Glidcop)

glidcop

*3GeV Synchrotron source
6.6 cm period undulator $K_{max}=5.7$
BL6.1*

1.5° grazing incidence

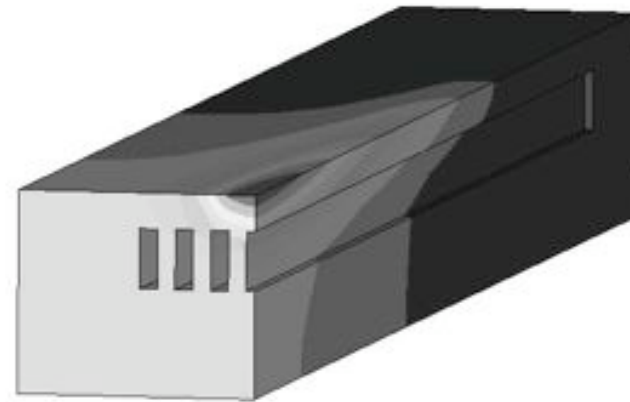
ARSTS 0.0



$\Delta h=17\mu m$ slope $26\mu rad$

1.5° grazing incidence

ARSTS 0.0



$\Delta T=7.7^\circ$

Invar & SuperInvar

	Density gm/cc	Young's modulus GPa	Thermal expansion (α) ppm/ $^{\circ}$ C	Thermal conductivity (k) W/m/ $^{\circ}$ C	Figure of merit k/ α
Silicon	2.33	131	2.60	156	60
SiC CVD	3.21	461	2.40	198	82
Aluminum	2.70	68	22.5	167	7.42
Copper	8.94	117	16.5	391	23.7
Glidcop	8.84	130	16.6	365	22
Molybdenum	10.22	324.8	4.80	142	29.6
Invar 36	9.05	141	0.5	10.4	20.8
SuperInvar	8.13	145	0.06	10.5	210

INVAR®

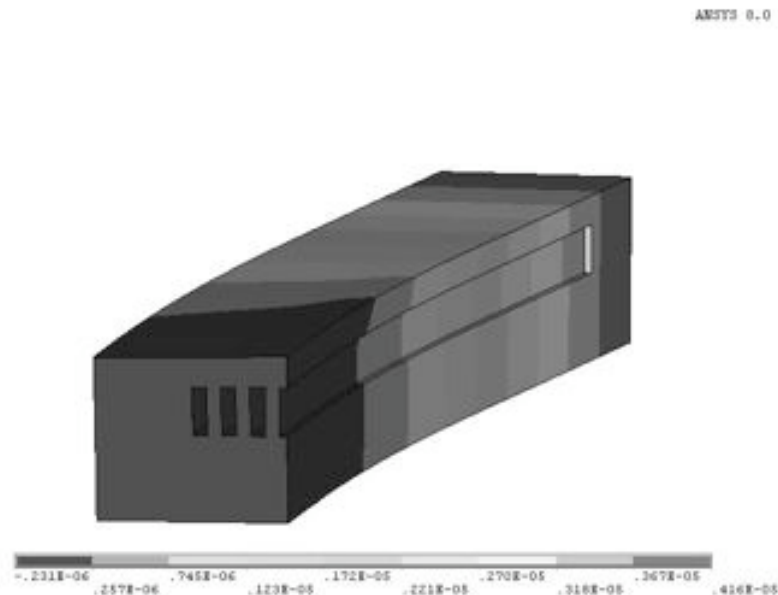
Carpenter Technology Inc.

Alloy 36 iron-nickel(36%) alloy with carbon (0.02%), manganese (0.35%), Silicon (0.2%)

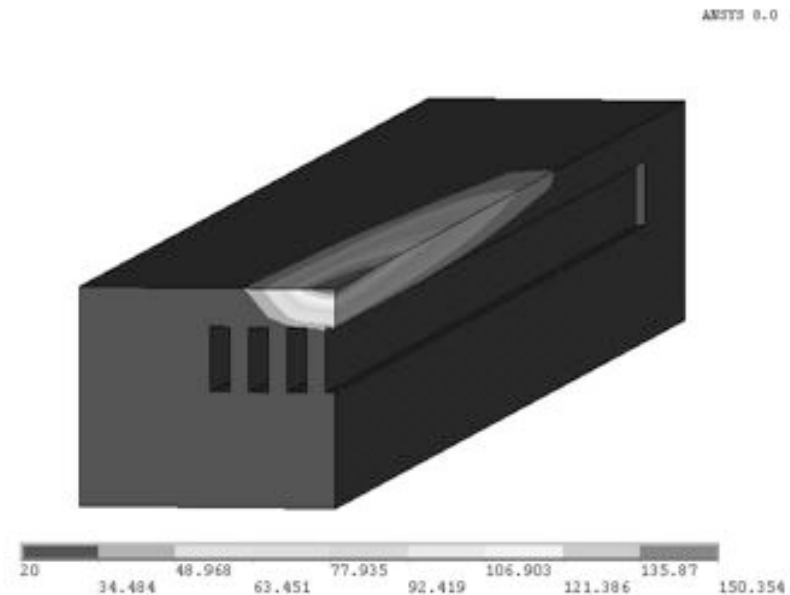
Supernvar: iron-nickel(32%) alloy with carbon (0.02%), manganese (0.40%), Silicon (0.25%), Cobalt (5.5%)

SuperInvar

	Density	Young's modulus	Thermal expansion	Thermal conductivity	Figure of merit
	gm/cc	GPa	(α) ppm/ $^{\circ}$ C	(k) W/m/ $^{\circ}$ C	k/ α
Glidcop	8.84	130	16.6	365	22
Molybdenum	10.22	324.8	4.80	142	29.6
SuperInvar	8.13	145	0.06	10.5	210



$$\Delta h = 6 \mu m$$



$$\Delta T = 130^{\circ}$$

Carbon Contamination

Contamination process:

Hydrocarbons adsorbed by the surface

Cracking induced by the incoming radiation

Formation of graphitic carbon layer (mixed C compound)

Effect of the contamination:

Strong adsorption at the carbon edge (≈ 270 eV)

Reduction of reflectivity due to enhancement of the surface roughness

general deterioration of the surface

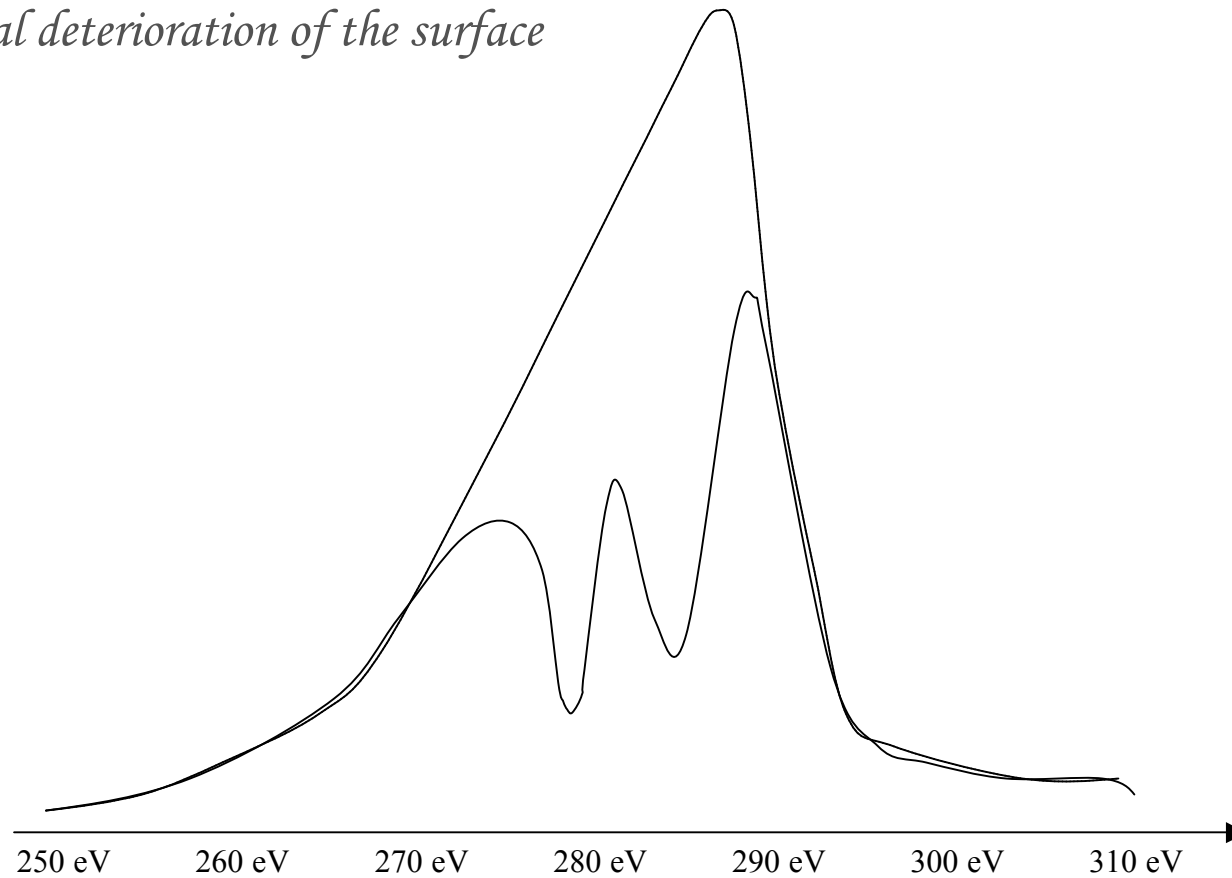
Carbon Contamination

Effect of the contamination:

Strong adsorption at the carbon edge (≈ 270 eV)

Reduction of reflectivity due to enhancement of the surface roughness

general deterioration of the surface



Carbon Contamination and Cleaning

Contamination process:

Hydrocarbons adsorbed by the surface

Cracking induced by the incoming radiation

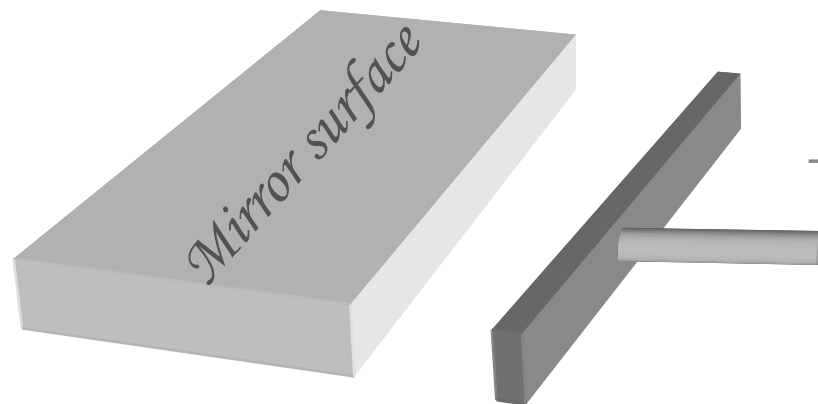
Formation of graphitic carbon layer (mixed C compound)

Effect of the contamination:

Strong adsorption at the carbon edge (≈ 270 eV)

Reduction of reflectivity due to enhancement of the surface roughness

general deterioration of the surface



UV lamp discharge

+ 300-500 V (DC)

I 100 mA-1A

P 0.5-1 mbar O₂



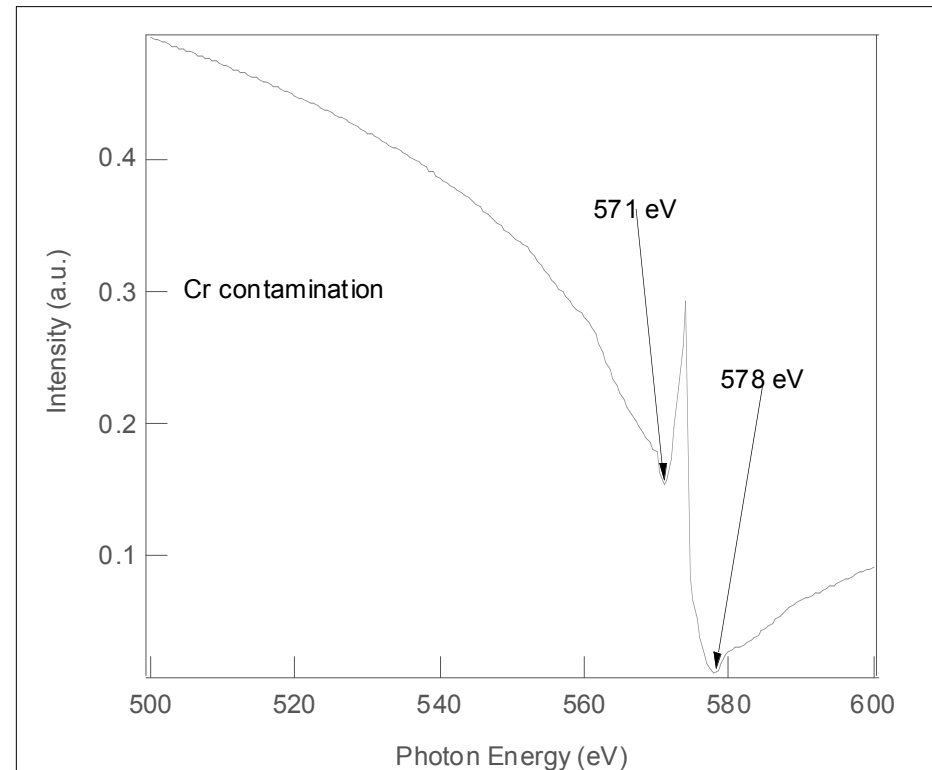
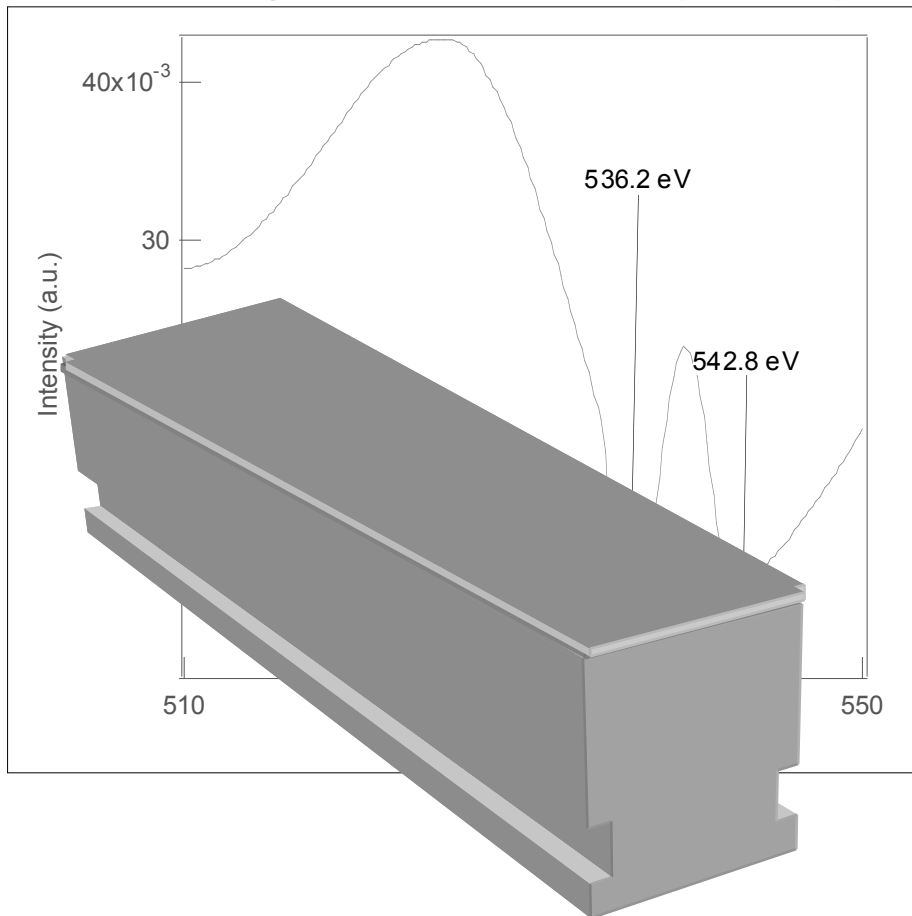
Other Contamination

Effect of the contamination:

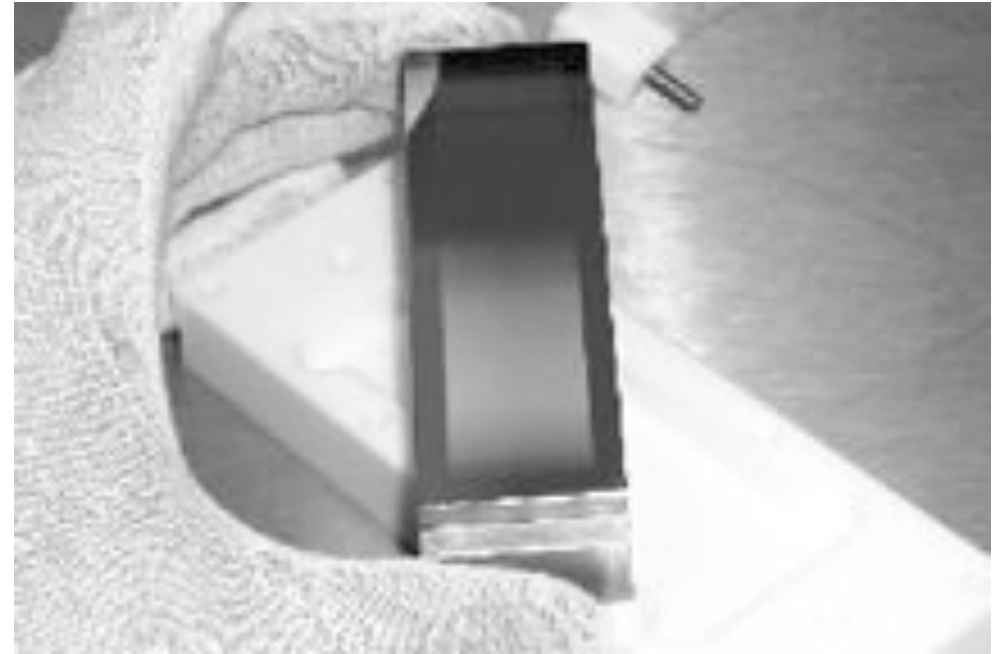
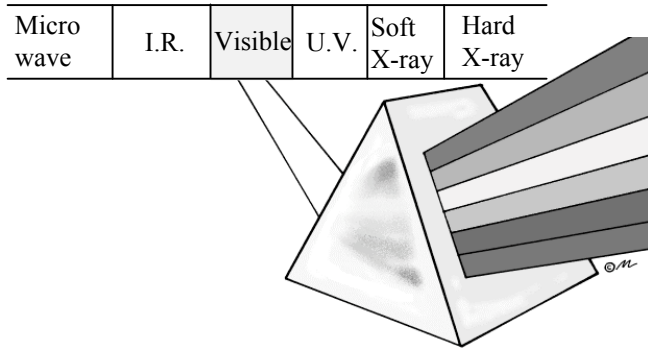
Strong adsorption at the O/Cr edge

Reduction of reflectivity due to enhancement of the surface roughness

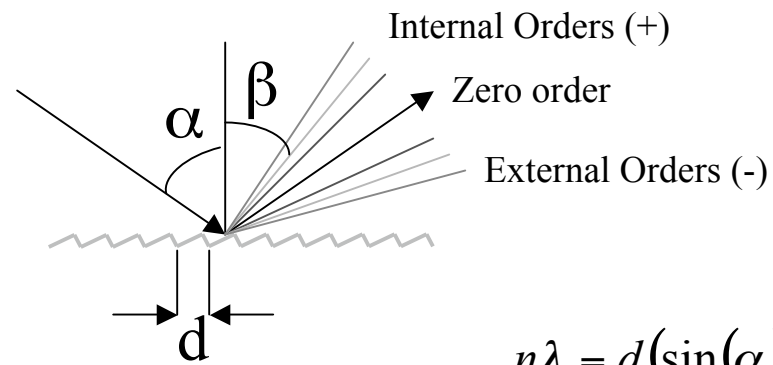
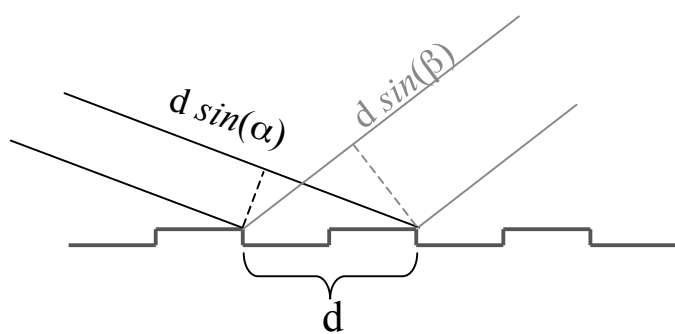
general deterioration of the surface



Dispersive elements

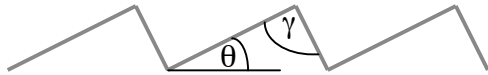


Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray
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$$n\lambda = d(\sin(\alpha) - \sin(\beta))$$

Grating's profiles



Blaze profile



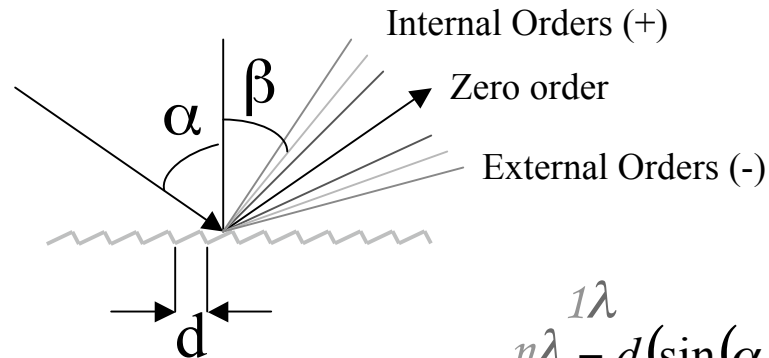
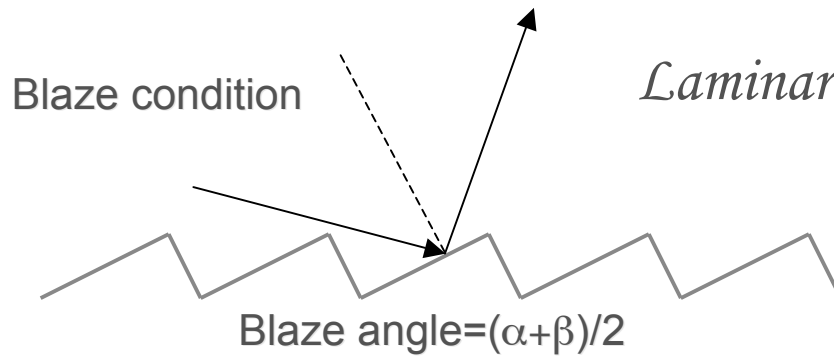
Lamellar profile

Blaze gratings:

higher efficiency

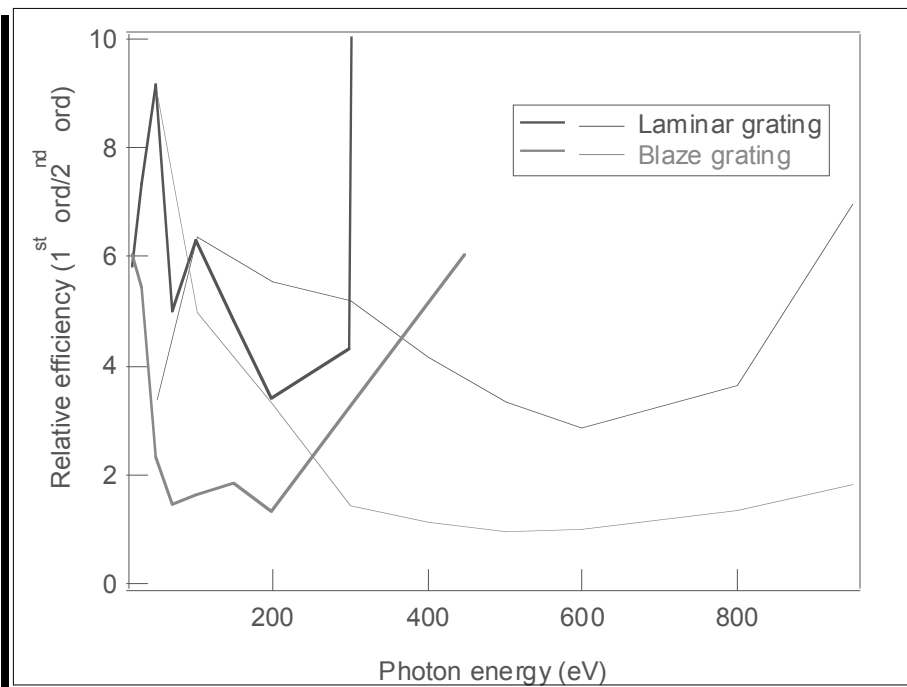
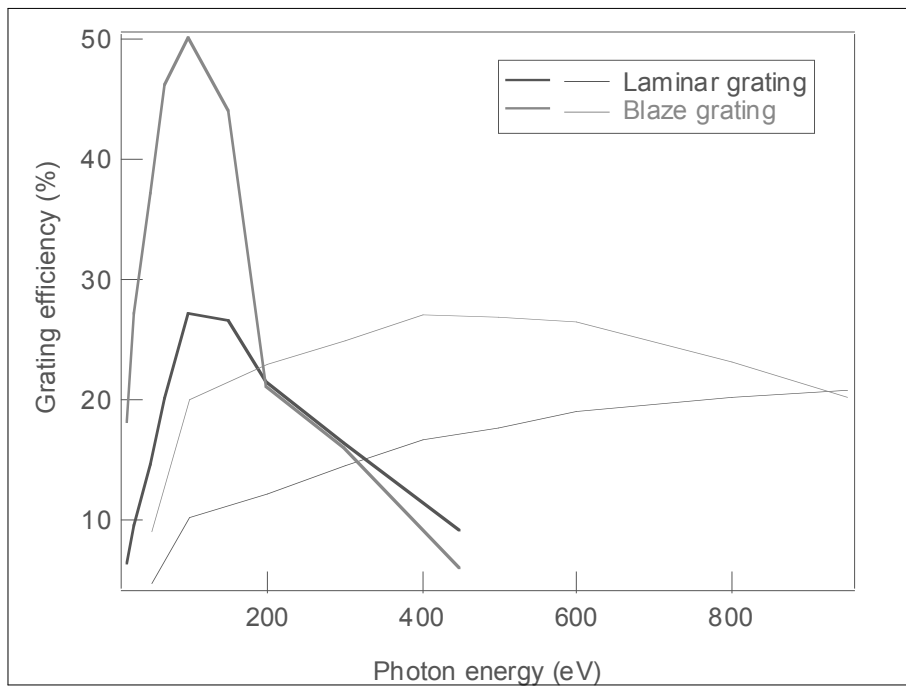
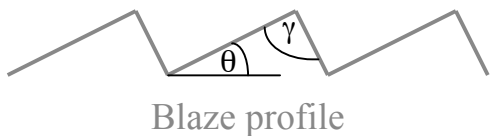
Lamellar gratings:

*Higher spectral purity
Higher resolution*



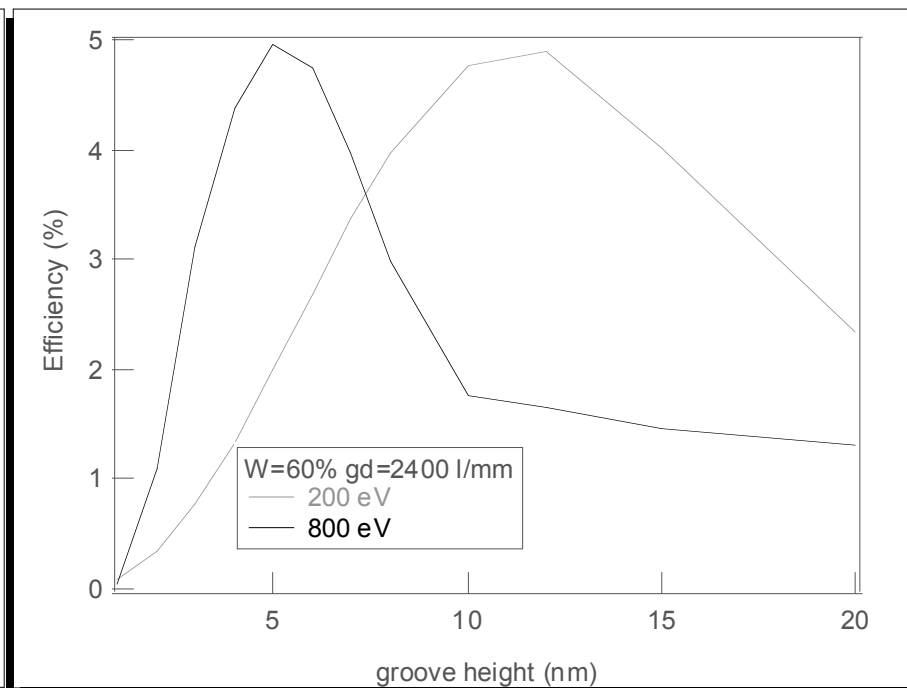
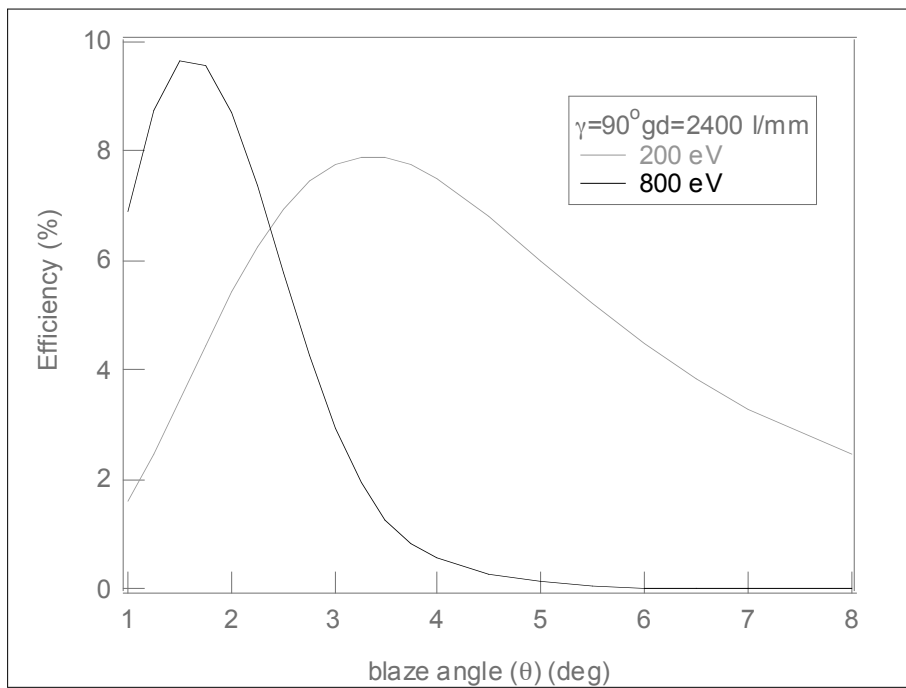
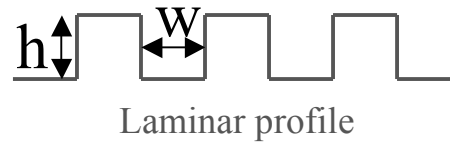
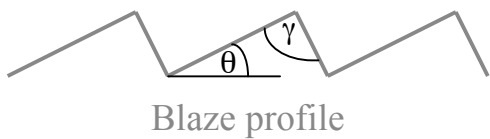
$$n\lambda = d(\sin(\alpha) - \sin(\beta))$$

Grating's efficiency



$$n\lambda = d(\sin(\alpha) - \sin(\beta))$$

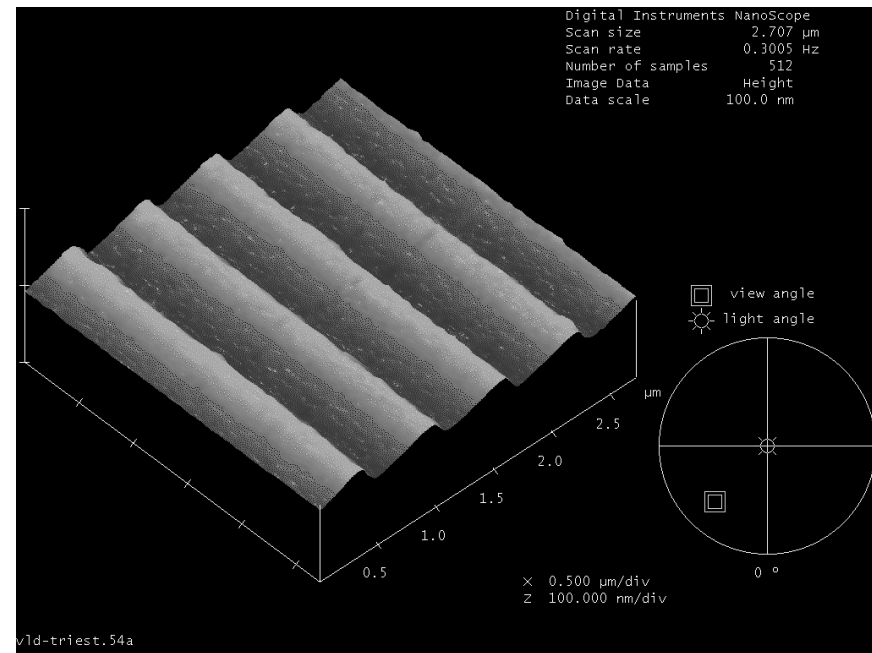
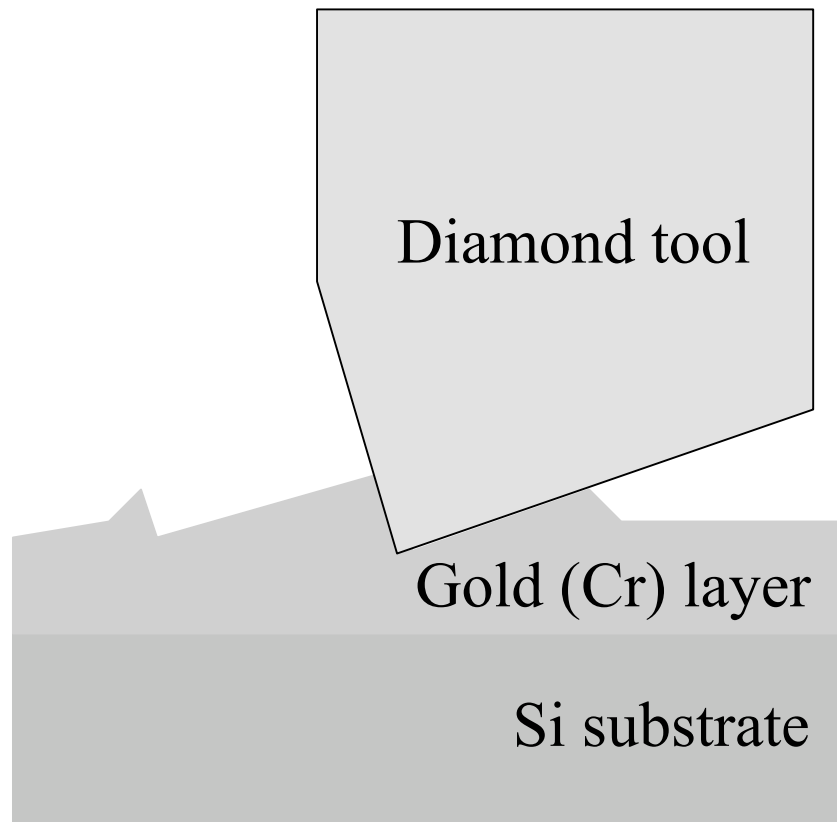
Grating's efficiency



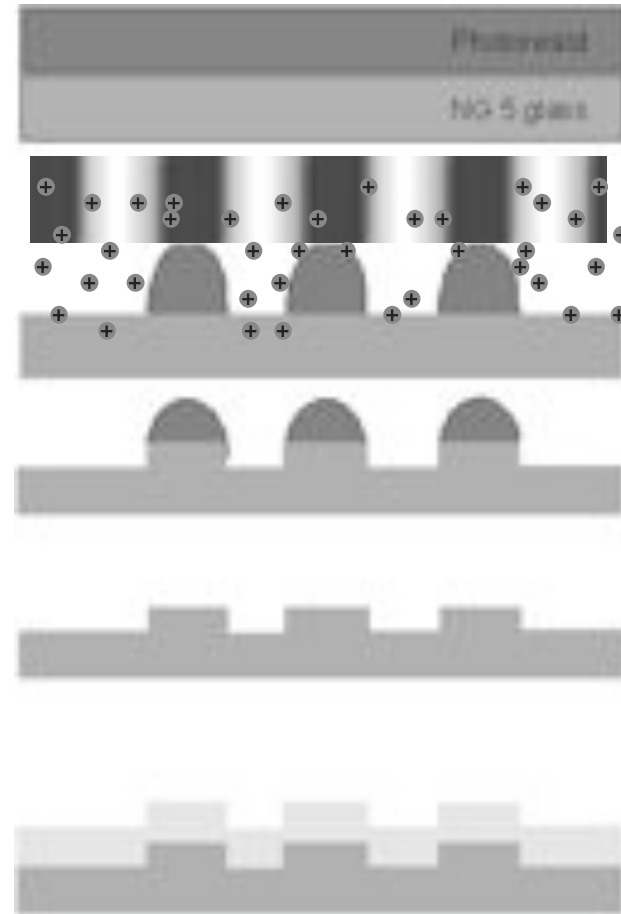
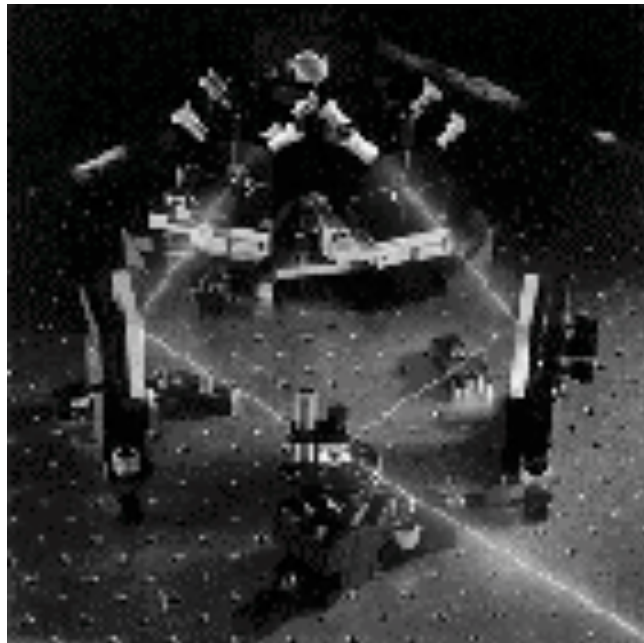
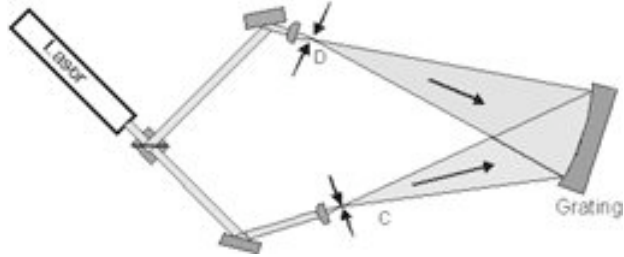
Grating's production

Mechanical ruling blaze profile \rightarrow smaller blaze angles; higher efficiency

Holographically recording laminar and blaze profile (large blaze angle)
 \rightarrow higher groove density; lower spacing disomogeneity



Holographic Recorded Gratings

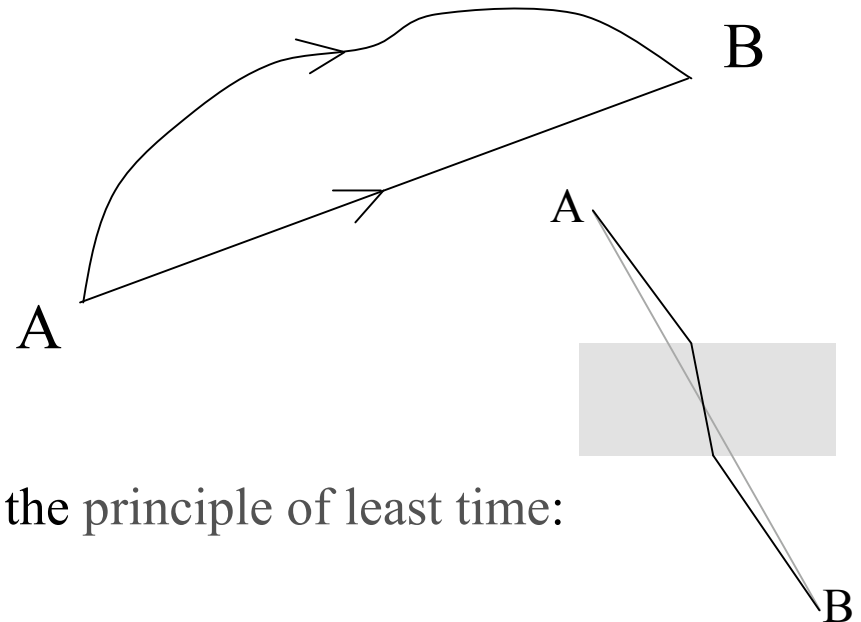


Fermat's principle

Light rays choose their paths to minimize the optical length

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

where $n(\vec{r})$ is the index of refraction of the medium and dl is the line segment along the path



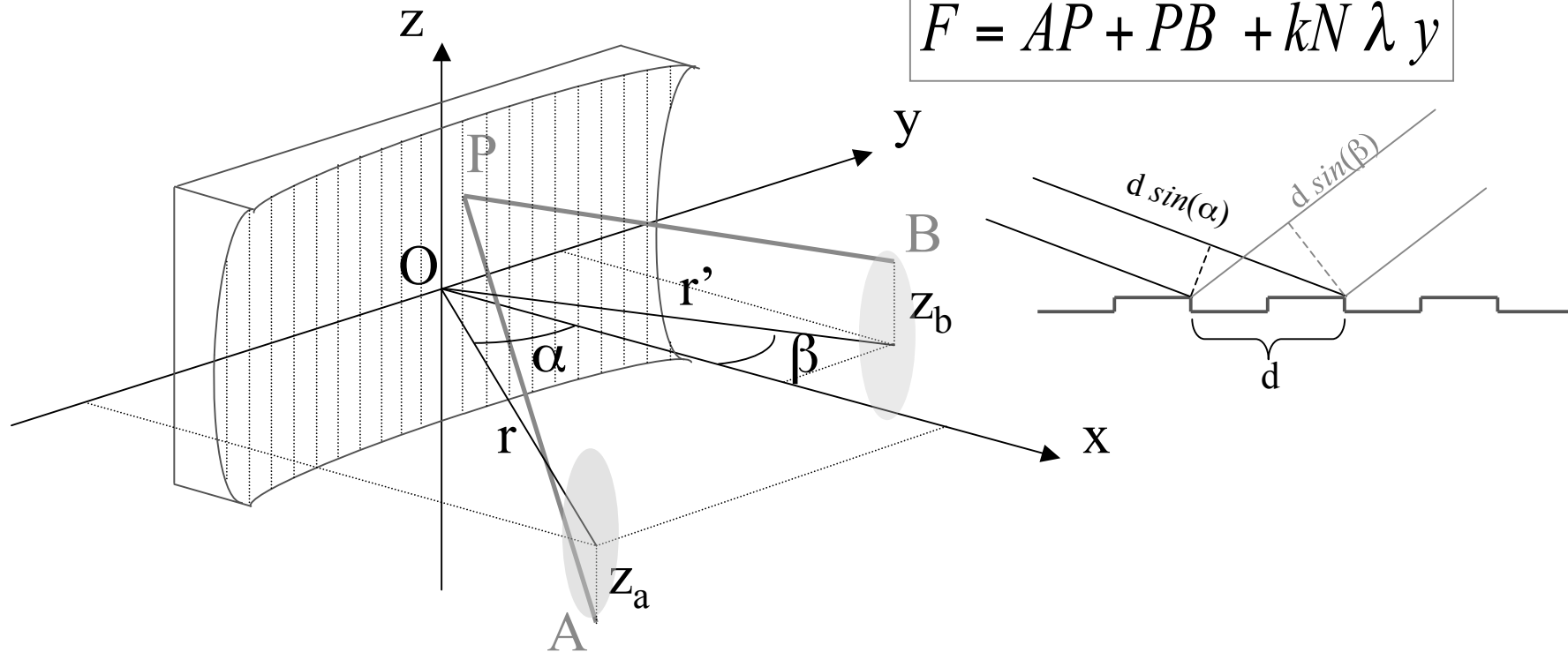
Fermat's principle is also known as the principle of least time:

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

Optical path

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

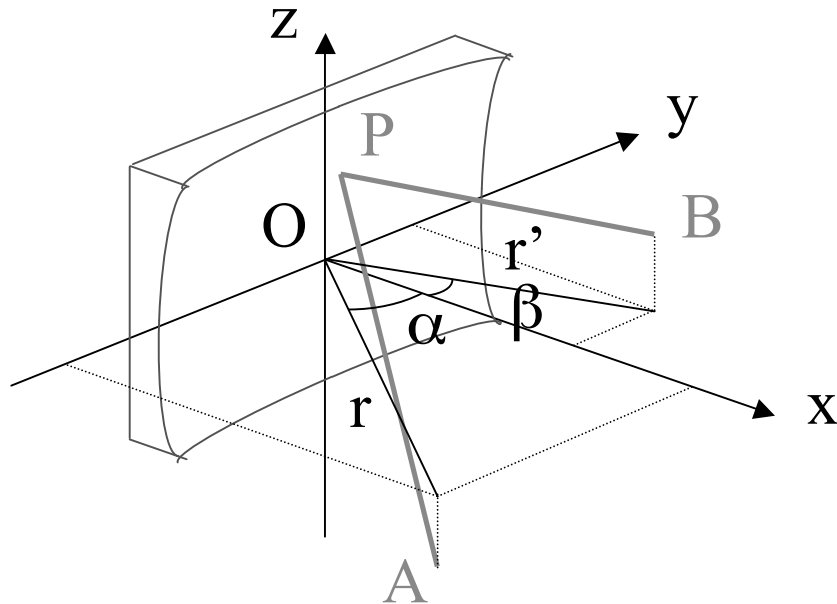
$$F = \overline{AP} + \overline{PB} + kN \lambda y$$



where λ is the wavelength of the diffracted light, k is the order of diffraction ($\pm 1, \pm 2, \dots$), $N=1/d$ is the groove density

Optical Path - focal condition

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:

$$\frac{\partial F}{\partial y} = 0 \quad \frac{\partial F}{\partial z} = 0$$

for any pair of (y,z)

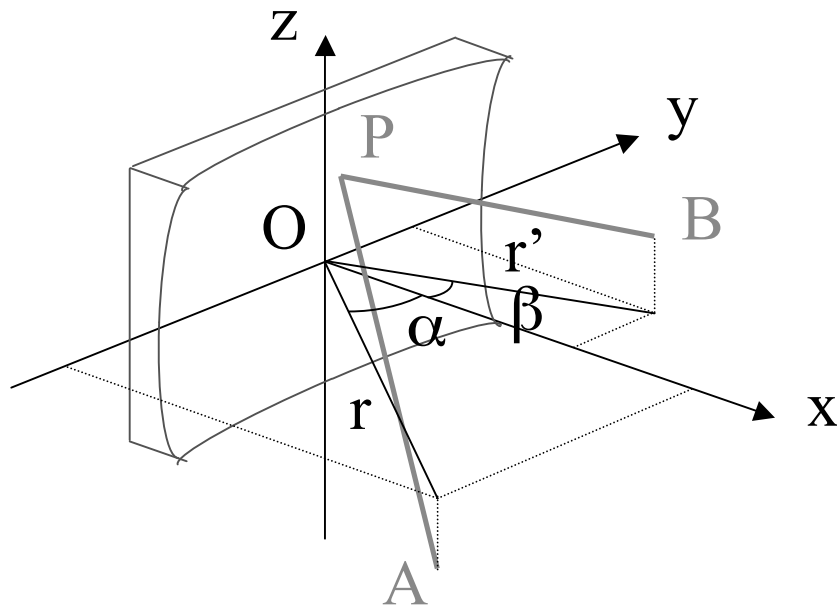
Optical Path - focal condition

Equations:

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

+

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

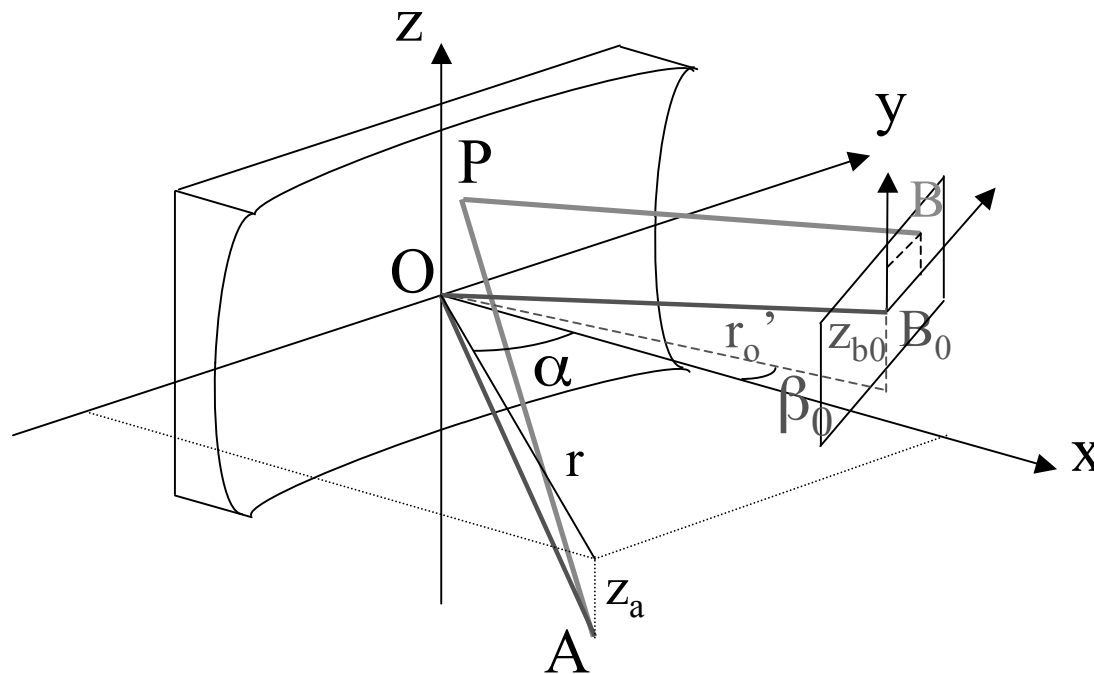


can be used to decide on the required characteristics of the diffraction grating, in particular the shape of the surface, the grooves density, the object and image distances.

Aberrated image

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

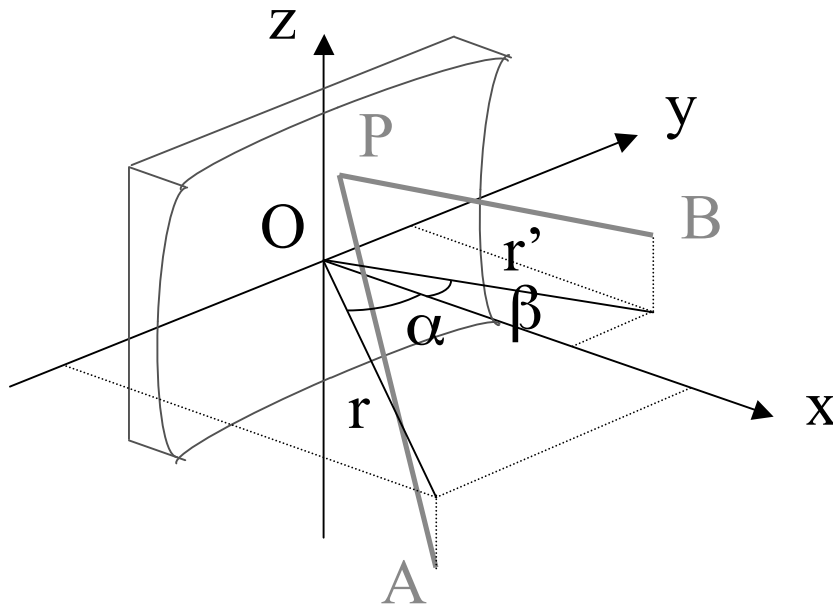
→ when the point P wanders over the grating surface, diffracted rays fall on slightly different points on the focal plane and an aberrated image is formed



Goal: produce simple expressions for the intersection points in the image plane produced by the rays diffracted from different points on the grating surface

Grating surface

The grating surface may 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
 $j = \text{even}$ 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.

Typical surfaces

Toroid

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

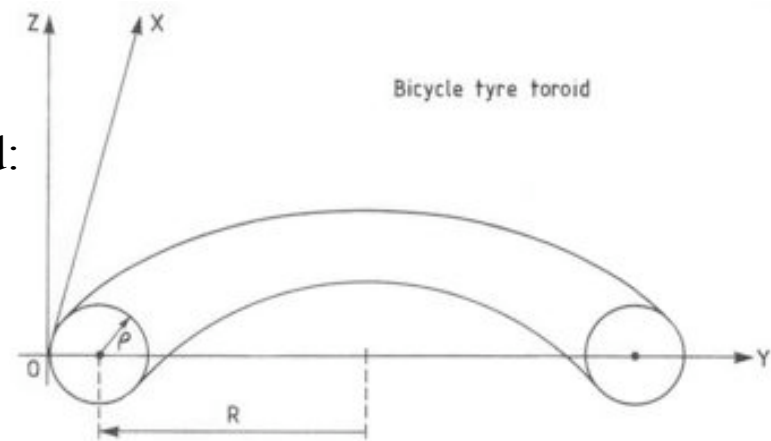
$$a_{04} = \frac{1}{8\rho^3}; \quad a_{12} = 0; \quad a_{30} = 0$$

Sphere, cylinder and plane are special cases of toroid:

$R=\rho \rightarrow$ sphere

$R= \infty \rightarrow$ cylinder

$R=\rho= \infty \rightarrow$ plane

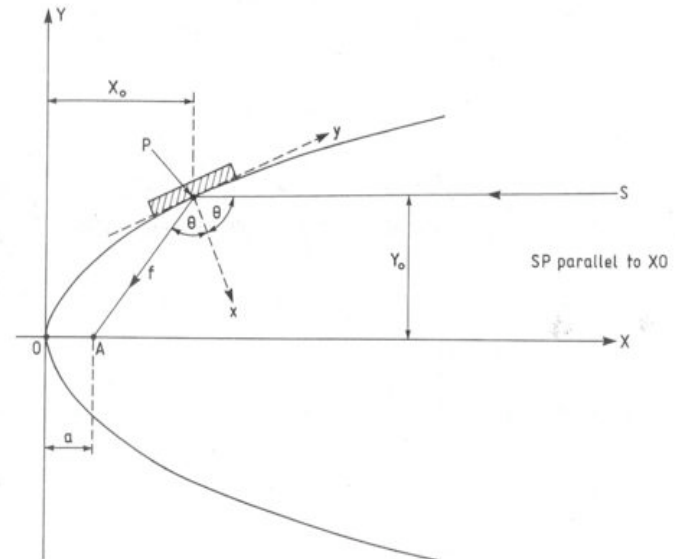


Paraboloid

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

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

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



Typical surfaces

Ellipsoid

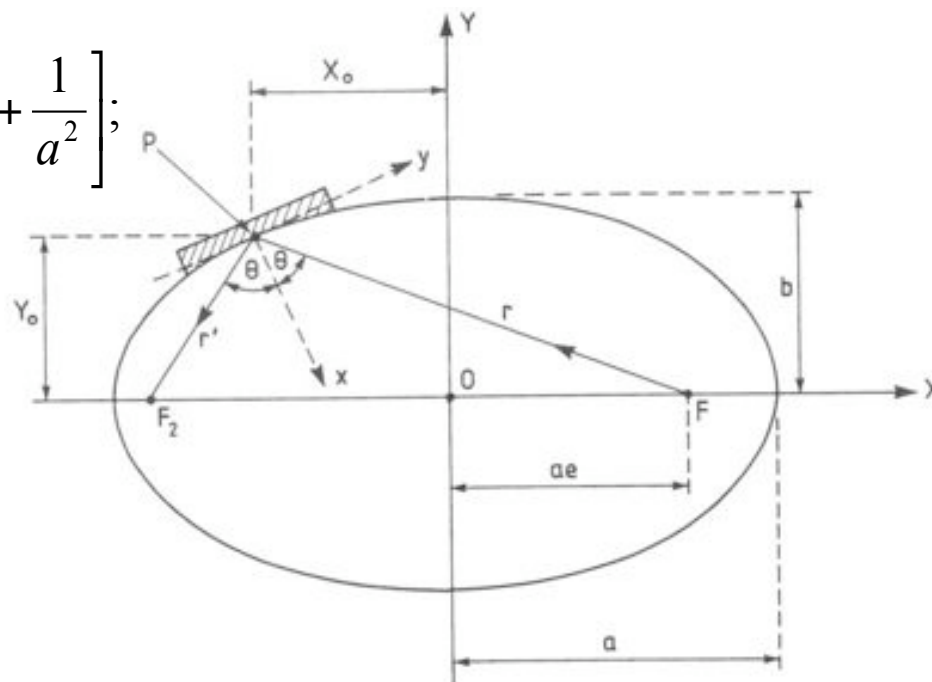
$$a_{02} = \frac{1}{4f \cos \vartheta}; \quad a_{20} = \frac{\cos \vartheta}{4f}; \quad a_{04} = \frac{b^2}{64f^3 \cos^3 \vartheta} \left[\frac{\sin^2 \vartheta}{b^2} + \frac{1}{a^2} \right];$$

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

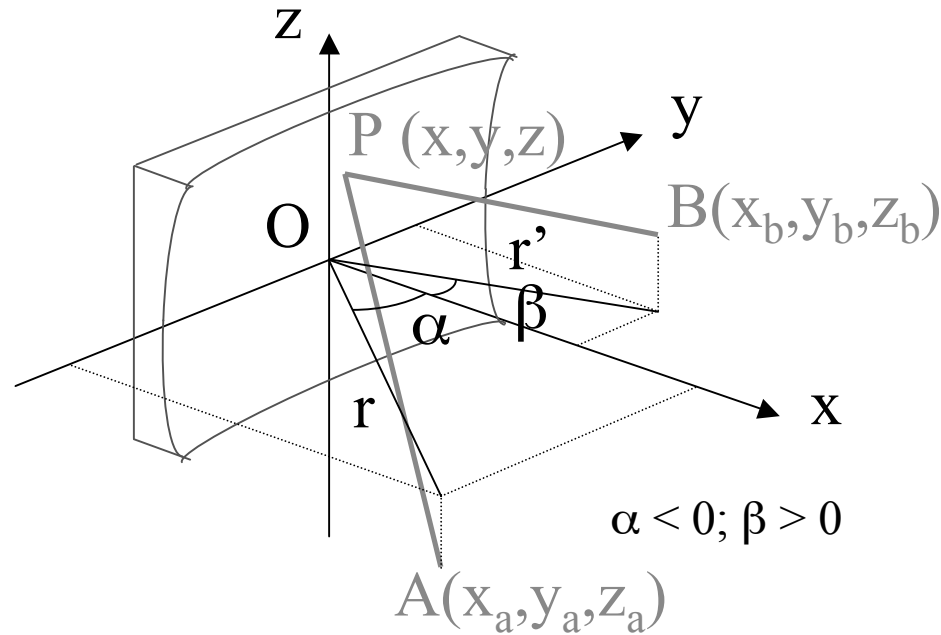
$$a_{40} = \frac{b^2}{64f^3 \cos^3 \vartheta} \left[\frac{5 \sin^2 \vartheta \cos^2 \vartheta}{b^2} - \frac{5 \sin^2 \vartheta}{a^2} + \frac{1}{a^2} \right];$$

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

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



Optical Path Function



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

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

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

$$x_a = r \cos \alpha$$

$$y_a = r \sin \alpha$$

$$x_b = r' \cos \beta$$

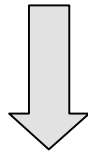
$$y_b = r' \sin \beta$$

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

$$\begin{aligned}
 &= F_{000} + yF_{100} + zF_{011} + \frac{1}{2} y^2 F_{200} + \frac{1}{2} z^2 F_{020} + \frac{1}{2} y^3 F_{300} \\
 &+ \frac{1}{2} yz^2 F_{120} + \frac{1}{8} y^4 F_{400} + \frac{1}{4} y^2 z^2 F_{220} + \frac{1}{8} z^4 F_{040} \\
 &+ yzF_{111} + \frac{1}{2} yF_{102} + \frac{1}{4} y^2 F_{202} + \frac{1}{2} y^2 zF_{211} + \dots
 \end{aligned}$$

Perfect focal condition

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



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

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

Aberrations Terms

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

for $r, r' \gg z_a, z_b$

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

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

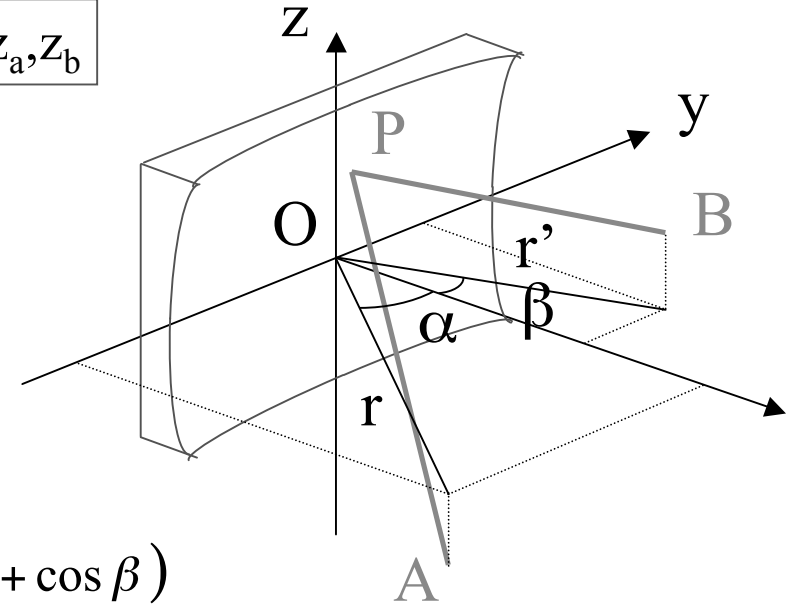
$$F_{020} = \frac{1}{r} + \frac{1}{r'} - 2a_{02} (\cos \alpha + \cos \beta)$$

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

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

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

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



Aberrations Terms

$$F_{100} = 0 \quad \Longrightarrow \quad \sin \alpha + \sin \beta_0 = Nk\lambda \quad \text{grating equation}$$

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!

Focal conditions

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

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

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

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

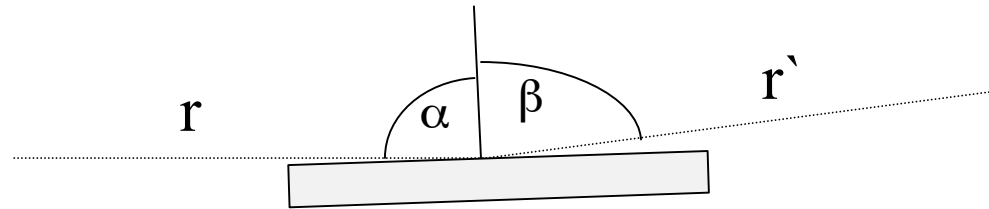
Example: toroidal mirror

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

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

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

Spherical Gratings



Optical path function

$$F_{100} = -n\lambda D_0 + (\sin \alpha - \sin \beta) \quad \textit{grating equation}$$

$$F_{200} = \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} + \frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right) \quad \textit{tangential focus}$$

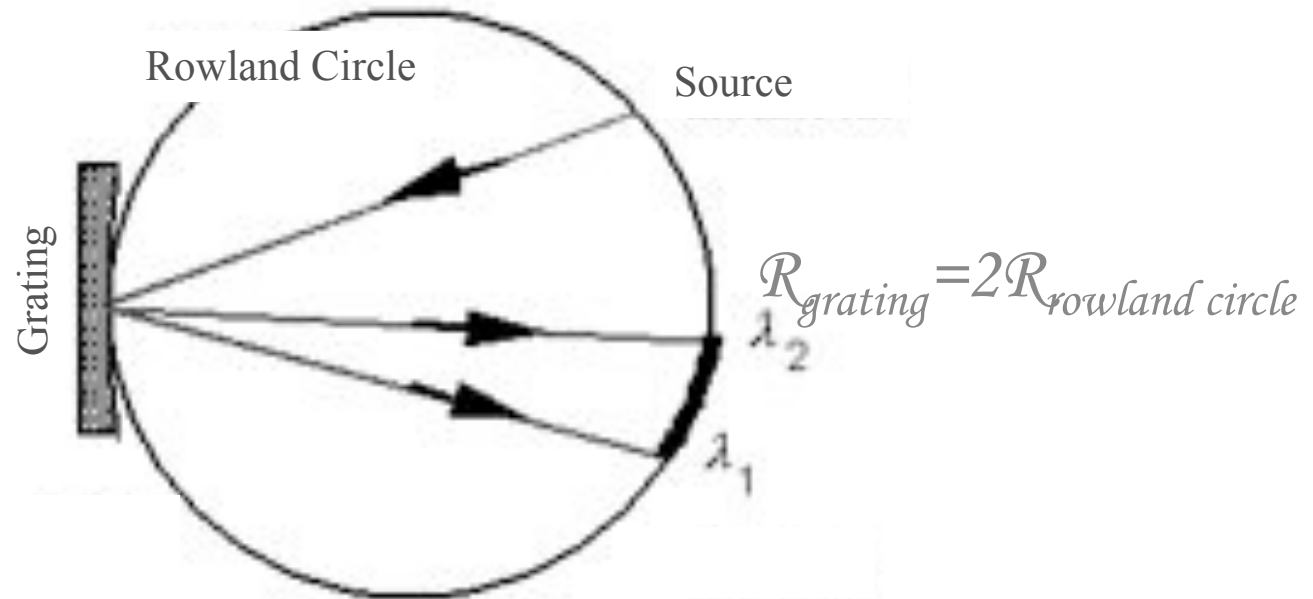
$$F_{300} = \left[\left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) \frac{\sin \alpha}{r} + \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right) \frac{\sin \beta}{r'} \right] \quad \textit{primary coma}$$

Spherical Gratings

$$F_{200} = F_{300} = 0$$

$$r' = R \cos \beta$$

$$r = R \cos \alpha$$



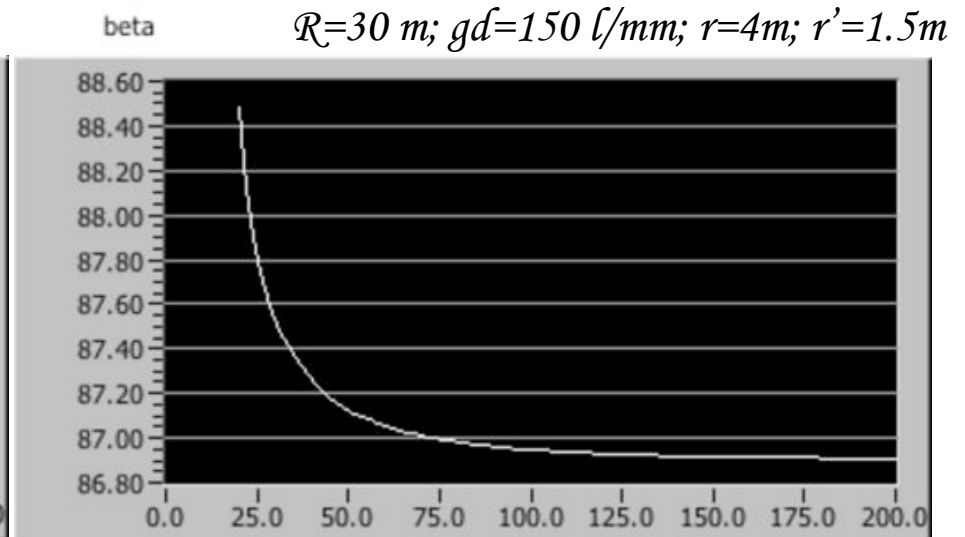
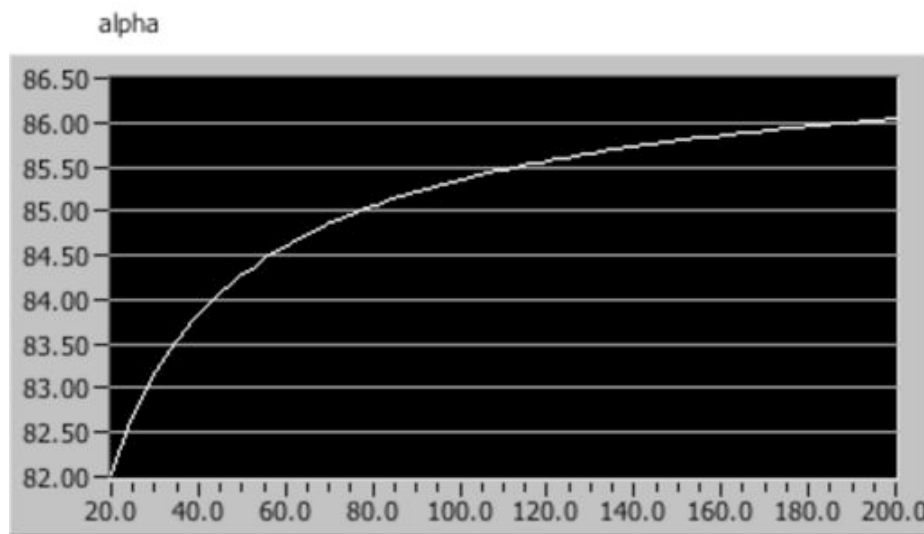
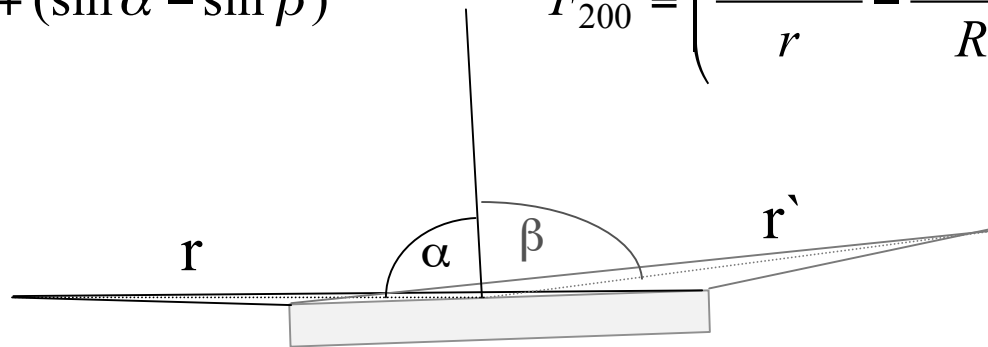
$$F_{200} = \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} + \frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right) \quad \text{tangential focus}$$

$$F_{300} = \left[\left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) \frac{\sin \alpha}{r} + \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right) \frac{\sin \beta}{r'} \right] \quad \text{primary coma}$$

Variable Included Angle Spherical Grating Monochromator

$$F_{100} = -n\lambda D_0 + (\sin \alpha - \sin \beta)$$

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

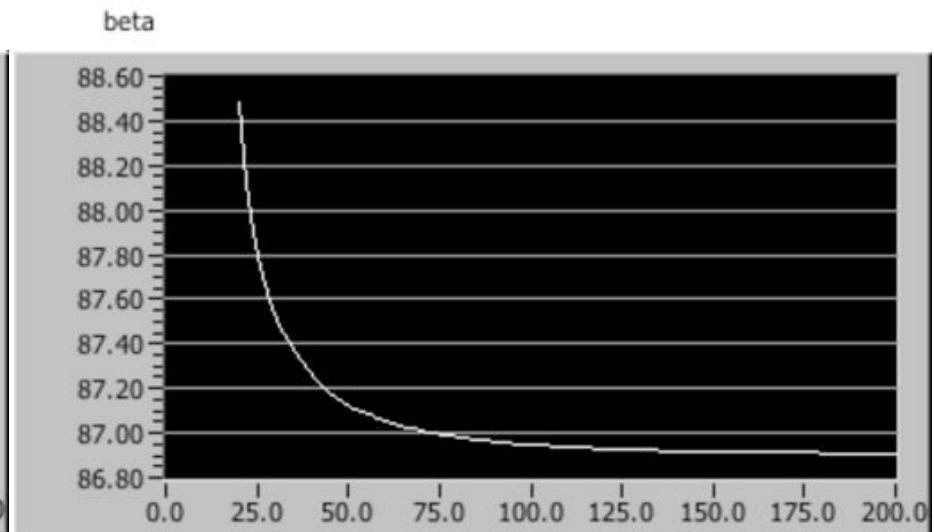
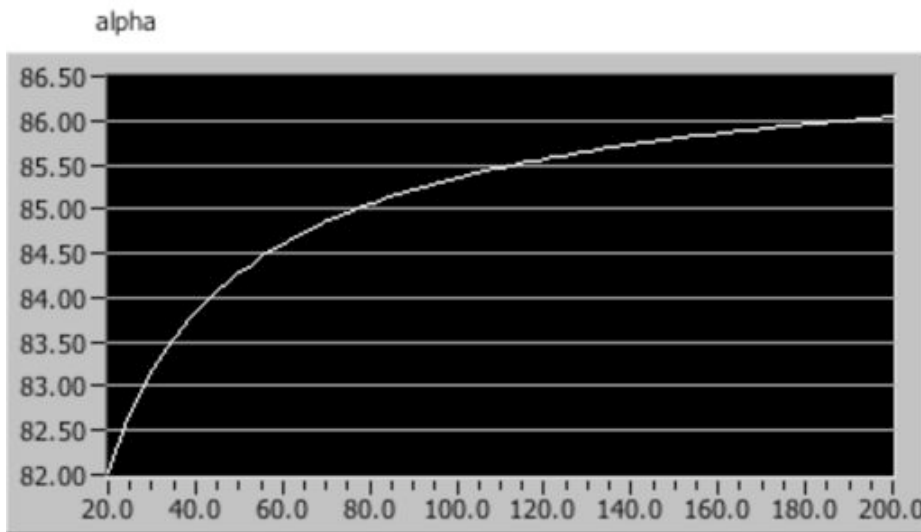
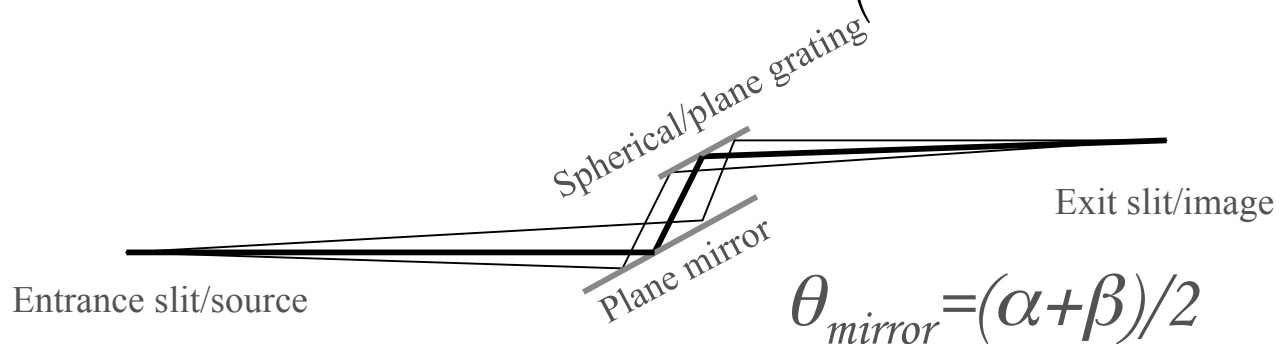


Maintain fixed source and image in position and direction

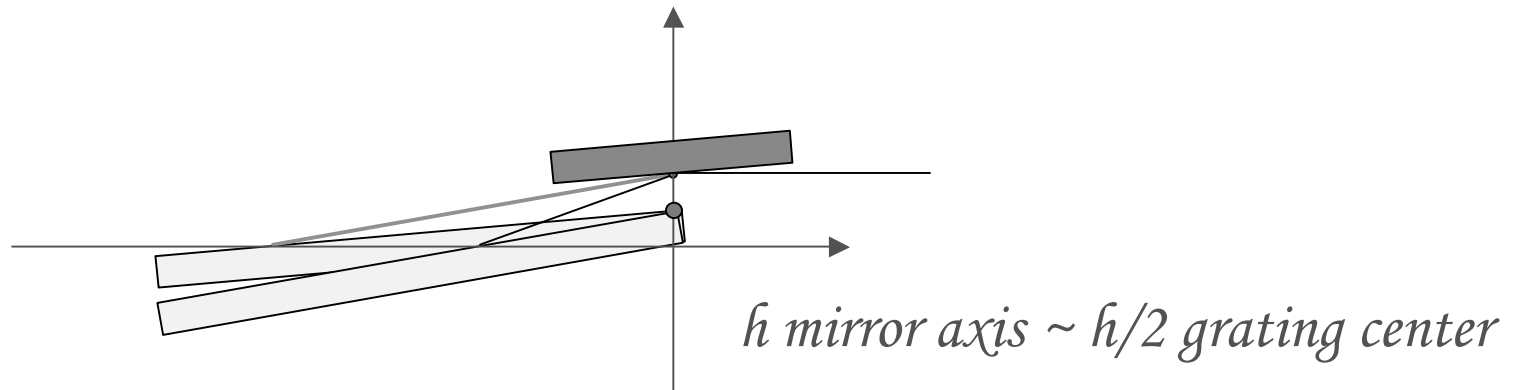
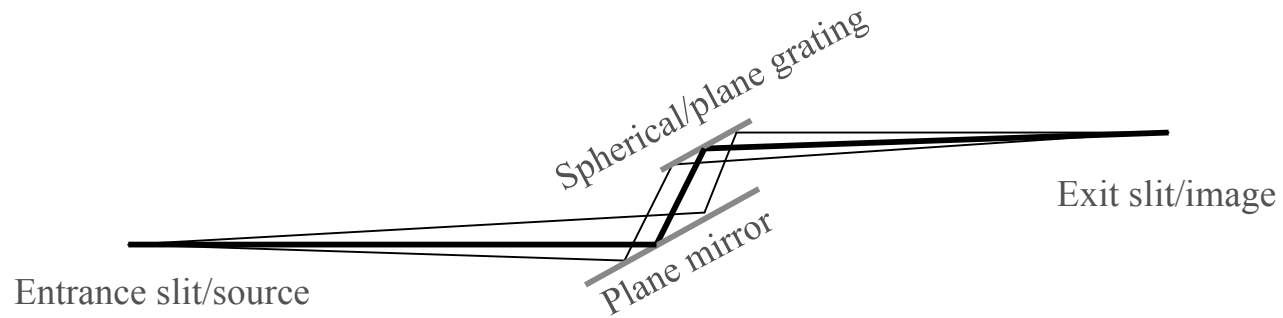
Variable Included Angle Spherical Grating Monochromator

$$F_{100} = -n\lambda D_0 + (\sin \alpha - \sin \beta)$$

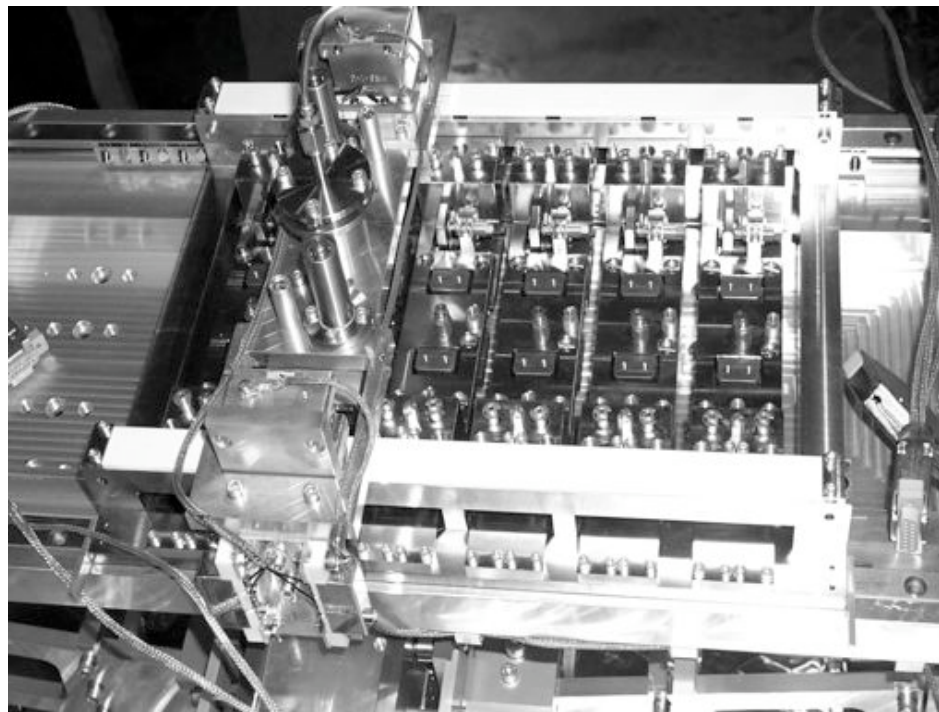
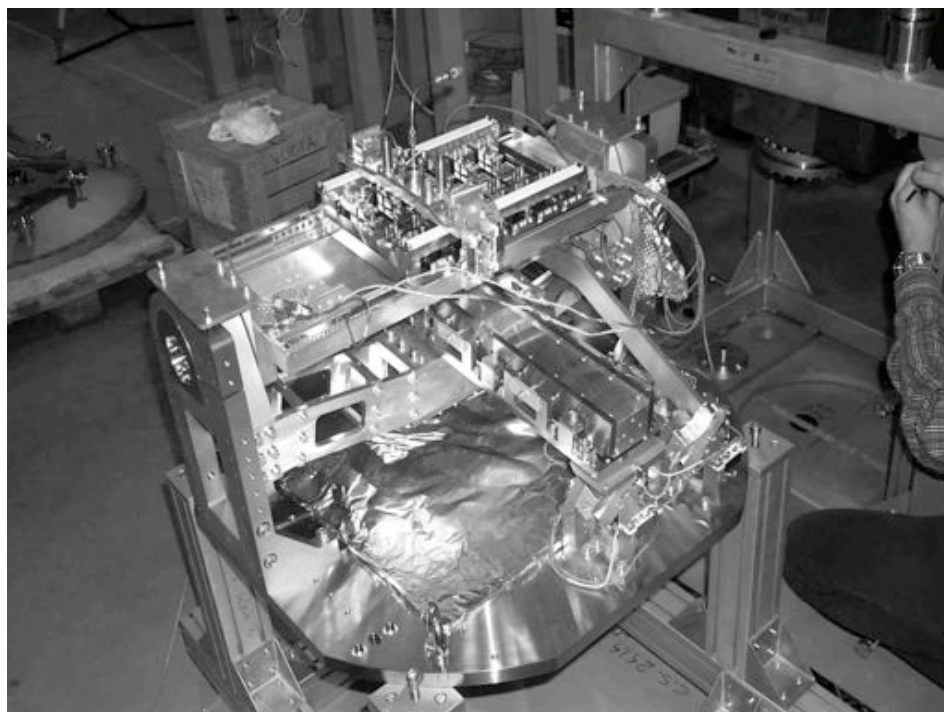
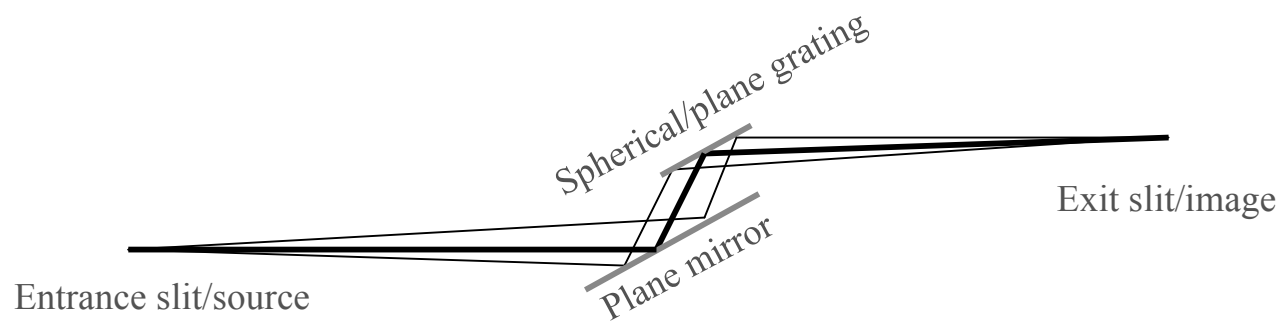
$$F_{200} = \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} + \frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right)$$



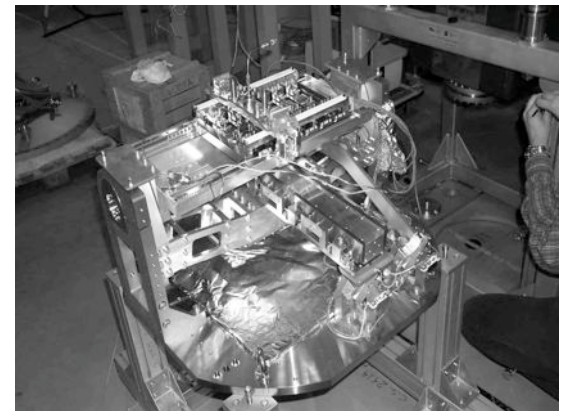
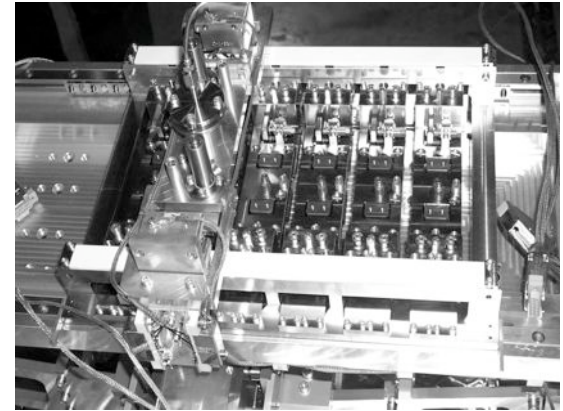
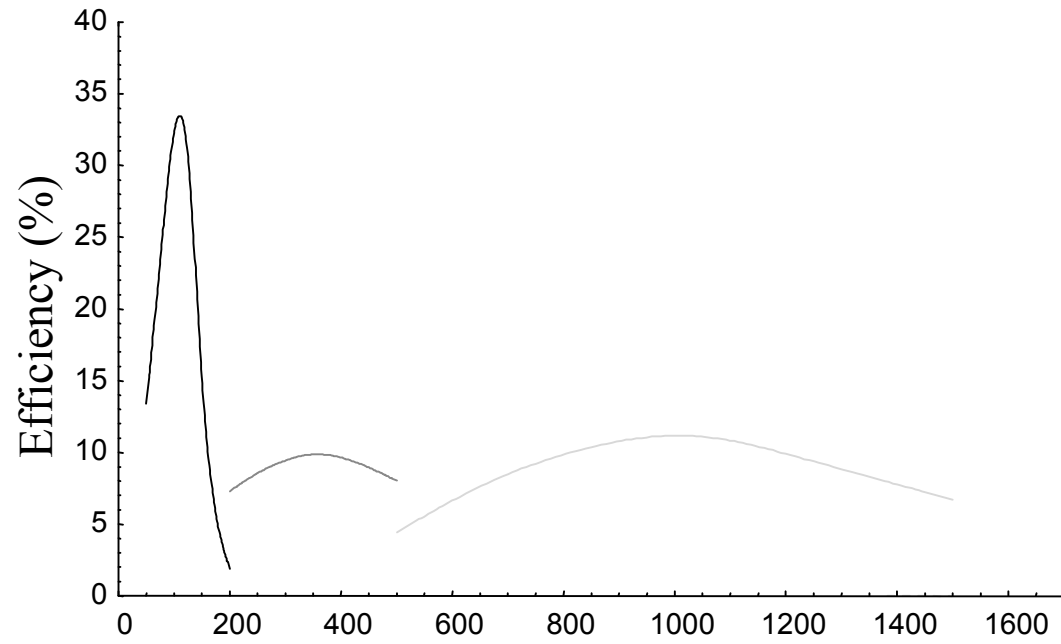
Variable Included Angle Spherical Grating Monochromator



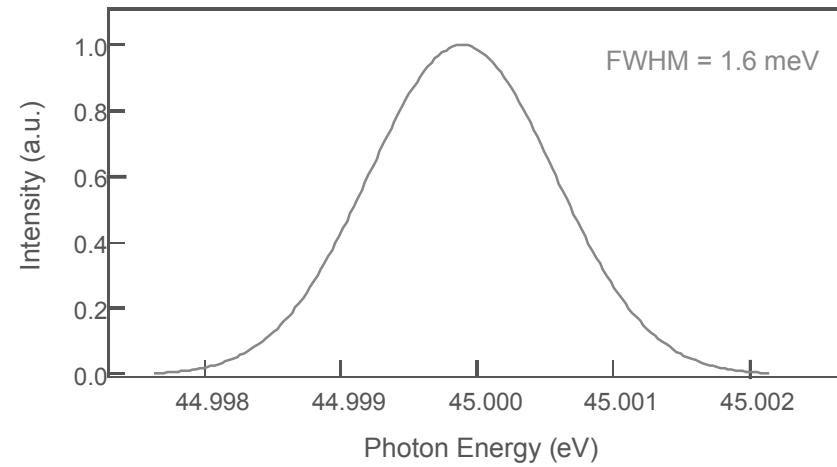
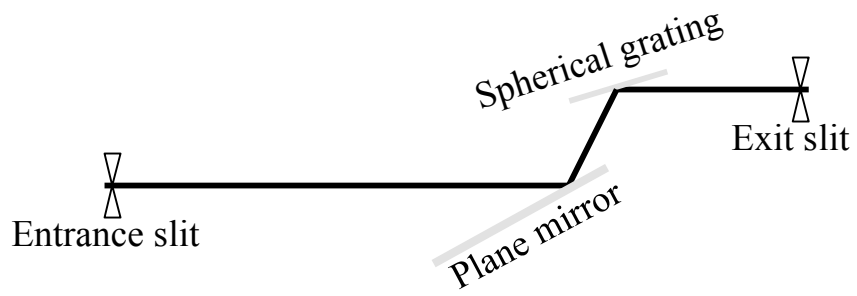
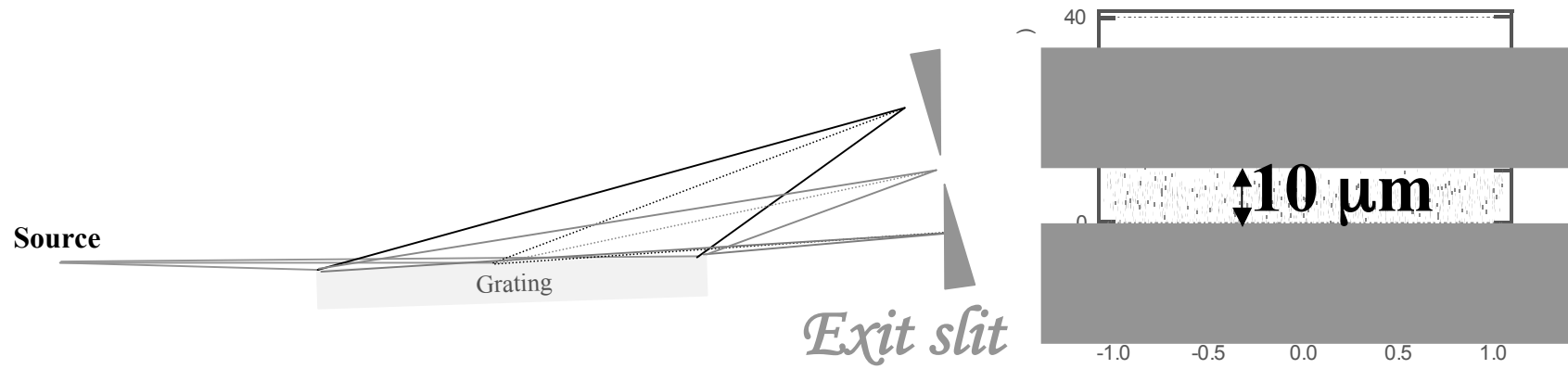
Variable Includ Angle Spherical Grating Monochromator



Efficiency Curves



Resolving Power



Resolving Power

$$Nk\lambda = \sin(\alpha) - \sin(\beta)$$

$$\left(\frac{\partial\lambda}{\partial\alpha}\right) = \frac{\cos(\alpha)}{Nk} \quad \Delta\alpha = \frac{s}{r}$$

$$\left(\frac{\partial\lambda}{\partial\beta}\right) = \frac{\cos(\beta)}{Nk} \quad \Delta\beta = \frac{s'}{r'}$$

$$\Delta\lambda_{\text{entrance}} = \frac{s \cdot \cos(\alpha)}{Nkr}$$

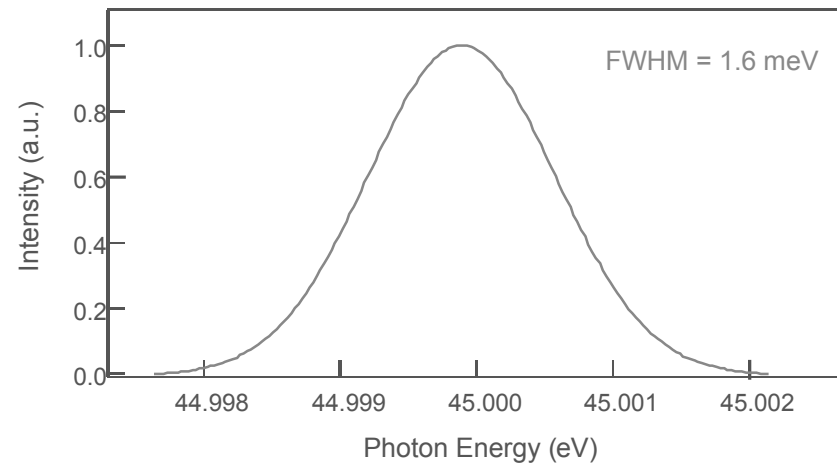
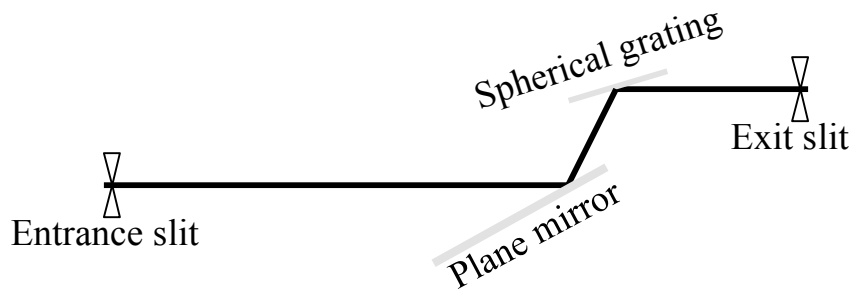
$$\Delta\lambda_{\text{exit}} = \frac{s' \cdot \cos(\beta)}{Nkr'}$$

smaller are s and s' ,
smaller will be the bandpass

entrance slit contribution

exit slit contribution

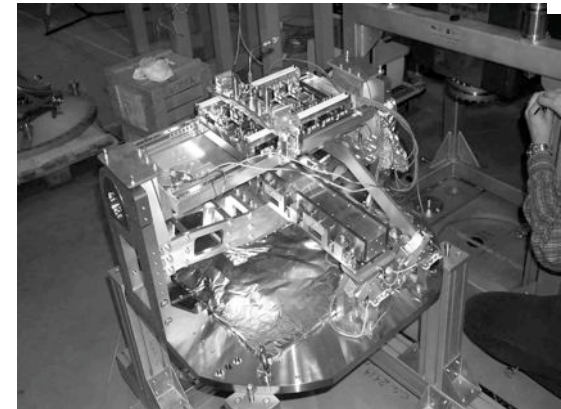
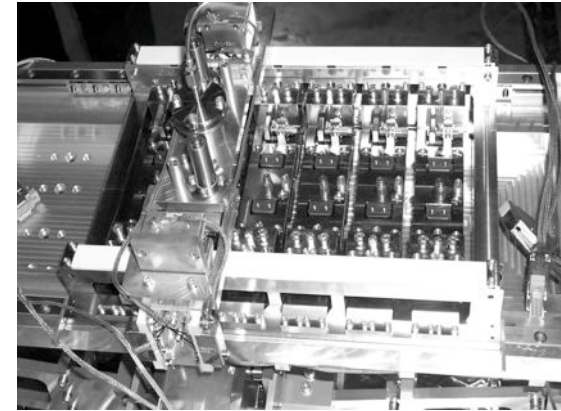
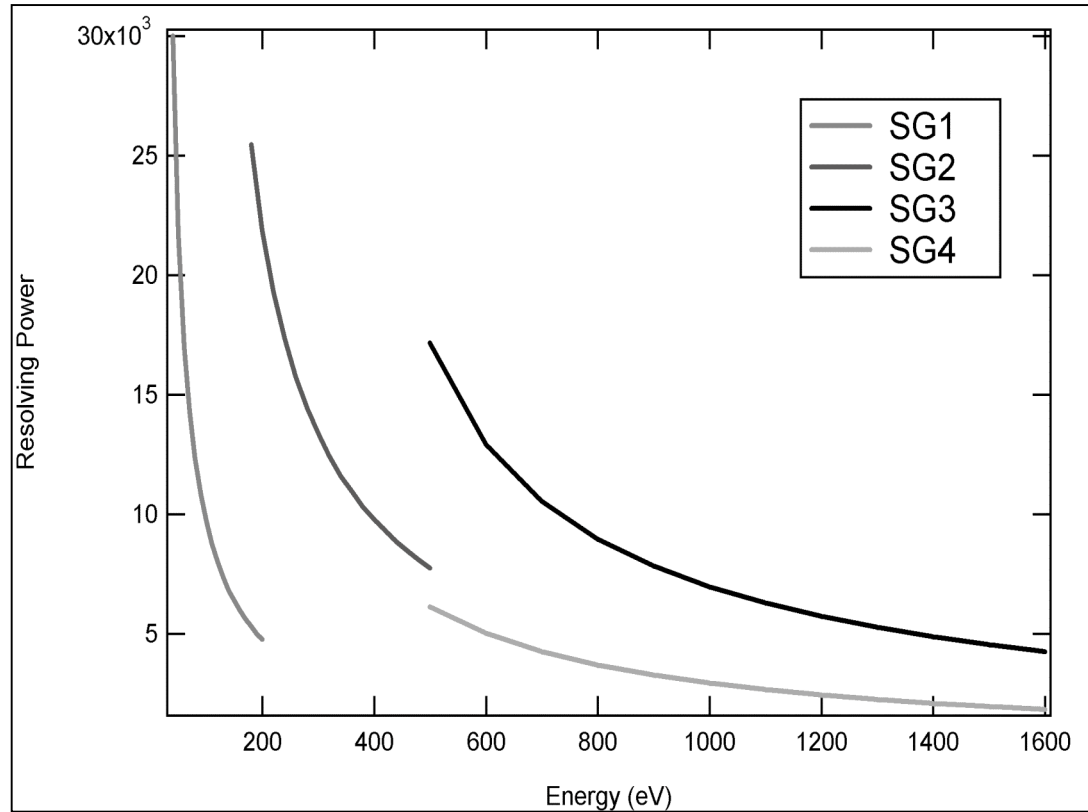
$$\mathcal{R}esolving\ power = \lambda/\Delta\lambda = E/\Delta E$$



$$45/0.0016 \approx 28000$$

Resolving Power

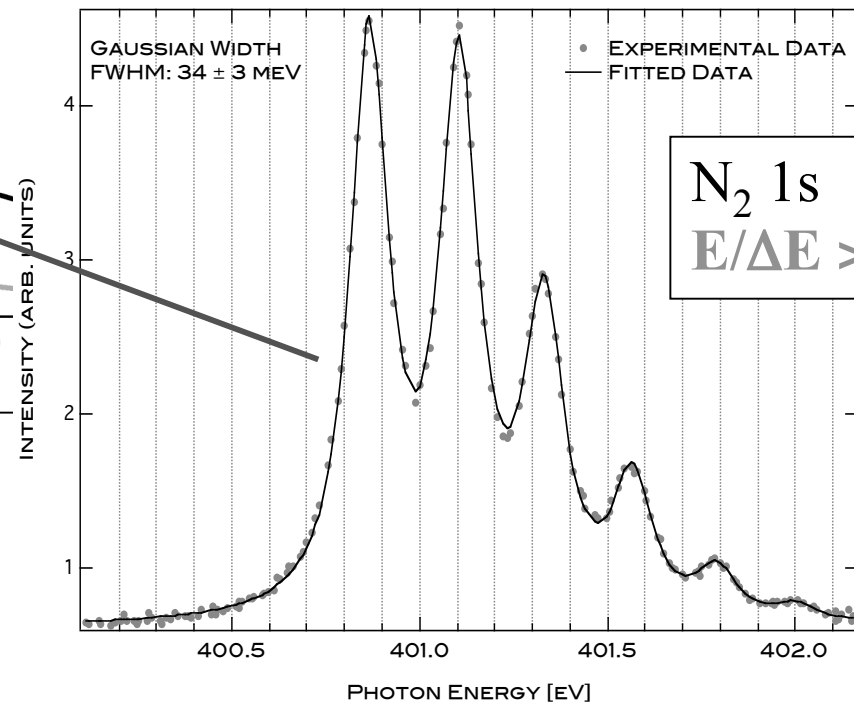
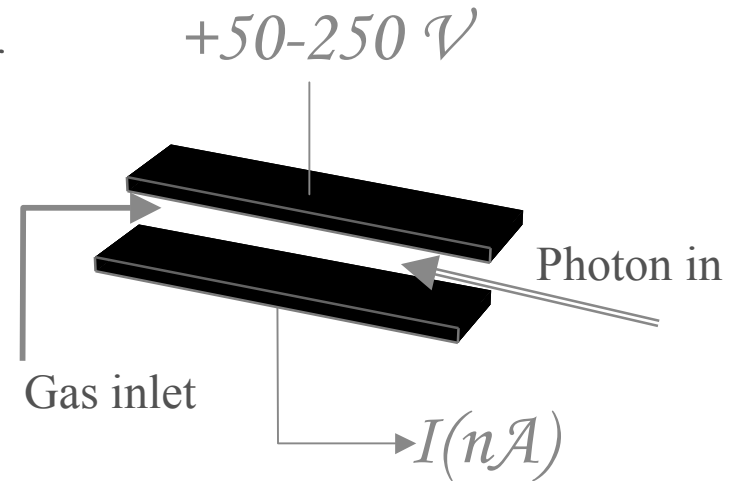
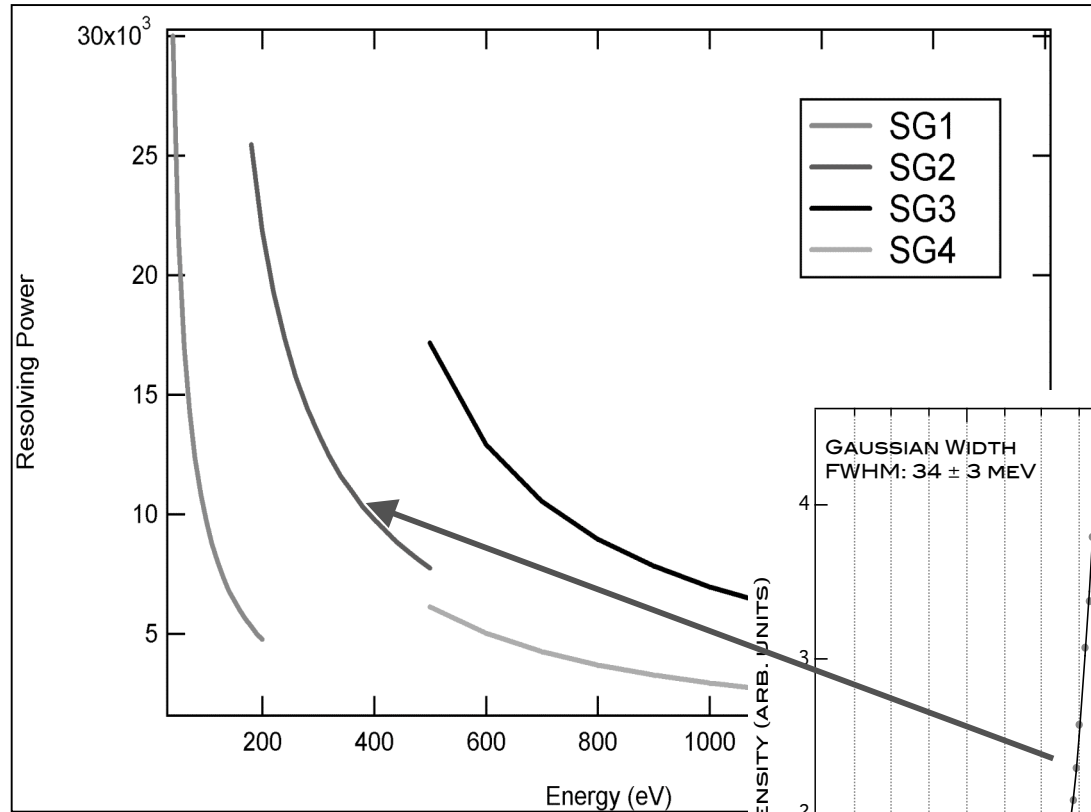
Typical Spherical grating monochromator resolving power



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

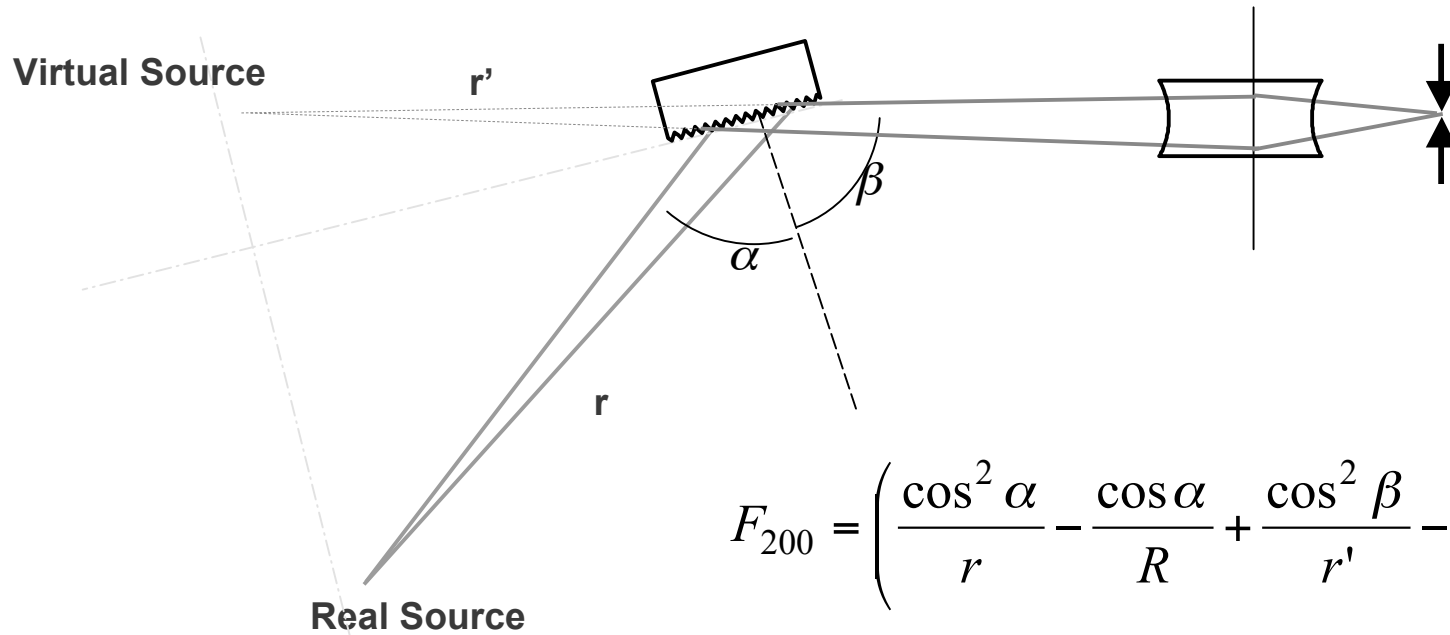
Resolving Power measurement

Typical Spherical grating monochromator resolving power



N₂ 1s
E/ΔE > 11000

Plane Grating



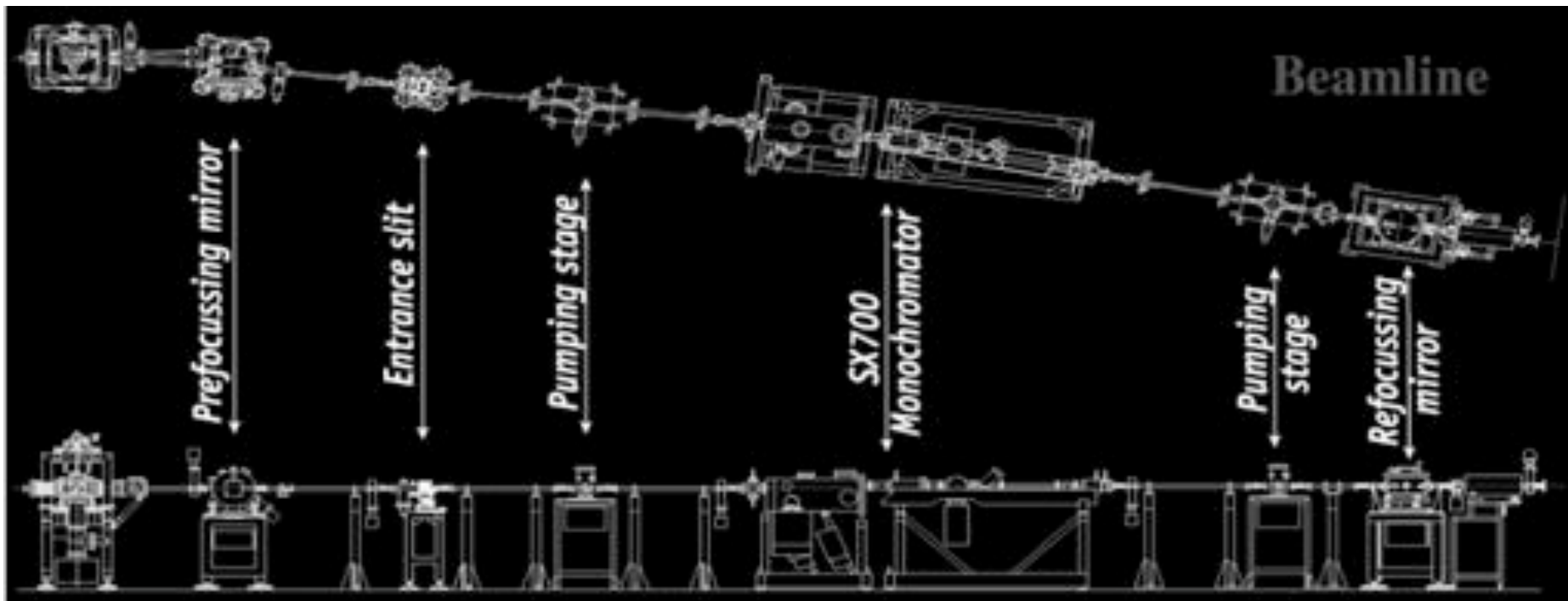
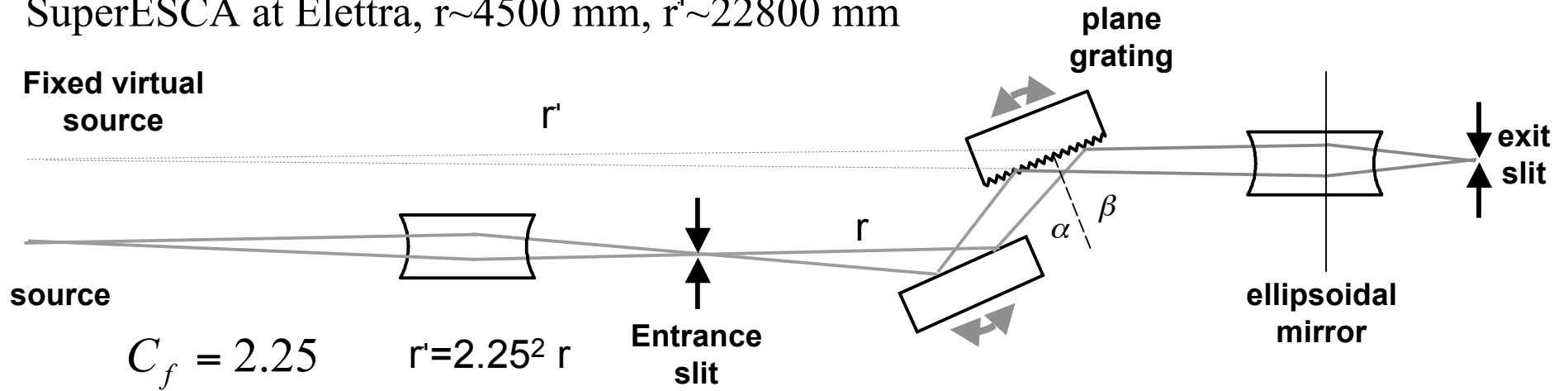
$$F_{200} = \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} + \frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right)$$

$$F_{200} = \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{\infty} + \frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{\infty} \right) = 0 \quad \frac{\cos^2 \alpha}{r} + \frac{\cos^2 \beta}{r'} = 0 \quad r' = -r \frac{\cos^2 \beta}{\cos^2 \alpha}$$

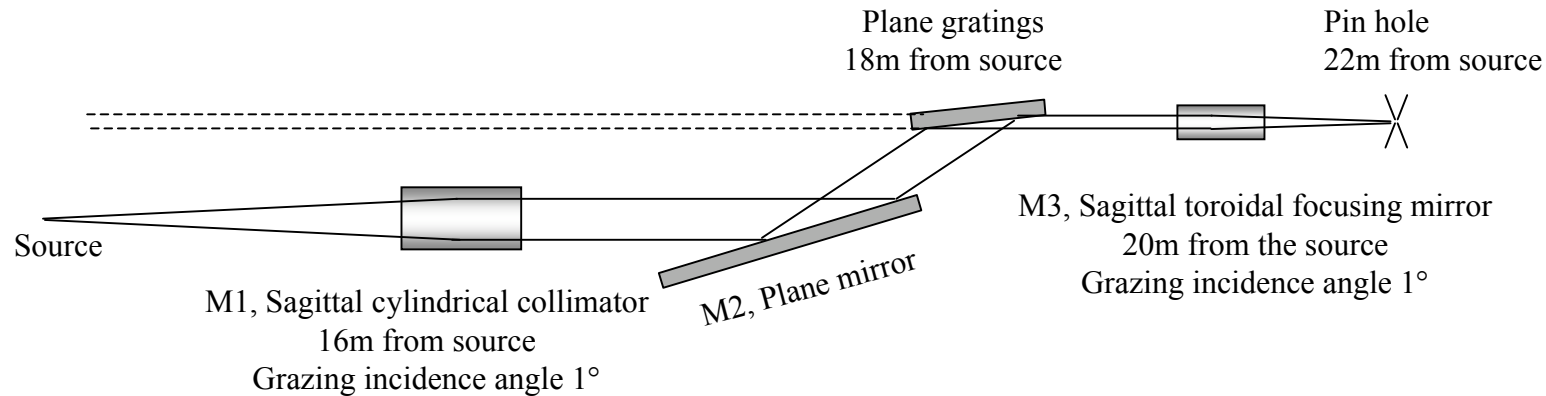
$$C_f = \frac{\cos \beta}{\cos \alpha} \quad |r'| = r C_f^2$$

SX 700

SuperESCA at Elettra, $r \sim 4500$ mm, $r' \sim 22800$ mm



Collimated light SX 700



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

One can select to work in:

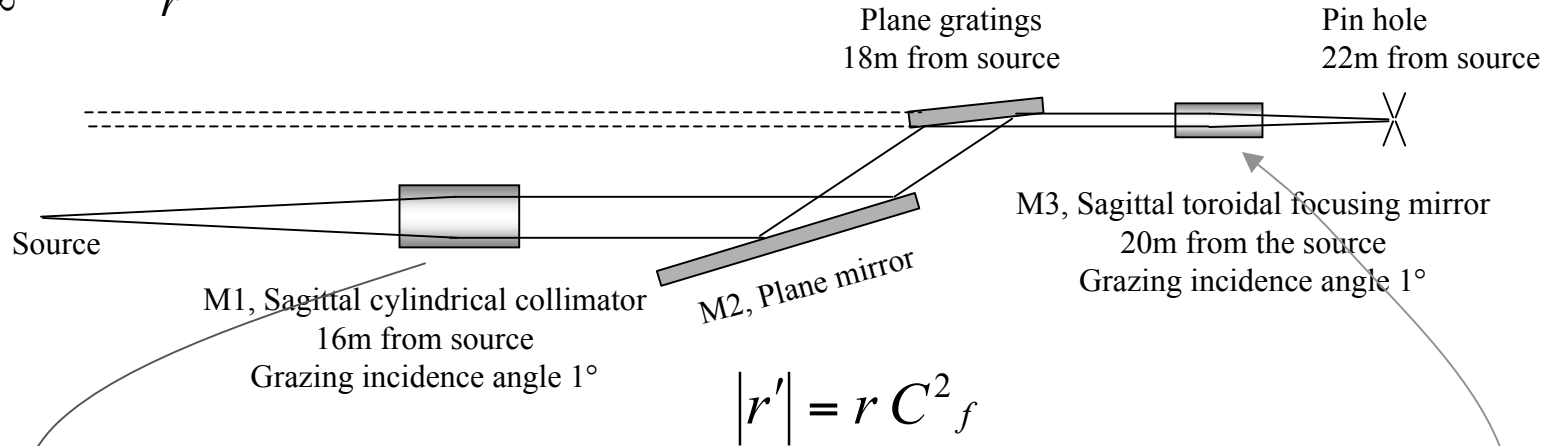
High resolution mode (accept to loose some flux)

High efficiency mode (accept a reduction of resolution)

High order suppression mode (with a typical appreciable reduction of flux)

Collimated Light SX 700

$$\frac{\cos^2 \alpha}{\infty} + \frac{\cos^2 \beta}{r'} = 0 \Rightarrow r' = \infty$$



In principle one can work with any C_f value, higher or lower than 1 but...

→ This mirror do not produce a perfectly collimated light (NEVER)

→ divergence changes with C_f

This mirror is no more able to focus the radiation

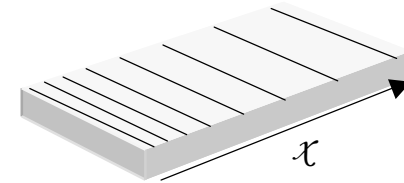
Problem amplified for C_f value lower than 1

Variable groove density gratings

Groove density D varies along the grating surface: $D(x) = D_0 + D_1x + D_2x^2 + D_3x^3 + \dots$

$$F_{200} = \frac{1}{2} \left(-n\lambda D_1 + \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{\mathcal{R}} + \frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{\mathcal{R}} \right) \right)$$

$$F_{300} = -\frac{1}{3} n\lambda D_2 + \frac{1}{2} \left[\left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{\mathcal{R}} \right) \frac{\sin \alpha}{r} + \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{\mathcal{R}} \right) \frac{\sin \beta}{r'} \right]$$



$$F_{200} = \frac{1}{2} \left(-n\lambda D_1 + \left(\frac{\cos^2 \alpha}{r} + \frac{\cos^2 \beta}{r'} \right) \right) \quad \text{A plane grating can focus!}$$

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

$$\sin \beta = \sin \alpha - n\lambda D$$

