

^{wnd} ILSF School on Synchrotron Radiation and Its Applications

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Optics of soft x-ray beamline

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Outline

- Beamline
- ✓ soft x-ray beamline optics

mirrors, Grating, monochromator, ...

- Example of some soft X-ray beamlines
- Ray-tracing of a SpectroMicroscopy beamline of ILSF`



Schematic figure of synchrotron and different part of beamline

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The beamline is the means of bringing the radiation from the source to the experiment transforming the phase volume in a controlled way, that is: demagnifying and monochromatizing the source and refocusing it onto a sample.





VUV, EUV and soft x-rays

Wavelength



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





mirrors

The mirrors which are included in a synchrotron radiation beamline perform different function:

- ✓ Focusing the radiation
- ✓ To split the radiation and send it to two or more beamline
- ✓ To filter off the high photon radiation or eliminating the higher order output of the monochromator

Geometric shape of mirrors:

- ✓ Plane
- ✓ Spherical
- Aspherical (elliptical, paraboloidal, and troidal)
- ✓ Bent plane mirrors





Toroid

The 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.







Parabola:

$$y^{2} = 4ax$$
$$a = f \cos^{2} \theta$$
$$x_{0} = a \tan^{2} \theta$$
$$y_{0} = 2a \tan \theta$$

b

ellipse

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KB confoguration

The two mirror designed to separate to the functions of horizontal and vertical focussing









Reflectivity of mirrors



 R_s = Reflectivity of the component whose E vector is perpendicular to the plane of incidence R_p = Reflectivity of the component whose E vector is parallel to the plane of incidence Complex refractive index:

 $\tilde{N}(E) = n(E) - ik(E)$

n(E) is the real part and the usual index of refraction

k(E) is the imagainary part and extinction coefficient

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Grazing angles

$$\operatorname{Re}(n_{1})Sin \theta_{1} = \operatorname{Re}(n_{2})Sin \theta_{2}$$

$$Sin \theta_{1} = (1 - \delta)Sin \theta_{2} \Longrightarrow \theta_{2} > \theta_{1}$$

$$\theta_{1}^{Crit} \rightarrow \theta_{2} = \pi / 2$$

$$\alpha^{Crit} = \pi / 2 - \theta_{1}^{Crit}$$

$$Sin \theta_{1}^{Crit} = Sin(\pi/2 - \alpha) = Cos \alpha^{Crit} = 1 - \delta$$

$$Cos \alpha^{Crit} = 1 - 1/2(\alpha^{Crit})^{2} = 1 - \delta$$

$$\Rightarrow \alpha^{Crit} = \sqrt{2\delta}$$

ρ: the number of electrons per unit volume $ε_0$: the electrical permittivity of free space m_e : the rest mass of the electron c: the speed of light in vacuum k: the wave-number of the X-ray radiation







Optical Path function

Fermat's principle: ligth rays choose their paths to minimize the optical length.



 $F = AP + PB + Nk\lambda y$

N: line density K: diffraction order, $(\pm 1, \pm 2 ...)$ λ : wavelength of the light being diffracted

Perfect focus condition:

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

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In general form of the surface is expressed by the equation:

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

$$a_{00} = a_{10} = 0; j = even$$

If x-y plane is a symmetry plane

a_{ii} coefficient:

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 apecial case of toroid:









;

a_{ij} coefficient

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:

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

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

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

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





Optical path function

$$\begin{split} F &= \sum_{ijk} F_{ijk} y^{i} z^{j} \\ &= F_{000} + y F_{100} + z F_{011} + \frac{1}{2} y^{2} F_{200} + \frac{1}{2} z^{2} F_{020} + \frac{1}{2} y^{3} \\ &+ \frac{1}{2} y z^{2} F_{120} + \frac{1}{8} y^{4} F_{400} + \frac{1}{4} y^{2} z^{2} F_{220} + \frac{1}{8} z^{4} F_{040} \\ &+ y z F_{111} + \frac{1}{2} y F_{102} + \frac{1}{4} y^{2} F_{202} + \frac{1}{2} y^{2} z F_{211} + \dots \end{split}$$

Perfect focus condition:

$$\frac{\partial F}{\partial z} = \frac{\partial F}{\partial y} = 0 \qquad \qquad F = \sum_{ijk} F_{ijk} y^i z^j \qquad \qquad F_{ijk} = 0 \text{ for all } ijk \neq (000)$$





Most important imaging errors

$$\begin{aligned} F_{100} &= 0 \Rightarrow \sin \alpha + \sin \beta = Nk\lambda & \text{Grating equation} \\ F_{200} &= 0 \Rightarrow \left(\frac{\cos^2 \alpha}{r} + \frac{\cos^2 \beta}{r'}\right) - 2a_{20}(\cos \alpha + \cos \beta) = 0 & \text{Tangential focus} \\ F_{020} &= 0 \Rightarrow \frac{1}{r} + \frac{1}{r'} - 2a_{02}(\cos \alpha + \cos \beta) = 0 & \text{Sagittal focus} \\ \text{Example: Toroidal mirror} & \left(\frac{1}{r} + \frac{1}{r'}\right) \frac{\cos \theta}{2} = \frac{1}{R} & \left(\frac{1}{r} + \frac{1}{r'}\right) \frac{1}{2\cos \theta} = \frac{1}{\rho} \\ \text{The dispersive contribution to resolution,} \Delta\lambda, \text{ caused by aberrations:} \\ \Delta\lambda &= \frac{1}{Nk} \left[yF_{200} + \frac{3}{2}y_2F_{300} + \frac{1}{2}z^2F_{120} + \frac{1}{2}y^3F_{400} + \frac{1}{2}yz^2F_{220} + zF_{111} + \frac{1}{2}F_{102} + \frac{1}{2}yF_{202} + yzF_{211}...\right] \end{aligned}$$

F ₂₀₀	defocus
F ₀₂₀	astigmatism
F ₃₀₀	primary coma
F ₁₂₀	astigmatic coma
$F_{400} F_{220} F_{040}$	spherical aberration







Slope errors

Slope errors = every deviation from the ideal surface with period larger then \sim 1, 2 mm (measured by the long trace profilometer (LTP))

There is a significant difference in the effectiveness of tangential errors and sagittal errors.









x,y

1mrad FWHM divergence in the x and

Angle of incidence θg=2°= 3.5×10⁻² radian Arm length r=r'=6000 mm

 $\Delta s'_{mer} = 2r' \Delta_{mer}$ 2×6000×1.14×10⁻⁵rad=0.14 mm

 $\Delta s'_{sag} = 2r'\theta g \Delta_{sag}$ 2×6000×3.5×10⁻²rad ×1.14×10⁻⁵rad=4.8×10⁻³ mm

 $\Delta s'_{sag} = 2r'\theta g \Delta_{sag}$ 2×6000×3.5×10⁻²rad ×1.14×10⁻⁵rad=4.8×10⁻³ mm

 $\Delta_{mer} = 1 \text{ sec}$ $\theta_g \Delta_{sag} = (1/29) \times 30 \approx 1$

 $\Delta s'_{mer} = 0.11 = 2 \times 6000 \times \Delta_{mer}$ $\Delta_{mer} = 0.81 \text{ sec}$ $\Delta s'_{sag} = 9.5 \times 10^{-3} = 2 \times 6000 \times 3.5 \times 10^{-2} \Delta_{sag}$ $\Delta_{sag} = 2.0 \text{ sec}$

	Δ _{sag} (sec)	Δ _{mer} (sec)	FWHM _{sag} (mm)	FWHM _{mer} (mm)
1	0	0	1.0×10 ⁻³	1.0×10 ⁻³
2	0	1	1.1×10 ⁻³	0.134
3	1	0	4.9×10 ⁻³	1.0×10 ⁻³
4	30	0	0.14	1.1×10 ⁻³
5	30	1	0.14	0.14
6	2	0.9	8-11×10 ⁻³	0.11

Source: 0.001mm²

y planes

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Surface roughness

Roughness: Every deviation from the ideal surface with period smaller then $\sim 0.5 - 1$ mm (determind by an interferometric microscope (IM))

 $R=R_0 \exp[-(4\pi \sigma \sin\theta_g/\lambda)^2]$

 R_0 : smooth surface reflectivity

- R: attenuated reflectivity
- σ : micro surface roughness in rms <0.5 nm
- θ_g : glancing angle of incidence

The effect of surface roughness on a platinum coated mirror for energies 50-1500 eV is shown. The loss of reflection at 100 eV is only 0.3% whereas at 1000 eV the loss is 25%.









Gratings

The core of a vacuum ultraviolet/soft x-ray monochromator is the diffraction grating. A reflection diffraction grating consist of a reflecting surface with a periodic array of lines.





 $Sin \alpha + Sin \beta = Nm \lambda$ $m = 0, \pm 1, \pm 2,...$

 α and β : incidence and diffraction angels m: order of the diffraction N: line density







The resolving power of a monochromator is a measure of how finely it is able to distinguish between photons of different energies.

The resolution, ΔE , is a measure of smallest amount by which two energies can differ and still be distinguished (or resolved)



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Contribution of the Grating Tangent Errors, σ_{te} , to resulution



The resolution, ΔE, being the Gassian sum of different terms such as the entrance and exit slit dimensions, the slope errors, and the residual aberrations.

dispersion

The angular dispersion is the rate at which the diffraction angle changes with energy. The spatial dispersion is the physical spacing on the focal plane of two lines of different energies.







Grating efficiency

The efficiency of a grating, or the fraction of incident photons that it successfully focuses onto the exit slit depend on ...

Geometric efficiency is the fraction of available photons that are successfully transmitted through the system as a result of the sizes of the optical elements.



Diffraction efficiency is the fraction of the photons incident on a grating that are diffracted into the desired diffraction order (m).

1) Line density (N), 2) Incidence angle (α), 3) Energy or wavelength of photons (E, λ), 4) Groove profile, 5) Grating material (coating)





Energy range

- High-energy region (> ~ 150 eV) Grazing incidence (> ~ 85 deg) monochoromator is inevitable Except for multilayer grating
- Low-energy region (< ~ 50 eV)
 Near normal incidence monochromator is also available
- Wide-energy beamline (e.g. 30 eV 1500 eV) Combination of grazing and normal incidence monochromators Variable included angle monochromator Interchangeable gratings



(α+β)





Exit slit

(wavelength

selection)

Parabolic mirror

(focusing)

Plane grating

Parabolic mirror

(collimation)

Resolution and intensity

1. Energy resolution depends on...

Dispertion & Focus

Focus size depends on ... Source size, demagnification, aberration, slope error, ...

Perfect monochromator, in principle,

(dispersion) Exce We must compromise !! Slop Intensity, resolution, energy range, ... – free monochromator

2. Intensity depend on ...

Number of optical elements

Incidence angle & acceptance (larger incidence needs larger mirror) **Diffraction efficiency** of the grating Point source High groove density large dispersion but low efficiency

> Minimum intensity loss (no mirror) Focal condition depends on wavelength Aberration might be serious



The simplest monochromator





Some hints for the choice

1. Grating shape (plane, spherical, ...)

Spherical: dispersion & focus \longrightarrow small number of optical elements be careful for aberrations

- 2. Groove density (uniform or varied)
- 3. Included angle (constant or varied)

Variable: higher degree of freedom \longrightarrow resolution & intensity in wide energy range Scanning mechanism is more complicated

4. Entrance slit

Without slit: source size of SR itself directly affects With slit: higher resolution can be achieved at the sacrifice of the resolution intensity Pre-focusing optics is necessary













Nanospectroscopy beamline

source:	2 undulators, with phase modulation electromagnet		
Period (mm)	100		
polarisation	linear horizontal, linear vertical, elliptical		
energy range	5-1000 eV		
Effective size of the source (FWHM)	240 μm × 40 μm		
Flux density (Ph/sec/µm²)	14		
beam defining aperture size (10 m behind the source)	1 × 2 mm ²		
Acceptance angle of beamline	0.1 mrad × 0.2 mrad		









Nanospectroscopy beamline

Variable included Angle Spherical Grating Monochromator:

It can provide very high resolving power To obtain very high resolving power, several gratings are required The included angle working curve is flat

A plane variable line spacing grating:

No high resolving power

It can cover a large energy rang with a relatively small change in the resolving power







Nanospectroscopy beamline

A second horizontally focusing mirror has a demagnification factor greater then 10, so it must be chosen carefully.

To produce a spot smaller then 5 μ m, 1 μ rad slope error is the minimum requirement.

			mage	
		Shape	Length	rms errors
		Spherical/flat	Up to 500 mm	< 0.5 µrad
		Spherical/flat	> 500 mm	1-2 µrad
		Toroidal	Up to 500 mm	< 1 µrad
		Toroidal	> 500 mm	> 1 µrad
	ia: KB configuration	Aspherical	Up to 500 mm	2 µrad
Source		Aspherical	> 500 mm	3-5 µrad

The only way to have a real micro-focus is to start from a flat or spherical surface and bent it to a ellipse.





brilliance

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

Photon flux = photons/sec I = electron current in the storage ring $\sigma_x \sigma_y$ = the transverse area from which SR is emitted $\sigma'_x \sigma'_z$ = the solid angle into which SR is emitted BW= spectral bandwidth, usually $\Delta E/E= 0.1\%$

The brilliance of the source and not just the number of photons/second must be transferred as completely as possible through the optical system to the experiment

- The surface error increase

- The cost increase



Small focus volumeHigher flux density

The source must be demagnified:

- The vertical aperture remains small
- The optical aberration decrease
- The surface error decrease
- The cost decreases





Spot size and divergence of the photon beam for two different undulators length (L=2.127 m and 6 m) at two energy values (1 KeV and 10 KeV).

E (KeV)		1			10		
$\epsilon_{\rm x}$ (nm.rad)		0.93		3.278	0.93		3.278
		Medium	Long	Medium	Medium	Long	Medium
L=	$\sigma_{t,x}(\mu m)$	58.1	153.4	156.4	57.0	153.4	156.2
2.127 m	$\sigma_{t,y}(\mu m)$	5.2	8.3	10.3	3.5	7.32	7.3
	$\sigma'_{t,x}(\mu rad)$	37.3	24.2	48.3	29.5	7.7	38.4
	$\sigma'_{t,y}(\mu rad)$	24.3	24.2	31.4	8.2	7.7	11
L=	$\sigma_{t,x}(\mu m)$	57.4	153.5	156.7	57.0	153.4	156.2
6 m	$\sigma_{t,y}(\mu m)$	7.6	9.96	14.7	3.9	7.5	7.9
	$\sigma'_{t,x}(\mu rad)$	31.9	14.4	41.7	28.8	4.6	37.6
	$\sigma'_{t,y}(\mu rad)$	14.7	14.4	19.6	5.4	4.6	7.7

Table shows the results, as it can be seen the spot size has been reduced by a factor of **2.7×2** in the medium straight section of low emittance case relative to high emittance, and so it is greatly appreciated. It should be noted that the decreasing of spot size is mostly due to using low value of β_y .





Spot size of the photon beam at the focal plane of KB mirrors (spherical mirrors) with undulator source in two values of emittance: 3.278 & 0.93 nm.rad.

Foot print of photon beam on the mirror with BM source



- Reduction of the photon beam aberration
- Reduction of foot prints on the optical elements (technically and budget)
- Simpler beamline design by using higher quality and simpler optical element or lower number of optical elements, etc.

Y (cm)

X (cm)

cm

0.3





Ray tracing:

In the vacuum ultraviolet and soft x-ray portion of the spectrum only three optical principle are required for basic ray trace program:

a) The optical path between physical elements of the optical system is a straight

b) The angle of reflection is equal to the angle of incidence

c) Diffraction phenomena are governed by Bragg's law



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$$p(\theta,\psi) = 10.84E^4 B_0 ING \left[1 - \left(\lambda \frac{\theta \times 0.001}{K} \right)^2 \right]^{0.5} \left[\frac{1}{\left[1 + (\gamma \psi \times 0.001)^2 \right]^{\frac{5}{2}}} + \frac{5(\gamma \psi \times 0.001)^2}{7\left[1 + (\gamma \psi \times 0.001)^2 \right]^{\frac{7}{2}}} \right]$$

$$G = K \times \frac{\left[K^{6} + \left(\frac{24}{7}K^{4}\right) + \left(4K\right)^{2} + \frac{16}{7}\right]}{\left(1 + K^{2}\right)^{\frac{7}{2}}}$$

θ: horizontal angular
displacement
Ψ: Vertical angular
displacement in mrad
K: deflection parameter
G: normalizing factor

 $P(\psi)$ is the angular power density function in W/mrad² in the vertical only ($\theta=0$). $\Psi=0$, 0.02, ..., 126.1 mrad $P(\psi)$ is the angular power density function in W/mrad² in the vertical only ($\theta=0$). $\theta=0$, 0.02, ..., 126.1 mrad)







A diverging beam







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