VUV & SX Beamline Design

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Outline

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   1.1. energy region
   1.2. resolution & intensity
   1.3. some hints for the choice
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   2.1. optimization of parameters
   2.2. analytical estimation of energy resolution
   2.3. ray-tracing simulation

3. Beamline installation
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   3.2. optical adjustments using SR
   2.3. experimental estimation of beamline performance
1.1. energy region

1. High-energy region (>~150 eV)
   **Grazing incidence** (>~85 deg) monochromator is inevitable
   *except for multilayer grating

2. Low-energy region (<~50 eV)
   (Near) **normal incidence** monochromator is also available
   *Medium incidence monochromator?
     **Strongly affects** the polarization

3. Wide-energy beamline (e.g. 30 eV – 1500 eV)
   (a) **Combination** of grazing and normal incidence monochromators
   (b) **Variable included angle** monochromator
   (c) Interchangeable gratings
1.2. resolution & intensity

1. Energy resolution depends on...

Dispersion & Focus

Focus size depends on...

Source size, demagnification, aberration, slope error, ...

Some of them drastically change according to technical progress

No absolute solution!!

e.g. aberration-free monochromator

Perfect monochromator, in principle, except for the reflectivity loss

Slope errors in parabolic mirrors are large
Use of cylindrical mirrors ⇒ large aberration

Recent progress in SR sources;
Small divergence ⇒ negligible aberration
1.2. resolution & intensity

2. Intensity depends on…

- Number of optical elements
- Incidence angle & acceptance (* more grazing needs larger mirror)
- Diffraction efficiency of the grating
  - * High groove density ⇒ large dispersion but low efficiency

  e.g. the simplest monochromator

We must compromise !!

Intensity, resolution, energy range,…
1.3. some hints for the choice

1. Grating shape (plane, spherical, …)
   Spherical: dispersion & focus ⇒ small number of optical elements
   be careful for aberrations

2. Groove density (uniform or varied)
   Varied line spacing: simpler optics (or higher resolution with the same optics)
   be careful for precision in the groove parameters

3. Included angle (constant or variable)
   Variable: higher degree of freedom ⇒ resolution & intensity in wide energy range
   scanning mechanism is more complicated ⇒ be careful for reproducibility

4. Entrance slit
   Without slit: Source size of SR itself directly affects the resolution
   Higher resolution than the source-size limit is never obtained!
   With slit: Higher resolution can be achieved at the sacrifice of intensity
    pre-focusing optics is necessary

5. Focusing elements in monochromator (upstream, downstream of G, or nothing)
   Effects of the slope errors in the focusing mirror are smaller in the upstream case

The choice depends on properties of light source, precision of mirrors, reliability of scanning mechanism, needs from applications, costs, …
1.4. examples for soft X-ray monochromator

(1) Plane grating monochromators

Collimated-light illumination

- Essentially no aberration
  \[ \Rightarrow \alpha \text{ and } \beta \text{ can be freely chosen} \]
  \[ \Rightarrow \text{Demagnification can be controlled} \]

- Precision of parabolic mirrors is relatively poor
  One can use cylindrical mirrors if divergence is small enough

1.4. examples for soft X-ray monochromator

(1) Plane grating monochromators

Diverging light illumination (SX-700)

Plane grating & post-focusing mirror (e.g. elliptical mirror) with variable included angle

Precision of elliptical mirrors was essential due to high demagnification factor

One can use cylindrical mirrors if divergence is small enough

Number of optical elements is reduced compared to the collimated case

Relation between $\alpha$ and $\beta$ must be properly chosen to keep focal condition
1.4. examples for soft X-ray monochromator

(2) Spherical (or cylindrical) grating monochromators

Rowland mount

Monochromator itself consists of a grating only

But…

Relation among $\alpha$, $\beta$, $r$, and $r'$ must be properly chosen

"Rowland condition": $r = R \cos \alpha$, $r' = R \sin \beta$

⇒ Many optical elements and complicated scanning mechanism

DRAGON mount

Monochromator consists of a spherical (cylindrical) grating only

Fixed included angle

⇒ Simple scanning mechanism

Kinds of aberration arises, but only the defocus term can be canceled by moving the exit slit

“Active grating” (variable radius) is developed to achieve fixed exit slit
1.4. examples for soft X-ray monochromator

(3) Varied-line-spacing (VLS) plane grating monochromators

Diverging light illumination

Monochromator itself consists of a **VLS plane grating** only
Relation between $\alpha$ and $\beta$ must be properly chosen

$\Rightarrow$ **A precise variable included angle system** is inevitable
1.4. examples for soft X-ray monochromator

(3) Varied-line-spacing (VLS) plane grating monochromators

Converging light illumination (Monk-Gillieson mount)

Pre-focusing mirror upstream of VLSG
Constant included angle ⇒ Simple scanning mechanism
Moderate aberration in spite of constant included angle
Variable included angle system is also adopted recently
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2. Design procedure
   2.1. optimization of parameters
   2.2. analytical estimation of energy resolution
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   2.3. experimental estimation of beamline performance
2.1. Optimization of the parameters

Overview of a typical soft X-ray beamline

**Pre-focusing optics:** focuses X rays onto the entrance slit

**Monochromator:** from the entrance slit to the exit slit

**Post-focusing optics:** focuses monochromatized X rays onto sample position

**Higher order suppression (Mc):**
utilizes energy dependence of reflectivity (or transmittance)
2.1. Optimization of the parameters

1. Source-size limit

Dispersion:

\[
\frac{dz}{d\lambda} = r' \frac{nm}{\cos \beta}
\]

Beam size at the exit slit

\[s' \text{ (lower limit)} = s \frac{r'}{r}\]

\[\Rightarrow \frac{\lambda}{\Delta \lambda} \propto \frac{nmr}{s \cos \beta}\]

(a) If the source size is the same, longer monochromator gives higher resolution.

(b) If the monochromator length \((r + r')\) is the same, longer entrance arm \((r)\) gives higher resolution. \(\Rightarrow\) Higher demagnification factor is better!

But…

(a') Long monochromator needs large mirrors to keep enough acceptance

\(\Rightarrow\) higher cost, or intensity loss by reduced acceptance

(b') High demagnification factor causes large aberration.

\(\Rightarrow\) Eventual decrease in energy resolution

Most people choose \(~1:1\) \((r \sim r')\) optics, though it might not be the best solution.

Groove density \(n\) and included angle are chosen, considering the balance among dispersion, demagnification, diffraction efficiency, etc.
2.1. Optimization of the parameters

2. Monochromator parameters (mirror radius, groove parameter, etc.)
   - highly depends on the type of monochromator

Design example: **Variable-included-angle Monk-Gillieson mount varied-line-spacing (VLS) grating monochromator**
2.1. Optimization of the parameters

Parameters:

- $\rho$ (sagittal radius of M1)
- Groove parameters of VLSG
  \[ N = N_0 (1 + a_1 w + a_2 w^2 + a_3 w^3) \]

1. Choose two energies ($E_1$ and $E_2$) and respective included angles ($K_1$ and $K_2$)
2. Optimize $\rho$ and $a_1$ so that the defocus vanishes at ($E_1$, $K_1$) and ($E_2$, $K_2$)
3. For other energies, included angles are set so that the defocus vanishes
4. Choose an energy ($E_3$) and optimize $a_2$ so that the coma aberration vanishes
5. Choose $E_4$ and optimize $a_3$ so that the spherical aberration vanishes

2.1. Optimization of the parameters

\[
N = N_0 \left(1 + a_1 w + a_2 w^2 + a_3 w^3\right)
\]
2.2. Analytical estimation of energy resolution

From light path function

$$F = p_A + q_A + r_B$$

$$+ M_{10}w + (M_{20}w^2 + M_{02}l^2 + M_{30}w^3 + M_{12}wl^2)/2$$

$$+ (M_{40}w^4 + M_{22}w^2l^2 + M_{04}l^4)/8 + \ldots$$

$$+ [n_{10}w + (n_{20}w^2)/2 + (n_{30}w^3)/2 + (n_{40}w^4)/8 + \ldots] m\lambda,$$
2.2. Analytical estimation of energy resolution

- Source size
- Defocus
- Coma
- Spherical
2.3. ray-tracing simulation

Source parameters:
\[ \sigma_x = 350 \ \mu m, \ \sigma_y = 20 \ \mu m, \ \sigma_x' = 20 \ \mu \text{rad}, \ \sigma_y' = 5 \ \mu \text{rad}, \ 4.5 \text{ m undulator} \]

Optimization conditions for \( N_0 = 600 \ \text{l/mm} \):
\[ E_1 = 50 \ \text{eV}, E_2 = 500 \ \text{eV}, K_1 = 164^\circ, K_2 = 174^\circ, E_3 = E_4 = 100 \ \text{eV} \]

Spot diagram at the exit slit

\[ \Rightarrow E/\Delta E \approx 26,000 \]
2.3. ray-tracing simulation

Simultaneous scan mode

Included angle is scanned simultaneously with the grating

- 600 l/mm (ray trace)
- 1200 l/mm (ray trace)
- source size limit
- slope error (0.1")

Resolution ($\Delta \lambda/\lambda$)

Source size or slope error limited resolution
2.3. ray-tracing simulation

Fixed included angle mode

Relatively high resolution over wide energy range

* Analytical estimation is consistent with ray tracing simulation
2.3. ray-tracing simulation

Comparison with diverging illumination optics

Monk-GIllieson
converging X rays
illuminate VLSG

non Monk-GIllieson
diverging X rays
illuminate VLSG
2.3. ray-tracing simulation

Monk-Gillieson (converging illumination)

Comparison with diverging illumination optics

non Monk-Gillieson (diverging illumination)

Simultaneous scan

Fixed included angle
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3.1. alignment

Determination of beamline center

Q-magnet to beamline

Undulator

Q-magnet

Hole on the Shield wall

Shield wall

Target on the Q-magnet
3.1. alignment

Grating adjustment
(roll and yaw)

Adjusted by using diffraction of Laser light

Mirror adjustment

Adjusted by using a dummy mirror and Laser light
3.2. optical adjustments using SR

Example: BL-16A at the Photon Factory

M0: vertical focusing to entrance slit (S1) \([r = 15 \text{ m}, r' = 5 \text{ m}]\)

M1: vertical focusing to 90 mm upstream of exit slit (S2) \([r = 4 \text{ m}, r' = 7.91 \text{ m}]\)
3.2. optical adjustments using SR  
Light intensity was monitored downstream of S1 during M0 roll-angle scan.  
**Upper and Lower parts of light were taken** by using an aperture.  

Sagittal radius of M0 is \(-0.1\%\) smaller than the designed value (262 mm).  
This coincides with the inspection report!
3.2. optical adjustments using SR

(2) Vertical focusing of M1

M1 is designed so that light is focused at 90 mm upstream of S2.

Intensity (arb. units)

Grating Angle (deg)

Zero-th order light intensity was monitored downstream of S2 during Grating angle scan.

Upper and Lower parts of light were taken by using an aperture.

A peak shift between the upper and lower parts means that the focal position is upstream of S2.

However…

The peak shift should be reduced by ~50 % when S2 is placed at -45 mm position.

⇒ Focal position is far from S2 !?
3.2. optical adjustments using SR

M1 pitch = 1.9535 deg (-2.3%)

The focal point became 90 mm upstream of S2 when the pitch angle of M1 was changed to 1.9535 deg (-2.3% from the designed value).

Sagittal radius of M1 is ~2.3 % smaller than the designed value !?
3.2. optical adjustments using SR

Problem of the Mirror Holders

Focal point of zero-th order depends on included angle !!

Plane mirror (M2) and/or Grating (VLSG) are not plane!

Mirror distortion by the holder?
3.2. optical adjustments using SR

Effect of Holder Improvement

![Graph showing the effect of holder improvement on focus shift. The graph plots focus shift (mm) against 2K (deg). The data points are differentiated between 'As Installed' and 'After M2 Improvement'.]
3.2. optical adjustments using SR

Focal position for diffracted light

High resolution is not necessary for adjustment!
3.2. optical adjustments using SR

**Focal position**

N = 1000 l/mm

2K = 173.0 deg

Photon Energy (eV)

Intensity (arb. units)

2K = 172.8 deg

Photon Energy (eV)

Intensity (arb. units)

2K = 172.7 deg

Photon Energy (eV)

Intensity (arb. units)

**S2 rotation (tilt angle)**

N = 500 l/mm

Tilt

Photon Energy (eV)

Intensity (arb. units)

Photon Energy (eV)

Intensity (arb. units)

2K = 173.0 deg

Photon Energy (eV)

Focal position

N = 1000 l/mm

S2 rotation (tilt angle)

N = 500 l/mm
3.3. experimental estimation of beamline performance

Absorption spectrum for $N_2$ gas

N = 500 l/mm, S1 = 25 $\mu$m, S2 = 25 $\mu$m

N = 1000 l/mm, 2K = 172.7 deg

S1 = 50 $\mu$m
S2 = 40 $\mu$m

S1 = 25 $\mu$m
S2 = 20 $\mu$m
3.3. experimental estimation of beamline performance

Absorption spectrum for Ar gas

\[ \lambda / \Delta \lambda > 30,000 \]
3.3. experimental estimation of beamline performance

Photon Flux: photodiode is available
3.3. experimental estimation of beamline performance

Beam size: knife-edge scan

Light intensity is monitored at downstream of the knife edge

![Graphs showing beam size and intensity](image)

**Vertical Size**
- Intensity (arb. units) vs. Vertical position (mm)
- 12 μm

**Horizontal Size**
- Intensity (arb. units) vs. Horizontal position (mm)
- 80 μm
(3.2.) optical adjustments using SR

Adjustment for the focus on the sample

Knife edge

Aperture

Horizontal Focus

M3 pitch = 2.0 deg

M3 pitch = 1.96 deg

M3 pitch = 1.99 deg

M3 pitch = 2.06 deg

M3 pitch = 1.994 deg

Intensity (arb. units)

Horizontal position (mm)

Vertical position (mm)

Tilt angle

M3 yaw = -0.25 deg

M3 yaw = -0.30 deg

M3 yaw = -0.289 deg

M3 yaw = -0.25 deg

Intensity (arb. units)

Vertical position (mm)
Thank you for your attention!