X-ray Optics

Daniele Cocco

Sincrotrone Trieste ScpA, S.S. 14 Km 163.5 in Area Science Park, 34012 Trieste, ITALY
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 \( \mu = 1 - \delta - i\beta \)

\[
\delta = \left( e^2 \lambda^2 / 2\pi mc^2 \right) N + \sum N_H \frac{\lambda}{\lambda_H} \ln \left[ \frac{\lambda_H}{\lambda^2} - 1 \right]
\]

\( \delta \) (unit decrement) related to the speed in the medium

\( \beta \) related to the absorption

\( N = \) electron density \((10^{23} - 10^{24} \text{ el./cm}^3)\)

\( \lambda_H = \) adsorption edge’s wavelength

\( \lambda \) far from \( \lambda_H \) \( \Rightarrow \delta = Ne^2\lambda^2 / 2\pi mc^2 \)

\( \beta = \lambda \mu / 4\pi \quad \mu = \) linear absorption coefficient
Snell Law

\[ n > 1 \]

\[ n < 1 \]

Snell’s law: \( n_1 \cos \gamma = n_2 \cos i \)
Snell Law

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

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

\[ \delta \approx 10^{-4} \quad HXR \Rightarrow f \approx 1m \quad if \quad R \approx 1mm \]
\[ \delta \approx 10^{-4} \quad HXR \Rightarrow f \approx 1m \quad \text{if} \quad R \approx 1\text{mm} \]
Snell’s law: \( \cos \gamma = \cos i / n \)

\( \gamma = 0 \quad n = \cos i_c \)

\( i_c \) critical angle: total external reflection

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

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

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (g/cm(^3))</th>
<th>( N ) (electron/cm(^3))</th>
<th>( \lambda_{\text{min}} ) (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pentadecane (oil)</td>
<td>0.77</td>
<td>( 7 \times 10^{22} )</td>
<td>64.1sin( i )</td>
</tr>
<tr>
<td>Glass</td>
<td>2.6</td>
<td>( 78 \times 10^{22} )</td>
<td>37.9sin( i )</td>
</tr>
<tr>
<td>Aluminum oxide</td>
<td>3.9</td>
<td>( 115 \times 10^{22} )</td>
<td>31.2sin( i )</td>
</tr>
<tr>
<td>Gold</td>
<td>19.3</td>
<td>( 466 \times 10^{22} )</td>
<td>15.4sin( i )</td>
</tr>
</tbody>
</table>

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

\( \lambda_{\text{min, gold}} = 1.34\text{nm} = 923\text{eV} \)

Shorter wavelength needs smaller angles of incidence.

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

Gold

reflectivity

Photon energy (eV)

0.0 0.2 0.4 0.6 0.8 1.0

0 500 1000 1500 2000

20° 10° 5° 3° 1° 2°
Hard X-ray reflectivity

\[ \theta \]

\[ \text{Reflectivity} \]

\[ \text{Angle (deg)} \]

\[ \text{W Rho=19.3, Sig=0 nm, P=1, E=20000 eV} \]

\[ \text{Pt Rho=21.45, Sig=0 nm, P=1, E=30000 eV} \]
Other coatings

Fused Silica

Ni

SiC

C

Al

Au

reflectivity vs. Photon energy (eV)

θ = 2°
Effect of Defects (slope errors)

\[ \Delta s' = 2r'\sigma \]
Image (spot) enlargement

\[ \Delta s' = 2r'\sigma \]

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

Tangential focusing

Object

Image

vertical position \((\mu m)\)

horizontal position \((\mu m)\)
Image (spot) enlargement

\[ \Delta s' = 2 \, r' \sigma \]

Slope error contribution FWHM (\(\mu m\))

Distance mirror-image = 1m

Slope error [rms] (\(\mu rad\))

Slope error = 2.5 \(\mu rad\)
Typical manufacturer capabilities (SESO, ZEISS, Winlight, Jobin Yvon)

<table>
<thead>
<tr>
<th>Shape</th>
<th>Length</th>
<th>rms errors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spherical/flat</td>
<td>Up to 500 mm</td>
<td>&lt; 0.5 µrad</td>
</tr>
<tr>
<td>Spherical/flat</td>
<td>&gt; 500 mm</td>
<td>1 µrad</td>
</tr>
<tr>
<td>Toroidal</td>
<td>Up to 500 mm</td>
<td>≥ 1 µrad</td>
</tr>
<tr>
<td>Toroidal</td>
<td>&gt; 500 mm</td>
<td>≥ 1-2 µrad</td>
</tr>
<tr>
<td>Aspherical</td>
<td>Up to 500 mm</td>
<td>≥ 1-2 µrad</td>
</tr>
<tr>
<td>Aspherical</td>
<td>&gt; 500 mm</td>
<td>≥ 2 µrad</td>
</tr>
</tbody>
</table>
Mirror profile precision

Typical manufacturer capabilities (SESO, ZEISS, Winlight, Jobin Yvon)
**Tangential and Sagital focusing geometries**

**Term $F_{20}$ of the optical path function**

$\frac{1}{r} + \frac{1}{r'} \cos \theta / 2 = 1/R$

spherical mirror

**Term $F_{02}$ of the optical path function**

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

cylindrical/toroidal mirror

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

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

Solution: work in 1:1 configuration

Spherical mirror suffer of spherical aberration

Deviations from perfect imaging are called aberrations
The bicycle tyre toroid is generated by rotating a circle of radius \( \rho \) 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: \[
\left(\frac{1}{r} + \frac{1}{r'}\right) \frac{\cos \theta}{2} = \frac{1}{R}
\]

Sagittal focus: \[
\left(\frac{1}{r} + \frac{1}{r'}\right) \frac{1}{2\cos \theta} = \frac{1}{\rho}
\]

Stigmatic image: \[
\frac{\rho}{R} = \cos^2 \theta
\]
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 Sagital focus
Other focusing geometries

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

Beam divergence 100X100 $\mu$rad

Spherical  
No slope errors

Elliptical  
No slope errors

Sagittal cylinder  
No slope errors

Source  
Image
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: \( a = f \cos^2 \theta \)

Position of the pole P:

\[
X_o = a \tan^2 \theta \\
Y_o = 2a \tan \theta
\]

Paraboloid equation:

\[
x^2 \sin^2 \theta + y^2 \cos^2 \theta + z^2 - 2xy \sin \theta \cos \theta - 4ax \sec \theta = 0
\]

J.B. West and H.A. Padmore, Optical Engineering, 1987
Other mirror defect - Roughness

Slope errors = every deviation from the ideal surface with period larger then ~ 1.2 mm

Typical definition is μrad or arcsec rms.
Alternative definition is λ/10 or λ/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 then ~ 0.5-1 mm

Typical definition is Årms.
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 then width 20-10 means 20/1000 of mm max scratch width 10/100 mm max dig dimension
Roughness

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

\[ \sigma = \sqrt{\frac{1}{n} \sum_{x=0}^{n} \left[ s(x) - \bar{s}(x) \right]^2} \]
Roughness
Power spectral density

Slope errors
($SF < 0.5-0.2 \text{ mm}^{-1}$)

Roughness ($SF > 1\text{ mm}^{-1}$)
Roughness
Flux reduction

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

<table>
<thead>
<tr>
<th>Shape</th>
<th>Spherical/Flat</th>
<th>Toroidal/aspherical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Roughness (Å)</td>
<td>3 standard 1 best</td>
<td>5 standard 3 best (1-2 if very lucky)</td>
</tr>
</tbody>
</table>
Synchrotron Radiation Beamlines

Prefocusing section:
- Adapt the source to the monochromator requirements
- Adsorb the unwanted power radiation

Monochromator: Select the proper photon energy

Refocusing section: Adapt the spot shape at the necessity of the experiment
There are several reasons to choose a mirror substrate, one is the power arriving on it.
SR sources

An electron travels towards an undulator at a speed, \( v \), close to the speed of light. Because of relativity, it “sees” the length \( L \) and the period \( L/n \) (\( n \) = number of periods) of the undulator shrinking by a factor \( \gamma \). The undulator forces an electron to wiggle emit synchrotron radiation with wavelength equal to (slurk) period. Because of the electron's motion (Doppler effect), when seen from a laboratory point of view, the wavelength further shrinks by a factor \( \gamma \).

\[ \lambda \approx L/2\gamma^2 n \]

\[ e^- \]

\[ h \nu \]

FWHM value: 28022.7
Integral is: 295.618
Peak at: (5600.00, 0.00873100)

Energy [eV]

Power [Watts/eV]

Horizontal

Vertical
Thermal deformations

400W → 1μm, 10 to 100 time larger than wished.
### Properties of typical mirror materials

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

**Reflecting coating**

**Bulk material**

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

[Image of silicon bulk mirrors with dimensions 600 mm and 110 mm indicated]
Direct side cooling
Direct side cooling

1st mirror sagittally oriented

\[ \Delta s'_s = 2 r' \cos \theta \sigma_s \]

Object  
Sagittal focusing  
Image

image

\( \sigma_s \)
# Internally cooled mirrors

<table>
<thead>
<tr>
<th>Shape</th>
<th>Spherical/Flat</th>
</tr>
</thead>
<tbody>
<tr>
<td>Roughness (Å)</td>
<td>3 standard 1 best</td>
</tr>
<tr>
<td>Glass/Silicon</td>
<td>5 standard 2-3 best</td>
</tr>
<tr>
<td>Metallic</td>
<td></td>
</tr>
</tbody>
</table>

**Roughness (Å)**

- Glass/Silicon: 10 Å
- Metallic: 5 Å

**Intensity reduction (%)**

- 3 Å rms
- 10 Å rms

---

D. Cocco X-Ray optics, Erice, 6-15 April 2011
Internally cooled mirrors (Glidcop)

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

$\Delta T = 7.7^\circ$

3GeV Synchrotron source
6.6 cm period undulator $K_{max} = 5.7$
BL6.1
## Invar & SuperInvar

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (gm/cc)</th>
<th>Young's Modulus (GPa)</th>
<th>Thermal Expansion ($\alpha$) ppm/$^\circ$C</th>
<th>Thermal Conductivity (k) W/m/$^\circ$C</th>
<th>Figure of Merit (k/$\alpha$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silicon</td>
<td>2.33</td>
<td>131</td>
<td>2.60</td>
<td>156</td>
<td>60</td>
</tr>
<tr>
<td>SiC CVD</td>
<td>3.21</td>
<td>461</td>
<td>2.40</td>
<td>198</td>
<td>82</td>
</tr>
<tr>
<td>Aluminum</td>
<td>2.70</td>
<td>68</td>
<td>22.5</td>
<td>167</td>
<td>7.42</td>
</tr>
<tr>
<td>Copper</td>
<td>8.94</td>
<td>117</td>
<td>16.5</td>
<td>391</td>
<td>23.7</td>
</tr>
<tr>
<td>Glidcop</td>
<td>8.84</td>
<td>130</td>
<td>16.6</td>
<td>365</td>
<td>22</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>10.22</td>
<td>324.8</td>
<td>4.80</td>
<td>142</td>
<td>29.6</td>
</tr>
<tr>
<td>Invar 36</td>
<td>9.05</td>
<td>141</td>
<td>0.5</td>
<td>10.4</td>
<td>20.8</td>
</tr>
<tr>
<td>SuperInvar</td>
<td>8.13</td>
<td>145</td>
<td>0.06</td>
<td>10.5</td>
<td>210</td>
</tr>
</tbody>
</table>

**INVAR®**
- Carpenter Technology Inc.
- Alloy 36 iron-nickel(36%) alloy with carbon (0.02%), manganese (0.35%), Silicon (0.2%)
- SuperInvar: iron-nickel(32%) alloy with carbon (0.02%), manganese (0.40%), Silicon (0.25%), Cobalt (5.5%)
SuperInvar

<table>
<thead>
<tr>
<th>Density</th>
<th>Young’s modulus</th>
<th>Thermal expansion</th>
<th>Thermal conductivity</th>
<th>Figure of merit</th>
</tr>
</thead>
<tbody>
<tr>
<td>gm/cc</td>
<td>GPa</td>
<td>($\alpha$) ppm/$^\circ$C</td>
<td>(k) W/m/$^\circ$C</td>
<td>k/$\alpha$</td>
</tr>
<tr>
<td>Glidcop</td>
<td>8.84</td>
<td>130</td>
<td>16.6</td>
<td>365</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>10.22</td>
<td>324.8</td>
<td>4.80</td>
<td>142</td>
</tr>
<tr>
<td>SuperInvar</td>
<td>8.13</td>
<td>145</td>
<td>0.06</td>
<td>10.5</td>
</tr>
</tbody>
</table>

$\Delta h = 6 \mu m$

$\Delta T = 130^\circ$
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 ($\approx 270$ eV)
- Reduction of reflectivity due to enhancement of the surface roughness
- General deterioration of the surface
Effect of the contamination:

Strong adsorption at the carbon edge ($\approx 270$ 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 ($\approx 270$ 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*

---

![Graph showing intensity vs. photon energy with peaks at 536.2 eV, 542.8 eV, and 571 eV for Cr contamination, and 578 eV for Other Contamination.](image-url)
Dispersive elements

$n\lambda = d (\sin(\alpha) - \sin(\beta))$
Grating’s profiles

Blaze profile

Laminar profile

Blaze gratings:
- Higher efficiency

Laminar gratings:
- Higher spectral purity
- Higher resolution

Blaze condition

Blaze angle = (α + β) / 2

Internal Orders (+)
Zero order
External Orders (-)

\[ \frac{1}{2} \lambda = d \left( \sin(\alpha) - \sin(\beta) \right) \]

D. Cocco X-Ray optics, Erice, 6-15 April 2011
Grating's efficiency

Blaze profile

Laminar profile

\[ n\lambda = d(\sin(\alpha) - \sin(\beta)) \]
Grating's efficiency

Blaze profile

Laminar profile

 Efficiency (%)

Blaze angle ($\theta$) (deg)

Efficiency (%)

groove height (nm)

$\gamma=90^\circ$, $gd=2400$ l/mm

$W=60\%$, $gd=2400$ l/mm

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

Diamond tool

Gold (Cr) layer

Si substrate
Holographic Recorded Gratings

Exposure

Development

Ion etching

Photoresist removal

Coating
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:

\[ \int_{A}^{B} n(\vec{r})dl = \int_{A}^{C} \frac{c}{v} dl = c \int_{A}^{B} dt \]
For a classical grating with rectilinear grooves parallel to \( z \) with constant spacing \( d \), the optical path length is:

\[
F = AP + PB + kN \lambda y
\]

where \( \lambda \) is the wavelength of the diffracted light, \( k \) is the order of diffraction (\( \pm 1, \pm 2, \ldots \)), \( N = 1/d \) is the groove density.
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 \((y,z)\).
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.

Equations:

\[ F = AP + PB + kN \lambda y \]

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

\( j = \) 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

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

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

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

\[ a_{02} = \frac{1}{4 f \cos \vartheta}; \quad a_{20} = \frac{\cos \vartheta}{4 f}; \quad a_{04} = \frac{b^2}{64 f^3 \cos^3 \vartheta} \left[ \frac{\sin^2 \vartheta}{b^2} + \frac{1}{a^2} \right]; \]
\[ a_{12} = \frac{\tan \vartheta}{8 f^2 \cos \vartheta} \sqrt{e^2 - \sin^2 \vartheta}; \quad a_{30} = \frac{\sin \vartheta}{8 f^2 \sqrt{e^2 - \sin^2 \vartheta}} ; \]
\[ a_{40} = \frac{b^2}{64 f^3 \cos^3 \vartheta} \left[ \frac{5 \sin^2 \vartheta \cos^2 \vartheta}{b^2} - \frac{5 \sin^2 \vartheta}{a^2} + \frac{1}{a^2} \right]; \]
\[ a_{22} = \frac{\sin^2 \vartheta}{16 f^3 \cos^3 \vartheta} \left[ \frac{3}{2} \cos^2 \vartheta - \frac{b^2}{a^2} \left( 1 - \frac{\cos^2 \vartheta}{2} \right) \right] \]

where \( f = \left[ \frac{1}{r} + \frac{1}{r'} \right]^{-1} \)
Optical Path Function

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

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

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

\[ + yz F_{111} + \frac{1}{2} y F_{102} + \frac{1}{4} y^2 F_{202} + \frac{1}{2} y^2 z F_{211} + \ldots \]

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

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

\[ x_a = r \cos \alpha \quad y_a = r \sin \alpha \]

\[ x_b = r' \cos \beta \quad y_b = r' \sin \beta \]
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

\[ F_{000} = r + r' \]
\[ F_{100} = Nk\lambda - (\sin \alpha + \sin \beta) \]
\[ F_{200} = \left( \frac{\cos^2 \alpha}{r} + \frac{\cos^2 \beta}{r'} \right) - 2a_{20}(\cos \alpha + \cos \beta) \]
\[ F_{020} = \frac{1}{r} + \frac{1}{r'} - 2a_{02}(\cos \alpha + \cos \beta) \]
\[ F_{300} = \left[ \frac{T(r, \alpha)}{r} \right] \sin \alpha + \left[ \frac{T(r', \beta)}{r'} \right] \sin \beta - 2a_{30}(\cos \alpha + \cos \beta) \]
\[ F_{120} = \left[ \frac{S(r, \alpha)}{r} \right] \sin \alpha + \left[ \frac{S(r', \beta)}{r'} \right] \sin \beta - 2a_{12}(\cos \alpha + \cos \beta) \]

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

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

For \( r, r' \gg z_a, z_b \)
Aberrations Terms

\[ F_{100} = 0 \quad \rightarrow \quad \sin \alpha + \sin \beta_0 = Nk\lambda \quad \text{grating equation} \]

Most important imaging errors:

<table>
<thead>
<tr>
<th>Term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>F_{200}</td>
<td>defocus</td>
</tr>
<tr>
<td>F_{020}</td>
<td>astigmatism</td>
</tr>
<tr>
<td>F_{300}</td>
<td>primary coma (aperture defect)</td>
</tr>
<tr>
<td>F_{120}</td>
<td>astigmatic coma</td>
</tr>
<tr>
<td>F_{400} F_{220} F_{040}</td>
<td>spherical aberration</td>
</tr>
</tbody>
</table>

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:

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

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

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

Example: toroidal mirror

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

and imposing \( \alpha = -\beta = \theta \)

\[
\left( \frac{1}{r} + \frac{1}{r''} \right) \frac{\cos \theta}{2} = \frac{1}{R} \quad \left( \frac{1}{r} + \frac{1}{r''} \right) \frac{1}{2 \cos \theta} = \frac{1}{\rho}
\]
Spherical Gratings

Optical path function

\[ F_{100} = -n \lambda D_0 + (\sin \alpha - \sin \beta) \quad \text{grating equation} \]

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

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

\[ F_{200} = F_{300} = 0 \]

\[ r' = R \cos \beta \]

\[ r = R \cos \alpha \]

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

\[ F_{300} = \left( \frac{\cos^2 \alpha - \cos \alpha}{r} \right) \sin \alpha + \left( \frac{\cos^2 \beta - \cos \beta}{r'} \right) \frac{\sin \beta}{r'} \]

Rowland Circle
Source
Grating

R_{\text{grating}} = 2R_{\text{rowland circle}}

tangential focus
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

\( R = 30 \text{ m}; \) \( gd = 150 \text{ l/mm}; \) \( r = 4 \text{ m}; \) \( r' = 1.5 \text{ m} \)
Variable Included Angle Spherical Grating Monochromator

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

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

\[ \theta_{\text{mirror}} = (\alpha + \beta)/2 \]
Variable Included Angle Spherical Grating Monochromator

Entrance slit/source

Spherical/plane grating

Plane mirror

Exit slit/image

$h \text{ mirror axis } \sim \frac{h}{2} \text{ grating center}$
Variable Included Angle Spherical Grating Monochromator

Entrance slit/source

Spherical/plane grating

Plane mirror

Exit slit/image
Source

Grating

Exit slit

Spherical grating

Plane mirror

Entrance slit

Resolving Power

FWHM = 1.6 meV

Photon Energy (eV)

Intensity (a.u.)

Photon Energy (eV)

Intensity (a.u.)
\[ Nk\lambda = \sin(\alpha) - \sin(\beta) \]

\[ \frac{\partial \lambda}{\partial \alpha} = \frac{\cos(\alpha)}{Nk}\Delta\alpha = \frac{s}{r} \]

\[ \frac{\partial \lambda}{\partial \beta} = \frac{\cos(\beta)}{Nk}\Delta\beta = \frac{s'}{r'} \]

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

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

Resolving Power

\[ \text{Resolving power} = \frac{\lambda}{\Delta\lambda} = \frac{E}{\Delta E} \]

\[ \text{FWHM} = 1.6 \text{ meV} \]

\[ 45/0.0016 \approx 28000 \]
Typical Spherical grating monochromator resolving power

\[
\frac{E}{\Delta E} = \frac{\lambda}{\Delta \lambda} = \frac{\lambda Nkr'}{s' \cdot \cos(\beta)}
\]
Resolving Power measurement

Typical Spherical grating monochromator resolving power

\[ +50-250 \, V \]

\[ I(nA) \]

\[ \text{N}_2 \, 1s \]

\[ E/\Delta E > 11000 \]
Plane Grating

Virtual Source

Real Source

$r'$

$\beta$

$\alpha$

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

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

$r' = -r \frac{\cos^2 \beta}{\cos^2 \alpha}$

$C_f = \frac{\cos \beta}{\cos \alpha}$

$|r'| = r C_f^2$
SuperESCA at Elettra, r~4500 mm, r'~22800 mm

\[ C_f = 2.25 \quad r' = 2.25^2 \times r \]
Collimated light SX 700

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

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

One can select to work in:
High resolution mode (accept to lose some flux)
High efficiency mode (accept a reduction of resolution)
High order suppression mode (with a typical appreciable reduction of flux)
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: 
\[
D(x) = D_0 + D_1 x + D_2 x^2 + D_3 x^3 + \ldots
\]

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

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

For \( F_{200} \): 
\[
F_{200} = \frac{1}{2} \left[ -n\lambda D_1 + \left( \frac{\cos^2 \alpha}{r} + \frac{\cos^2 \beta}{r'} \right) \right]
\]

A plane grating can focus!

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

\[
\sin \beta = \sin \alpha - n\lambda D
\]