VUV & SX Beamline Design

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1. Choice of monochromator type
   1.1. energy region
   1.2. resolution & intensity
   1.3. some hints for the choice
   1.4. examples for soft X-ray monochromator

2. Design procedure
   2.1. optimization of parameters
   2.2. analytical estimation of energy resolution
   2.3. ray-tracing simulation

3. Beamline installation
   3.1. alignment
   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

   Included angle

   Included angle

   Included angle

   Included angle
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 (* larger incidence needs larger mirror)
   - Diffraction efficiency of the grating
     * High groove density ⇒ large dispersion but low efficiency

   e.g. the simplest monochromator

   ![Diagram of a monochromator with a point source, concave grating, and exit slit.]

   Minimum intensity loss (no mirrors)

   Focal condition depends on wavelength
   Aberration might be serious

   We must compromise !!
   Intensity, resolution, energy range,…
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, 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 monochromators

(1) Plane grating monochromators

**Collimated light illumination**

- Essentially no aberration
- $\Rightarrow \alpha$ and $\beta$ can be freely chosen
- $\Rightarrow$ Demagnification can be controlled
- Precision of parabolic mirrors is relatively poor
- One can use cylindrical mirrors if divergence is small enough

**Diverging light illumination (SX-700)**

- Plane grating & post-focusing mirror (e.g. elliptical mirror) with variable included angle
- Precision of elliptical mirrors is relatively poor
- 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": $r = R \cos \alpha$, $r' = R \sin \beta$

$\Rightarrow$ Many optical elements and complicated scanning mechanism

DRAGON mount

Monochromator consists of a spherical (cylindrical) grating only

Fixed included angle

$\Rightarrow$ Simple scanning mechanism

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

Converging light illumination (Monk-Gillieson mount)

Pre-focusing mirror upstream of VLSG

Constant included angle $\Rightarrow$ Simple scanning mechanism

Moderate aberration in spite of constant included angle

Variable included angle system is also adopted recently
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:

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

Beam size at the exit slit

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

\[ \Rightarrow \frac{\lambda}{\Delta \lambda} \propto \frac{r}{s} \]

(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 \(~1:1\) demagnification 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 $N = N_0 (1+a_1w+a_2w^2+a_3w^3)$

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

\[
N = N_0 \left(1 + a_1w + a_2w^2 + a_3w^3 \right)
\]

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<thead>
<tr>
<th>Parameter</th>
<th>Value 1</th>
<th>Value 2</th>
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### 2.2. Analytical estimation of energy resolution

<table>
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<tr>
<th>Included angle (deg)</th>
<th>Energy (eV)</th>
<th>( \lambda ) (Å)</th>
<th>( \sigma_\lambda ) (Å)</th>
<th>Source size (μm)</th>
<th>( \Sigma ) (μm)</th>
<th>( \sigma_\Sigma ) (μm)</th>
<th>( \Sigma_\lambda ) (μm)</th>
<th>( \sigma_\Sigma_\lambda ) (μm)</th>
<th>( \alpha )</th>
<th>( \beta )</th>
<th>( w ) (m)</th>
<th>( \Delta \lambda 20/\lambda )</th>
<th>( \Delta \lambda 30/\lambda )</th>
<th>( \Delta \lambda 40/\lambda )</th>
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- **defocus**: Included angle (deg)
- **Source size**: Error (µ rad)
- **slope error**: Incidence angle (deg)
2.2. Analytical estimation of energy resolution
2.3. ray-tracing simulation

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

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

Spot diagram at the exit slit

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

Simultaneous scan mode

Included angle is scanned simultaneously with the grating

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

2.3. ray-tracing simulation

Monk-Gillieson (converging illumination)

Comparison with diverging illumination optics

non Monk-Gillieson (diverging illumination)

Simultaneous scan

Fixed included angle
3.1. alignment

Determination of beamline center

Q-magnet  Undulator  Q-magnet

Hole on the Shield wall
to beamline

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) \([r = 4 \text{ m}, r' = 7.91 \text{ m}]\)
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!
M1 is designed so that light is focused at 90 mm upstream of S2.

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

(2) Vertical focusing of M1

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 !?
3.3. experimental estimation of beamline performance

Absorption spectrum for Ar gas

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

Absorption spectrum for $N_2$ gas

- $N = 500$ l/mm, $S_1 = 25$ μm, $S_2 = 25$ μm
- $N = 1000$ l/mm, $2K = 172.7$ deg

- $S_1 = 25$ μm, $S_2 = 20$ μm
- $S_1 = 50$ μm, $S_2 = 40$ μm
3.3. experimental estimation of beamline performance

Photon Flux: photodiode is available

![Graph showing photon flux vs. photon energy (eV)]
3.3. experimental estimation of beamline performance

Beam size: knife-edge scan

Light intensity is monitored at downstream of the knife edge

![Graphs showing vertical and horizontal size](image)