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# Optical path function

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#### Outline

•Main properties of SR, brilliance

•Main properties of VUV, EUV and soft x-rays mirrors and gratings

• Conserving brilliance up to the experiment

• Determining optical paths from Fermat's principle: general theory of aberrations

#### Main properties of Synchrotron Radiation

- Very broad and continuous spectral range, from infrared up to soft and hard x-rays
- High intensity
- The emitted radiation is highly collimated and emanates from a very small source: the electron beam
- Pulse time structure
- High degree of polarization

#### Spectral range



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

#### Brilliance

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

I = electron current in the storage ring  $\sigma_x \sigma_z$  = transverse area from which SR is emitted  $\sigma'_x \sigma'_z$  = solid angle into which SR is emitted BW = spectral bandwidth, usually:  $\frac{\Delta E}{E} = 0.1\%$ 



#### SR brilliance at ELETTRA



Why is brilliance important? (1)

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

#### more flux $\rightarrow$ more signal for 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)  $\rightarrow$   $(\sigma\sigma')_{\text{final}} \ge (\sigma\sigma')_{\text{initial}}$ 



#### Meaning of x',z'

• transverse momenta  $p_x$ ,  $p_z$  can be expressed in terms of the direction cosines:

$$p_x = p \cos \alpha$$
$$p_z = p \cos \gamma$$

• defining:  $x' = \cos \alpha$   $z' = \cos \gamma$ 

and assuming:  $p_y \gg p_x, p_z \rightarrow p \cong p_y$ ,

the transverse momenta are proportional to x', z':

$$p_x = p_y x'$$
  $p_z = p_y z'$ 





### Why is brilliance important? (2)

#### Liouville's theorem: $(\sigma\sigma')_{\text{final}} \ge (\sigma\sigma')_{\text{initial}}$

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

High beam divergence along the beamline:

 $\rightarrow$  large optical devices

 $\rightarrow$  high costs and low optical qualities

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

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

#### The beamline

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

The beamline:

- is the means of bringing radiation from the source to the experiment transforming the phase volume in a controlled way: it demagnifies, monochromatizes and refocuses the source onto a sample
- must preserve the excellent qualities of the radiation source

### VUV, EUV and soft x-rays

We restrict ourselves to photon energies from 10 to 2000 eV.



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

 $\rightarrow$  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
- → No windows → The entire optical system must be kept under vacuum

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

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

#### Grazing incidence optics

Strong absorption of radiation by all materials:  $\rightarrow$  no lenses: the only optical elements that can work are mirrors and diffraction gratings, used in reflection

Reflectivities drop down fast with the increasing of the grazing incidence angle → only reflective optics at grazing incidence angles (1-2 degrees)



#### Focusing properties

The meridional or tangential plane contains the central incidence 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.



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

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

# 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: $a = \frac{r+r'}{2}$ ; $b = a\sqrt{1-e^2}$ $e = \frac{1}{2a}\sqrt{r^2 + r'^2 - 2rr'\cos(2\theta)}$

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)

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



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

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



#### 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.

#### Gratings

The diffraction grating separates the different components of the spectrum by redirecting the radiation by an amount which depends upon the wavelength.



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

#### VUV, EUV and soft x-rays beamline

Basic elements:

- mirrors to focus, deflect and filter
- gratings to diffract
- slits to spatially select the radiation

Optical elements have to preserve the quality (brilliance) of the radiation

#### Conserving brilliance

Brilliance decreases because of:

- roughness and slope errors on optical surfaces
- thermal deformations of optical elements due to heat load produced by the high power radiation
- aberrations of optical elements

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

#### Perfect imaging and aberrations

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



Deviations from perfect imaging are called aberrations.

#### Aberrations theory

Image quality is essential for achieving high energy and spatial resolution  $\rightarrow$  knowledge of aberrations theory is necessary It shows what the different aberration terms are and how they play a role in the image formation  $\rightarrow$  it teaches how aberrations can be reduced

Goal: understand in general terms how to treat mathematically the focusing properties of a concave optical element. We will study the case of a grating.

The general theory of aberrations of diffraction gratings applies Fermat's principle to derive expressions for the aberration coefficients.

#### Fermat's principle

Light-rays choose their paths to minimize the optical length



A more accurate statement:

a light-ray going from A to B must traverse an optical path length which is stationary with respect to small variations of that path

### Theory of conventional diffraction gratings

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



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

#### Perfect focus condition (1)

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



B is the point of a perfect focus if:

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

for any pair of (y,z)

#### Perfect focus condition (2)

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:

•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

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



B<sub>0</sub>: gaussian image, produced by the central ray
B: ray diffracted by the generic point P on the grating surface
Aberrations: displacement

• Aberrations: displacements of B with respect to B<sub>0</sub>

#### 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.

 $a_{ij}$  coefficients (1)

Toroid 
$$a_{02} = \frac{1}{2\rho}; \quad a_{20} = \frac{1}{2R}; \quad a_{22} = \frac{1}{4R^2\rho}; \quad a_{40} = \frac{1}{8R^3};$$
  
 $a_{04} = \frac{1}{8\rho^3}; \quad a_{12} = 0; \quad a_{30} = 0$ 

Sphere, cylinder and plane are special cases of toroid:

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

Paraboloid  $a_{02} = \frac{1}{4f\cos\vartheta}; \quad a_{20} = \frac{\cos\vartheta}{4f}; \quad a_{22} = \frac{3\sin^2\vartheta}{32f^3\cos\vartheta};$  $a_{12} = -\frac{\tan\vartheta}{8f^2}; \quad a_{30} = -\frac{\sin\vartheta\cos\vartheta}{8f^2}$  $a_{40} = \frac{5\sin^2\vartheta\cos\vartheta}{64f^3}; \quad a_{04} = \frac{\sin^2\vartheta}{64f^3\cos^3\vartheta}$ 

### $a_{ij}$ coefficients (2)

**Ellipsoid** 

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

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

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

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

http://xdb.lbl.gov/Section4/Sec\_4-3Extended.pdf

#### Optical path function (1)



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

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

$$x_{a} = r \cos \alpha \qquad y_{a} = r \sin \alpha$$
$$x_{b} = r' \cos \beta \qquad y_{b} = r' \sin \beta$$

Optical path function (2)

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

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

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

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

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

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

#### Perfect focus condition (3)



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

$$F_{ijk}$$
 coefficients (1)

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

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

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

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

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

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

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

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

## F<sub>ijk</sub> coefficients (2)

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

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

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

## $F_{ijk}$ coefficients (3)

$$\begin{split} F_{011} &= -\frac{z_a}{r} - \frac{z_b}{r'} \\ F_{111} &= -\frac{z_a \sin \alpha}{r^2} - \frac{z_b \sin \beta}{r'^2} \\ F_{102} &= \frac{z_a^2 \sin \alpha}{r^2} + \frac{z_b^2 \sin \beta}{r'^2} \\ F_{202} &= \left(\frac{z_a}{r}\right)^2 \left[\frac{2 \sin^2 \alpha}{r} - T(r, \alpha)\right] + \left(\frac{z_b}{r'}\right)^2 \left[\frac{2 \sin^2 \beta}{r'} - T(r', \beta)\right] \\ F_{211} &= \frac{z_a}{r^2} \left[T(r, \alpha) - \frac{2 \sin^2 \alpha}{r}\right] + \frac{z_b}{r'^2} \left[T(r', \beta) - \frac{2 \sin^2 \beta}{r'}\right] \end{split}$$

#### Gaussian image point (1)

If we apply Fermat's principle to the central ray:

$$\left(\frac{\partial F}{\partial y}\right)_{y=0,z=0} = 0 \quad \left(\frac{\partial F}{\partial z}\right)_{y=0,z=0} = 0$$

$$F_{100} = 0 \implies \sin \alpha + \sin \beta_0 = Nk\lambda$$

$$F_{011} = 0 \longrightarrow \frac{\frac{Z_a}{r}}{r} = -\frac{\frac{Z_{b0}}{r_0'}}{r_0'}$$

#### grating equation

law of magnification in the sagittal direction

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

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

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

### Gaussian image point (2)



#### Sagittal focusing

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

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

Example: toroidal mirror

#### Aberrations terms

Most important imaging errors:

F <sub>200</sub>	defocus
F <sub>020</sub>	astigmatism
F <sub>300</sub>	primary coma (aperture defect)
F <sub>120</sub>	astigmatic coma
$F_{400} F_{220} F_{040}$	spherical aberration

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

#### Ray aberrations (1)

The generic ray starting from A will arrive at the focal plane at a point B displaced from the Gaussian image point  $B_0$  by the ray aberrations  $\Delta y_b$  and  $\Delta z_b$ :



#### Ray aberrations (2)

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

$$\Delta y_{b}^{\ ijk} = \frac{r_{0}'}{\cos \beta_{0}} F_{ijk} \ i \ y^{i-1} \ z^{j}$$

$$\Delta z_{b}^{\ ijk} = r_{0}' F_{ijk} y^{i} j z^{j-1}$$

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

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

#### Aberrated image

Example of footprint on the grating:



Substituting  $y=\pm w$  and  $z=\pm l$  in the ray aberrations  $\Delta y_b^{ijk}$  and  $\Delta z_b^{ijk}$ , we evaluate the contributions of the rays which are more distant from the pole of the grating

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

#### Defocus and coma contributions

The defocus contribution is linear in the ruled length  $(\pm w)$  of the grating, the error in the dispersive direction is symmetric about the Gaussian image point:

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

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

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

#### Comparison ray trace - aberration calculations



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

Aberration-based calculations specify the different contributions

#### Aberrations contribution to resolution

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

Substituting:  $\Delta \beta = \frac{\Delta y_b}{r'} \rightarrow \qquad \Delta \lambda = \frac{\cos \beta}{Nk} \frac{\Delta y_b}{r'}$ Substituting:  $\Delta y_b = \frac{r'_0}{\cos \beta_0} \frac{\partial F}{\partial y} \rightarrow \qquad \Delta \lambda = \frac{1}{Nk} \frac{\partial F}{\partial y}$ 

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

#### Aberration theory: conclusions

• Perfect focus condition:  $\frac{\partial F}{\partial y} = 0$   $\frac{\partial F}{\partial z} = 0$  for each pair (y,z)  $\rightarrow$  all the coefficients  $F_{ijk}$  must be zero

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

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

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

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