Hard X-ray Beamline Optics

~Engineering of x-ray beamline ~

Haruhiko Ohashi
JASRI / SPring-8
Experimental station

Where is “beamline”? 

Light source

Bending magnet

Insertion device

Storage ring

Optics & transport

Monochromator, mirror shutter, slit, pump, ...

Interlock & Shielding hutch

Front-end

Absorber, beam shutter, slit, pump, ...

Experimental station

Today’s lecture

Beamline
Introduction

“X-ray beamline looks complicated?”

Inside shielding tunnel (front end)

Outside shielding tunnel (optics hutch)

What function of each component?
Light source (IDs/BM)  
Front end (FE)  
Interlock system  
Radiation shield hutch  
X-ray beamline  

Light source (Power)  
Engine  
Brake Air-bags  
Radiator Body  
Transmission Gear  
Tailoring x-rays (Power control)  
User Interface  
Application (drive)  
Monochromator  
Mirrors  
End station  

Human safety  
Machine protection  

A vehicle  
Steering wheel  
Dashboard Gear lever  

Power  
Power control
Today’s contents

Light source (IDs/BM)

Front end (FE)

X-ray beamline

Radiation shield hutch

Interlock system

Heat management

Machine protection

Tailoring x-rays

X-ray Optics

Monochromator

Mirrors

User Interface

Utilities

Application

Experimental station

Today’s contents

Human safety

Light source

Machine protection

Tailoring x-rays

User Interface

Utilities

Application

Experimental station

Today’s contents

Front end (FE)

Light source (IDs/BM)

Human safety

Heat management

Machine protection

Tailoring x-rays

User Interface

Utilities

Application

Experimental station

Today’s contents

Front end (FE)

Light source (IDs/BM)

Human safety

Heat management

Machine protection

Tailoring x-rays

User Interface

Utilities

Application

Experimental station
Heat management for human safety & machine protection

↓

Front end (FE)
SPRing-8 Tunnel

Front end (15~18m)
Schematic Layout inside the SPring-8 Tunnel

Tunnel of the storage ring (1/16)

Experimental Hall

BL10XU Front end

Standard in-vacuum undulator
Power density:
500 kW/mrad$^2$
Total power: 13 kW

Front end (FE)
(15～18m)

Optics Hatch

Experimental Hall

To a Transportation Channel SR

Shielding Wall

Tunnel

BL10XU Front End

Q7 S5 Q6 S4 Q5 S3 Q4 CR B1 Q5 S2 Q2 S1 Q1

18.612m

Why so long FE?
Key functions & components of FE

- **Shielding for human safety**
- **Handling high heat load for safety**
- **Handling high heat load for optics**
- **Monitoring the x-ray beam position**
- **Protection of the ring vacuum**

Beam shutter (BS), collimator
Absorber, masks
XY slit, filters
XBPM (x-ray BPM), SCM (screen monitor)
FCS (fast closing shutter), Vacuum system

FE section inside the tunnel of storage ring

(cont.) FE in the tunnel

Exp. hall
What’s “Main Beam Shutter”?
MBS ( = ABS + BS ) is closed $\rightarrow$ MBS accepts the incident power form ID.
When we operate a main beam shutter (MBS), what happens?

X-ray → **Absorber (Abs)** to protect BS from heat load

- A block of 33 kg is moved

**Glidcop**® (copper that is dispersion-strengthened with ultra-fine particles of aluminum oxide)

**Beam shutter (BS)** to shield you against radiation

- A block of 30~46 kg is moved

**Heavy metal** (alloy of tungsten) the thermal conductivity not so high
When we operate a main beam shutter (MBS), what happens?

Absorber (Abs) → Beam shutter (BS)

Absorber (Abs) to protect BS from heat load

Beam shutter (BS) to shield you against radiation

A block of 33 kg is moved

A block of 30~46 kg is moved

Glidcop®
(copper that is dispersion-strengthened with ultra-fine particles of aluminum oxide)

Heavy metal (alloy of tungsten)

the thermal conductivity not so high

Move

For safety

X-ray

After BS is fully opened, Abs is opened.
After Abs is fully closed, BS is closed.
The sequences are essential to keeping safety.

ABS and BS work on ways together

to protect us from radiation when we enter the hutch.
What components remove most “power” from ID?

Total power from ID = 14 kW
The power through FE section = 0.6 kW

For managing heat load
What components remove most “power” from ID?

Absorber, masks (to prevent BS from melting)

XY slit, filters (to prevent optics from distorting)

These components (①, ② and ③) cut off the power to prevent optics from distorting by heat load.

Someone may enlarge opening of XY slit to get more “flux” → You can NOT get it!
FE: “For users to take lion’s share”

Adding a spatial limitation to photon beam, supplying only a good quality part around the central axis of ID to transport optical system safely and stably.

The size of XY slit is set to 1.05mm □. XY slit is installed ~30m away from ID.

1st harmonic Flux Density

Higher order

Power Density

Helical Mode Operation at BL15XU 17
Comparison of the **Spatial Distribution**

between **1\textsuperscript{st} harmonic Flux density** and **Power density**

- Standard in vacuum undulator
  - $K=2.6$ $E_{1\text{st}}=4.3\text{keV}$

- FE slit
  - $V: 15 \, \mu\text{rad} = 0.5\, \text{mm} / 30\, \text{m}$
  - $H: 40 \, \mu\text{rad} = 1.2\, \text{mm} / 30\, \text{m}$

\[
\text{Power} \leftarrow \int \text{Flux} \, dE
\]
If an optical component is irradiated by too much power ....

One user opened FE slit excessively.

2kW

LN2-cooled Si crystal

Slit: “Too much is as bad as too little”
How to manage high heat load by FE XY slit?

Incident angle 0.08 deg (1.5 / 100)

Spatial distribution of power

1st harmonic flux

For managing heat load

SR

29 kg

2m
Key issues of front end

1. **Key functions of components in front end**:  
   They have their proper functions, proper missions based on the principles of human **radiation safety**, **vacuum protection**, **heat-load** and **radiation damage** protection of themselves.  
   They have to deal with every mode of ring operation and every mode of beamline activities.

2. **Any troubles in one beamline should not make any negative effect to the other beamlines**.

3. **Strongly required to be a reliable and stable system**.  
   We have to adopt key technologies which are reliable, stable and fully established as far as possible.  
   *Higher the initial cost, the lower the running cost from the long-range cost-conscious point of view.*
Tailoring x-rays to application

↓

X-ray mirrors design, errors, metrology & alignment
The functions of x-ray mirrors

- Deflecting
- Low pass filter
- Focusing
- Collimating

- Separation from γ-ray
- Branch / switch beamline
- Higher order suppression
- Micro- / nano- probe
- Imaging
- Energy resolution
  
  *w. multilayer or crystal mono.*
Tailoring x-rays to application

\[ \downarrow \]

X-ray mirrors

design, errors, metrology & alignment
Design parameters of x-ray mirror

Requirement

**the beam properties both of incident and reflected x-rays**

*(size, angular divergence / convergence, direction, energy region, power...)*

We have to know well what kinds beam irradiate on the mirror.

**Design parameters**

- Coating material: Rh, Pt, Ni, Cr (w/o binder), thickness multilayers, laterally graded ML
- Incident angle: grazing angle (mrad)
- Surface shape: flat, sphere, cylinder, elliptic... adaptive (mechanically bent, bimorph)
- Substrate shape: rectangular, trapezoidal...
- Substrate size: length, thickness, width
- w/o cooling: indirect or direct, water or LN₂...
- Substrate material: Si, SiO₂, SiC, Glidcop...

In addition, some errors such as:

- figure error
- roughness...
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In addition,

some errors such as figure error, roughness...
How to select coating material and incident angle?

Reflectivity for grazing incident mirrors

\[ R(\lambda, \theta, n) = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2 \]

\[ k_1 = \frac{2\pi}{\lambda} \cos \theta, \quad k_2 = \frac{2\pi}{\lambda} \sqrt{n^2 - \cos^2 \theta} \]

The complex index of refraction
Coating material (1)

**“the complex index of refraction”**

The complex atomic scattering factor for the *forward scattering*

\[ f = f_1 + if_2 \]

The complex index of refraction

\[ n = 1 - \delta - i\beta \]

\[ \begin{align*}
\delta &= \frac{Nr_0 \lambda^2}{2\pi} f_1(\lambda) \\
\beta &= \frac{Nr_0 \lambda^2}{2\pi} f_2(\lambda)
\end{align*} \]

\[ r_0 = \frac{e^2}{4\pi mc^2} = 2.82 \times 10^{-15} m \]

N: Number of atoms per volume

\[ \beta = \frac{\mu \lambda}{4\pi} \quad \mu: \text{linear absorption coefficient} \]

Small for x-ray region

<table>
<thead>
<tr>
<th>Material</th>
<th>$\delta \times 10^{-5}$</th>
<th>$\beta \times 10^{-7}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>0.488</td>
<td>0.744</td>
</tr>
<tr>
<td>Quartz</td>
<td>0.555</td>
<td>2.33</td>
</tr>
<tr>
<td>Pt</td>
<td>3.26</td>
<td>20.7</td>
</tr>
<tr>
<td>Au</td>
<td>2.96</td>
<td>19.5</td>
</tr>
</tbody>
</table>
Coating material (2)

“total reflection”

\[ \cos(\theta_1)/\cos(\theta_2) = n_2/n_1 \]

\[ \theta_1 > \theta_c \]

\[ \theta_1 = \theta_c \]

\[ \theta_1 < \theta_c \]

\[ \cos(\theta_c) = n = 1 - \delta, \cos(\theta_c) \approx 1 - \theta_c^2/2 \]

\[ \theta_c \approx \sqrt{2\delta} = 1.6 \times 10^{-2} \lambda \sqrt{\rho} = 20 \sqrt{\rho} / E \]

For example,

\[ \theta_c (\text{rad}), \rho (\text{g/cm}^3), \lambda (\text{nm}) , E (\text{eV}) \]

Rh (\( \rho = 12.4 \text{ g/cm}^3 \)) \( \lambda=0.1 \text{nm} \), \( \theta_c = 5.68 \text{ mrad} \)
Coating material (3): “cut off, absorption”

The cut off energy of total reflection $E_c$

$$E_c \approx 20\sqrt{\rho / \theta_i}$$

$E_c$ (eV), $\rho$ (g/cm$^3$), $\theta_c$ (mrad)

Rh (12.4 g/cm$^3$)

Pt (21.4 g/cm$^3$)

Cut off energy, absorption $\rightarrow$ incident angle

Opening of the mirror, length, width of mirror, power density
Atomic scattering factors, Reflectivity

You can easily find optical property in “X-Ray Data Booklet” by Center for X-ray Optics and Advanced Light Source, Lawrence Berkeley National Lab.

In the site the reflectivity of x-ray mirrors can be calculated.

http://xdb.lbl.gov/

Many thanks to the authors!
Surface shape (1)

Purpose of the mirror:
- deflecting
- low pass filter
- focusing
- collimate
- meridional
- sagittal

For example,
- flat
- spherical
- cylindrical
- toroidal
- elliptical
- parabolic...

Easy to make or cost:
- ○ ○ ○ ○ ○

Take care of aberration:
- △ △ △ △ △
Surface shape (2) radius and depth

\[
R_m = \frac{2}{(1/p + 1/q) \sin(\theta_i)}
\]

\[
R_s = \frac{2 \sin(\theta_i)}{(1/p + 1/q)} = R_m \sin^2(\theta_i)
\]
Surface shape (2) radius and depth

\[
R_m = \frac{2}{(1/p + 1/q) \sin(\theta_i)} \\
R_s = \frac{2 \sin(\theta_i)}{(1/p + 1/q)} = R_m \sin^2(\theta_i)
\]

For parallel beam \( q \to \infty, 1/q = 0 \)

Depth at the center \( D = R - \sqrt{R^2 - \left(\frac{L}{2}\right)^2} \approx \frac{L^2}{8R} \)

For example,

- \( p = 15 \sim 50m, q = 5 \sim 20m, \theta_i = 1 \sim 10mrad \)
- \( R_m = 0.1 \sim 10 km, R_s = 30 \sim 100 mm \)
- \( R_m = 1 km, L = 1m \) \( \rightarrow D = 125 \mu m \)
- \( R_s = 30 mm, L = 20mm \) \( \rightarrow D = 1.7 mm \)
Surface shape (3) elliptical

\[ \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \]

For example,

\[ p = 975 \text{ m}, q = 50 \text{ mm}, \theta = 3 \text{ mrad} \]

Precise fabrication is not easy.
Design parameters of x-ray mirror

Requirement

the beam properties both of incident and reflected x-rays
  ( size, angular divergence / convergence, direction, energy region, power... )

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In addition,
  some errors such as figure error, roughness...
Tailoring x-rays to application

↓

X-ray mirrors
design, errors, metrology & alignment
“An actual mirror has some errors.”

The tolerance should be specified to order the mirror

- Roughness
- Density of coating material
- Radius error
- Figure error

The cost (price and lead time) depends entirely on tolerance. We must consider or discuss how to measure it.

- Deformation by self-weight, coating and support...
- Figure error of adaptive mechanism
- Misalignment of mirror
- Stability of mirror’s position (angle)
- Deposition of contamination by use
- Decomposition of substrate by use

- Reflectivity
- Beam size
- Distortion
- Deformation ...

- Environment
- Manipulator
- Cooling system ...
Contamination and removal

**before**

**After cleaning**

*It takes from 10 min to a few hours.*
Errors (1)

"Density $\rho$ and surface roughness $\sigma$"

\[ E_c \approx 20 \sqrt{\rho / \theta_i} \quad \text{and} \quad R = R_0 e^{-\left(\frac{4\pi\sigma \sin(\theta_i)}{\lambda}\right)^2} \]

Coating on sample wafer at the same time is helpful to evaluate the density and roughness.
Errors (2)

“the self-weight deformation”

Material: SiO₂
Density: 2.2 g/cm³
Poisson's ratio: 0.22
Young’s modulus: E = 70 GPa

FEA (finite element analysis)

Supported by 2 lines

17 nm PV

This value for nano-focusing is larger than figure error by Rayleigh’s rule.

Improvement for nano-focusing

a) Substrate → Si (E ~ 190 GPa)
b) Optimization of supporting points and method
c) Figuring the surface in consideration of the deformation

\[ D \propto \frac{L^4}{E \times t^3} \]
Errors (3a)

“figure error estimated by Rayleigh’s rule”

\[ \phi = 2hk \sin(\theta) \rightarrow \frac{\pi}{2} \]

\[ h_{\lambda/4} = \frac{\lambda}{8\theta} \]

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>Angle (mrad)</th>
<th>Distance (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>15</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>1</td>
<td>10</td>
<td>12</td>
</tr>
</tbody>
</table>

\[ \theta \]
Errors (3b)

“estimation by wavefront simulation”

Errors of short range order decreases intensity. → Roughness
Errors (3c)

“ estimation by wavefront simulation ”

Errors of long range order

Integrity profiles of focusing beam by wavefront simulation

Errors of long range order loses shape. → Figure
“estimation by wavefront simulation”

If the figure error $< 3\text{nmPV}$ for all spatial range, the estimated focusing size performs 25 nm. The value corresponds to the result of Rayleigh’s rule.

The focusing beam of 25 nm was realized using high precision mirror with figure error of 3 nm PV

Tailoring x-rays to application

↓

X-ray mirrors design, errors, metrology & alignment
How to evaluate the errors?

- Designed surface
- Errors (short range)
- Errors (long range)
Metrology instruments for x-ray optics

Field of view, lateral resolution

**Short**
- ~10 μm, 0.1 nm
  - Roughness, figure
  - Scanning probe microscope
- z (0.1nm)

**Short / middle**
- ~10 mm, 1 μm
  - Roughness, figure
  - Scanning white light interferometer
- z (0.1nm)

**Long / middle**
- ~0.1 m, 0.1 mm
  - Figure
  - Fizeau interferometer
- z (0.1nm)

**Long /**
- ~1 m, 1 mm
  - Slope
  - Long Trace Profiler (LTP)
  - slope (0.1μrad)

**Vertical resolution (rms)**
Scanning white light interferometer

Interference fringe $\rightarrow$ **Height**

**Commercially available**

Fringes on CCD

White light source (Lamp or LED)

Reference

Beam splitter

Mirau or Michelson objective lens scanned

Under the test

**Zygo Corp. NewVeiw**, **Bruker AXS (Veeco) Contour GT** .......

**FOV (=lens) 50um $\sim$ 10 mm**

**Lateral resolution** 1 μm $\sim$

**Vertical resolution** 0.1 nm

**Figure error**

Short / middle range order
Fizeau interferometer

Interference pattern $\rightarrow$ Height

Monochromatic point light source

Zygo Corp. VeriFire®, 4DS technologies, FujiFILM ……

Beam splitter

Collimator

Cavity

Reference

Under the test

Fizeau fringes on CCD

FOV (=reference) $\sim 0.1$ m
Lateral resolution $\sim 0.1$ mm
Vertical resolution 0.1 nm

Figure error

Not easy to measure large mirror

Long / mid range
Long trace profiler (LTP)

Direction of laser reflected on the surface → **Slope**

\[
Z' = \frac{d}{2F} \quad \text{where} \quad d \; \mu m \quad F \; 1 m \\
Z' < \text{sub-μrad}
\]

Scanning penta prism

**Slope**

Easy to measure slope of sub-μrad on large mirror by **NO reference**

Many kinds of LTPs are developing among SR facilities.

Stitching interferometer for large mirror

**Homemade**

**MSI**
( micro-stitching interferometer )

**RADS**
( relative angle determinable stitching interferometer )

Collaboration with Osaka Univ., JTEC and SPring-8

**Height error of wide range order for a long and aspherical mirror**
**with 1μm of lateral and 0.1 nm of vertical resolution.**

_Necessity is the mother of invention._
Tailoring x-rays to application

X-ray mirrors design, errors, metrology & alignment
Introduction of KB mirrors

In 1948, P. Kirkpatrick and A. V. Baez proposed the focusing optical system. 


Advantages
- Large acceptable aperture and High efficiency
- No chromatic aberration
- Long working distance

Disadvantages
- Difficulty in mirror alignments
- Difficulty in mirror fabrications
- Large system

Suitable for x-ray nano-probe
# Overview of x-ray focusing devices

<table>
<thead>
<tr>
<th>Device Type</th>
<th>focus size, focal length [energy]</th>
<th>energy range</th>
<th>aberration</th>
<th>energy range</th>
<th>aberration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffraction</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fresnel Zone Plate</td>
<td>12 nm, ( f = 0.16 \text{ mm} ) [0.7 keV], 30 nm, ( f = 8 \text{ cm} ) [8 keV]</td>
<td>soft x-ray hard x-ray</td>
<td>-coma small -chromatic exist -figure error small</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sputter sliced FZP</td>
<td>0.3 µm, ( f = 22 \text{ cm} ) [12.4 keV], 0.5 µm, ( f = 90 \text{ cm} ) [100 keV]</td>
<td>8-100 keV</td>
<td>-coma small -chromatic exist -figure error large→small</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bragg FZP</td>
<td>2.4 µm, ( f = 70 \text{ cm} ) [13.3 keV]</td>
<td>mainly hard x-ray</td>
<td>-coma small -chromatic exist -figure error small</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Multilayer Laue Lens</td>
<td>16 nm(1D), ( f = 2.6 \text{ mm} ) [19.5 keV], 25nm×40nm, ( f=2.6\text{mm,}4.7\text{nm} ) [19.5 keV]</td>
<td>mainly hard x-ray</td>
<td>-coma large -chromatic exist -figure error small</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reflection</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressed Lens</td>
<td>1.5 µm, ( f = 80 \text{ cm} ) [18.4 keV], 1.6 µm, ( f = 1.3 \text{ m} ) [15 keV]</td>
<td>mainly hard x-ray</td>
<td>-coma small -chromatic exist -figure error large</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Etching Lens</td>
<td>47nm×55nm, ( f = 1\text{ cm,}2\text{ cm} ) [21 keV]</td>
<td>mainly hard x-ray</td>
<td>-coma small -chromatic exist -figure error small</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kirkpatrick-Baez Mirror</td>
<td>7 nm × 8nm, ( f = 7.5\text{cm} ) [20 keV]</td>
<td>soft x-ray hard x-ray</td>
<td>-coma large -chromatic not exist -figure error small</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wolter Mirror</td>
<td>0.7 µm, ( f = 35 \text{ cm} ) [9 keV]</td>
<td>&lt;10 keV</td>
<td>-coma small -chromatic not exist -figure error large</td>
<td></td>
<td></td>
</tr>
<tr>
<td>X-ray Waveguide</td>
<td>95 nm, [10 keV]</td>
<td>soft x-ray hard x-ray</td>
<td>-coma large -chromatic not exist -figure error large</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
How small is x-ray focused?

For example, by elliptical mirror

Geometrical size

\[ d_G = \frac{q}{p} \times S_0 \]

\[ p = 975 \, \text{m}, \quad q = 50 \, \text{mm}, \quad \theta = 3 \, \text{mrad}, \quad l = 50 \, \text{mm}, \quad \lambda = 0.083 \, \text{nm}, \quad S_0 = 100 \, \text{\mu m} \]

Mag. = 1 / 19500

\[ d_G = 5 \, \text{nm} \]

Diffraction limited size (FWHM)

\[ d_{DL} = \lambda \times \frac{0.88q}{l \sin(\theta)} \]

\[ (15 \, \text{keV}) \]

\[ d_{DL} = 25 \, \text{nm} \]

The opening of the mirror restricts the focused size even if magnification is large.
Nano-focusing by KB mirror
History since the century

World Record of spot size is 7 nm (by Osaka Univ., in 2009 *).

*Routinely obtained spot size is up to 30 nm.*

Difficulty in mirror alignments

Positioning two mirrors is difficult because there are at least 7 degree of freedom.

It is difficult to use KB mirrors.

- Pitching: $\theta_1, \theta_2$
- Yawing: $\psi_1, \psi_2$
- Orthogonality: $\Phi$
- Focal length: $f_1, f_2$
KB optics installed in BL29XU-L

![KB optics diagram]

<table>
<thead>
<tr>
<th></th>
<th>1st Mirror</th>
<th>2nd Mirror</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glancing angle (mrad)</td>
<td>3.80</td>
<td>3.60</td>
</tr>
<tr>
<td>Mirror length (mm)</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Mirror aperture (µm)</td>
<td>382</td>
<td>365</td>
</tr>
<tr>
<td>Focal length (mm)</td>
<td>252</td>
<td>150</td>
</tr>
<tr>
<td>Demagnification</td>
<td>189</td>
<td>318</td>
</tr>
<tr>
<td>Numerical aperture</td>
<td>0.75x10⁻³</td>
<td>1.20x10⁻³</td>
</tr>
<tr>
<td>Coefficient a of elliptic function (mm)</td>
<td>23.876 x 10³</td>
<td>23.825 x 10³</td>
</tr>
<tr>
<td>Coefficient b of elliptic function (mm)</td>
<td>13.147</td>
<td>9.609</td>
</tr>
<tr>
<td>Diffraction limited focal size (nm, FWHM)</td>
<td>48</td>
<td>29</td>
</tr>
</tbody>
</table>

Tolerance limits of mirror alignments

Severe positioning of two mirrors is required. The manipulator should be designed for these freedom of axis with the resolution & the range.

Freedom of axis, Resolution, range

A typical manipulator of KB optics

- Precise manipulation of mirrors
- Highly stable system
- Ultra-high vacuum (or He environment)

For example,
- Resolution of pitching axis = 0.1 μrad
  → Res. of the actuator at 100 mm = 10 nm
- The focal length = 1 m and beam size = 1 μm
  → Angular stability of the mirror \( \sim 0.1 \, \mu\text{rad} \)
Image on X-ray CCD camera

\[ L \times 2\theta = x \]

\[ \theta = \frac{x}{2L} \]
Image of reflected x-ray

1m from focal point (CCD)

8.28mm (1.150 m × 3.6 mrad × 2)

Upper

x-z plane

Focal plane

Reflection in a vertical direction

1.92mm (0.252 m × 3.8 mrad × 2)

Focal point

Reflection in a horizontal direction

Max 360μm

(0.150 m × 3.6 mrad × 2)

Max 380μm

1.08mm

(0.150 m × 3.6 mrad × 2)

Direct x-ray
(Mirror aperture)

Reflection in a vertical direction

Max 360μm

(0.252 m × 3.8 mrad × 2)

Focal plane

Reflection in a horizontal direction

Max 380μm

1.08mm

(0.150 m × 3.6 mrad × 2)

Direct x-ray
(Mirror aperture)

Reflection in a vertical direction

Max 360μm

(0.252 m × 3.8 mrad × 2)

Focal plane

Reflection in a horizontal direction

Max 380μm

1.08mm

(0.150 m × 3.6 mrad × 2)

Direct x-ray
(Mirror aperture)
Alignment of in-plane rotation (Horizontal focusing mirror)

θ: 3.8mrad → 2θ: 7.6mrad

Reflected angle of vertical-focusing mirror needs to be considered, in the alignment of in-plane rotation of horizontal-focusing mirror.
Alignment

Alignment of incident angle

- Foucault test
  *Rough* assessment of focusing beam profile. This method is used for *seeking focal point*.

- Wire (Knife-edge) scan method
  *Final* assessment of *focusing beam profile*.

*Precise adjustment of the glancing angle and focal distance is performed until the best focusing is achieved, while monitoring the intensity profile.*
Alignment of incident angle

Diagram showing the alignment of X-ray with X-ray Mirror and CCD camera.
Foucault test

Image on CCD

Projection image

Downstream

Focal plane

Upstream

Whole bright-area gradually becomes dark.

Knife edge shadow

Focusing beam

Downstream

Focal point

OK
Foucault test 1

Wire is at downstream of focal point.
Image on CCD become dark from lower side.

X-ray camera
Foucault test 2

Wire is at upstream of focal point. Image on CCD become dark from upper side.
Foucault test 3

Wire is at the focal point.
Whole bright-area gradually becomes dark.
Relationship between incident angle and focal position

Tolerance of the incident angle → only a few micro-rad

Incident angle → Large  ⇒  Focal point → downstream
Incident angle → Small  ⇒  Focal point → upstream
Wire (Knife-edge) scan method for measuring beam profiles

The sharp knife edge is scanned across the beam axis, and the total intensity of the transmitting beam is recorded along the edge position.

The line-spread function of the focused beam was derived from the numerical differential of the measured knife-edge scan profiles.
Relationship between Beam size and Source size

Beam size changes depending on source size (or virtual source size).

Beam size = Source size / M \quad (M: \text{demagnification})

\text{Beam size} \geq \text{Diffraction limit}

Beam size is selectable for each application.
Scanning X-ray Fluorescence Microscope: SXFM

Scanning samples

Focused X-ray

X-ray fluorescence

X-ray spectrometer

Measurement principle

X-ray Fluorescence spectrum

Key issues of x-ray mirror

1. To select the functions of x-ray mirror
   Deflecting, low pass filtering, focusing and collimating → Shape of the mirror

2. To specify the incident and reflected beam properties
   Energy range, flux
   → absorption, cut off energy → coating material → incident angle
   The beam size and the power of incident beam
   → opening of the mirror, incident angle
   → absorbed power density on the mirror → w/o cooling, substrate
   Angular divergence / convergence, the reflected beam size
   → incident angle, position of the mirror (source, image to mirror)
   Direction of the beam
   → effect of polarization, self-weight deformation

4. To specify the tolerance of designed parameters
   Roughness, density of coating material, radius error, figure error
   The cost (price and lead time) depends entirely on the tolerance.

5. To consider the alignment
   The freedom, resolution and range of the manipulator
Tailoring x-rays to application

↓

X-ray monochromator

- Principle
  - Introduction of diffraction theory
  - Dynamical theory
  - DuMond diagram

- Engineering
X-ray Monochromator

X-ray monochromator is key component for SR experiments:
✓ length gauge for structure analysis,
✓ energy gauge for spectroscopy,...

Principle of x-ray monochromator
✓ Photon energy tuning $\leftrightarrow$ Bragg’s law
✓ Energy resolution $\leftrightarrow$ source divergence, Darwin width,..
✓ Flux (throughput) $\leftrightarrow$ related to Darwin width

⇒ Understanding the dynamical theory for large & perfect crystal

Practical of the monochromator
✓ Double-crystal monochromator for fixed-exit
✓ Crystal cooling to manage high heat load

⇒ Mechanical engineering issues
Tailoring x-rays to application

X-ray monochromator

Principle

- Introduction of diffraction theory
- Dynamical theory
- DuMond diagram

Engineering
**Bragg reflection (kinematical)**

**Bragg’s law**
in real space

\[ 2d \sin \theta = m\lambda \]

**Laue condition**
in reciprocal space

\[ \mathbf{Q} = \mathbf{h} \]

Scattering vector \( \mathbf{Q} = \) Reciprocal lattice vector \( \mathbf{h} \)

1) Phase matching on the single net plane by mirror-reflection condition.
2) Phase matching between net planes.

Reciprocal lattice vector \( \mathbf{h} \)
- Normal to net plane
- Length = \( 1/d \)

\[ |\mathbf{K}_s| = |\mathbf{K}_0| = k = 1/\lambda \]

\[ |\mathbf{Q}| = 2k \sin \theta = |\mathbf{h}| = 1/d \]

Laue condition equivalent to Bragg’s law
Ewald sphere:

*Radius* = \( \frac{1}{\lambda} = K_0 \)

\[ K_s - K_0 = h \]

*When a reciprocal lattice point is on the Ewald sphere, Bragg reflection occurs.*
Miller indices and $d$-spacing for silicon

\[ d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \]

**Top view**

- Silicon: $a = 5.431\, \text{Å}$
  - $d$-spacing:
    - $(400): 1.3578\, \text{Å}$
    - $(111): 3.1356\, \text{Å}$
    - $(311): 1.6375\, \text{Å}$
    - $(511): 1.0452\, \text{Å}$

**Side view**

- Diamond: $a = 3.567\, \text{Å}$
Crystal structure factor for diamond structure

Structure factor \( \Rightarrow \) Sum of atomic scattering with phase shift in the unit cell

\[
F(h) = \sum_j f_j(h, E) \exp\left(2\pi i h \cdot r_j\right)
\]

Atomic scattering factor

\[
F(h) = \sum_j f_j(h, E) \exp\left(2\pi (hx_j + ky_j + lz_j)\right)
\]

For diamond structure

\[
\begin{align*}
\begin{cases}
  h, k, l & \text{Mixture of odd and even numbers} \\
  h, k, l & \text{All odd, or, all even numbers, and } m: \text{ integer,}
\end{cases}
\end{align*}
\]

\[
\begin{align*}
\begin{cases}
  h + k + l = 4m & F = 8f \\
  h + k + l = 4m \pm 1 & F = 4(1 \pm i)f \\
  h + k + l = 4m \pm 2 & F = 0
\end{cases}
\end{align*}
\]

\( \leftarrow \) 8 atoms in phase

\( \leftarrow \) Half contribute with phase shift \( \pm \pi /2 \)

\( \leftarrow \) Half cancel with \( \pi \)

Position of atoms in the unit cell for diamond structure

\[
(x_j, y_j, z_j) =
\begin{align*}
(0, 0, 0)_1, (1/4, 1/4, 1/4)_2, \\
(1/2, 1/2, 0)_3, (3/4, 3/4, 1/4)_4, \\
(0, 1/2, 1/2)_5, (1/4, 3/4, 3/4)_6, \\
(1/2, 0, 1/2)_7, (3/4, 1/4, 3/4)_8
\end{align*}
\]
Crystal structure factor for diamond structure

(400), (220),...
All in phase

\[ F = 8f \]

(111), (311),...
Half contribute with phase shift \( \pm \pi/2 \)

\[ F = 4(1 \pm i)f \]

(011), (200),...
Half cancel with \( \pi \)

\[ F = 0 \]
Total intensity in **kinematical approximation**

3-dimensional periodic structure of unit cell with number $N_x, N_y, N_z$

Total scattering intensity becomes:

$$ I = I_e |F(Q)|^2 \cdot |G(Q)|^2 $$

Laue function:

$$ |G(Q)|^2 = \frac{\sin^2(\pi N_x h)}{\sin^2(\pi h)} \cdot \frac{\sin^2(\pi N_y k)}{\sin^2(\pi k)} \cdot \frac{\sin^2(\pi N_z l)}{\sin^2(\pi l)} $$

$h, k, l$: integer $\rightarrow$ Intense peaks

$\rightarrow$ (hkl) reflection

Crystal size $(N)$ becomes larger

$\rightarrow$ narrower & higher, approaching delta function

Peak intensity $N_x^2$

FWHM $\Delta h \approx 0.8858/N_x \sim 1/N_x$
X-ray monochromator using *perfect crystal*

→ Perfect single crystal: *silicon, diamond,* ..

Photon energy tuning:
✓ Crystal & lattice plane
✓ Bragg angle range

\[ E \text{ [keV]} = \frac{12.3984}{2d_{hkl} \text{ [Å]} \sin \theta_B} \]

ex) for SPring-8 standard DCM

Bragg angle: 3~27°
Total intensity in *kinematical approximation*

3-dimensional periodic structure of unit cell with number $N_x, N_y, N_z$

Total scattering intensity becomes:

$$I = I_e |F(Q)|^2 \cdot |G(Q)|^2$$

Laue function:

$$|G(Q)|^2 = \frac{\sin^2(\pi N_x h)}{\sin^2(\pi h)} \cdot \frac{\sin^2(\pi N_y k)}{\sin^2(\pi k)} \cdot \frac{\sin^2(\pi N_z l)}{\sin^2(\pi l)}$$

One-dim. Laue function, $N_z = 10$

<table>
<thead>
<tr>
<th>$h$</th>
<th>$I$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2.5</td>
<td>120</td>
</tr>
<tr>
<td>-1.5</td>
<td>100</td>
</tr>
<tr>
<td>-0.5</td>
<td>80</td>
</tr>
<tr>
<td>0.5</td>
<td>60</td>
</tr>
<tr>
<td>1.5</td>
<td>40</td>
</tr>
<tr>
<td>2.5</td>
<td>20</td>
</tr>
</tbody>
</table>

Peak intensity $N_x^2$

FWHM $\Delta h \approx 0.8858/N_x \sim 1/N_x$

Crystal size $(N)$ becomes larger

$\rightarrow$ narrower & higher, approaching delta function

$N \uparrow$

$FWHM \rightarrow 0, I \rightarrow \infty$
Diffraction theory for large and perfect crystal

Kinematical to dynamical theory

“Large & perfect” single crystal:
1) Multiple scattering in crystal
2) Extinction (Diffraction by “finite” number of net planes)

Kinematical diffraction is invalid for large and perfect crystal. Dynamical theory must be applied.
Tailoring x-rays to application

\[ \downarrow \]

X-ray monochromator

- Principle
  - Introduction of diffraction theory
  - Dynamical theory
  - DuMond diagram

- Engineering
Dynamical theory

C. G. Darwin (1914)
the crystal as an finite stack of atomic planes
\[ \text{difference equation} \]

P. P. Ewald (1917)
Max von Laue (1931)
the crystal as a periodic dielectric constant
\[ \text{Maxwell's equation} \]

\[ T_n = t T_{n-1} e^{i\phi} + r R_n e^{2i\phi} \]
\[ R_n = r T_n + t R_n e^{i\phi} \]
\[ T_0 = 1, R_{-1} = 0 \]
\[ \phi = K d \sin \theta \]
Fundamental equation

Fundamental equation is derived using Maxwell’s equations and introducing Bloch wave for 3-dimensional periodic medium (= perfect single crystal):

Maxwell’s equations

\[ \rot (\rot E) = K^2 (1 + \chi) E \]

\[ E = \exp(-i \omega t) \sum_{g} E_g \exp(i k_g \cdot r) \]

\[ k_g = k_0 + h \]

\[ \chi(r) = \sum_{g} \chi_g \exp(i g \cdot r) \]

\[ \chi_g \propto F(g) \]

\[ K = \frac{2\pi}{\lambda} \]

\[ \frac{k_h^2 - K^2}{K^2} E_h = \sum_{g} \chi_{h-g} P \cdot E_g \]
Fundamental equation

Fundamental equation is derived

\[
E_h = \sum_{g} \chi_{h-g} P \cdot E_g
\]

\[\frac{k_h^2 - K^2}{K^2} \]

\(h, g, \ldots\) : Reciprocal lattice points

\(E_h, E_g\) : Fourier components of electric field

\(K\) : Incident wave vector in vacuum

\(k_h\) : Wave vectors in the crystal

\(\chi_h\) : Fourier components of the polarizability (Negative values, \(10^{-6}\sim10^{-5}\))

\(P\) : Polarization factor between \(h\) and \(g\) waves

\(k_h = k_0 + h\) : Momentum conservation
When one wave $E_0$ in crystal

**Fundamental equation**

\[
\frac{k_h^2 - K^2}{K^2}E_h = \sum_g \chi_{h-g} P \cdot E_g
\]

Waves $E$ in the crystal

\[
E = \sum_g E_g \exp(ik_g \cdot r)
\]

\[k_h = k_0 + h \rightarrow \text{Bloch wave}\]

When one wave $E_0$ in the crystal

\[
\frac{k_0^2 - K^2}{K^2}E_0 = \chi_0 E_0
\]

\[\therefore \left\{1 + \chi_0 \right\} K^2 - k_0^2 \right\} E_0 = 0\]

\[k_0 = K \sqrt{1 + \chi_0} \equiv k\]

\[k \approx K \left(1 + \chi_0/2\right)\]

$k$ : *Mean* wave number in the crystal
Boundary condition of wave vector

We must consider connections of waves from vacuum into the crystal and from the crystal to vacuum, to solve the equations.

 Incident wave in vacuum $K_0$
→ Refracted wave in the crystal $k_0$
→ Reflected wave in the crystal $k_h$
→ Reflected wave in vacuum $K_h$

Tangential component of wave vector must be continuous
Two-beam approximation

Fundamental equation is reduced to the equation for two beams (waves) of incidence $E_0$ and “one” intense diffraction $E_h$

$$k_h^2 - K^2 \frac{E_h}{K^2} = \sum_g \chi_{h-g} P \cdot E_g$$

(A) $$\frac{k_0^2 - K^2}{K^2} E_0 = \chi_0 E_0 + P\chi_{-h} E_h$$

(B) $$\frac{k_h^2 - K^2}{K^2} E_h = P\chi_h E_0 + \chi_0 E_h$$

Fourier components of the polarizability

Negative values, $10^{-6} \sim 10^{-5}$

$$\chi_h = \chi_{-h} \quad \text{for Si}$$

Polarization factor

$$\sigma : P = 1, \quad \pi : P = \cos 2\theta_B$$
Two-beam approximation

Two beams (waves) of incidence $E_0$ and “one” intense diffraction $E_h$

What means these equations:

(A) $\frac{k_0^2 - K_0^2}{K_0^2} E_0 = \chi_0 E_0 + P \chi_{-h} E_h$

(B) $\frac{k_h^2 - K^2}{K^2} E_h = P \chi_h E_0 + \chi_0 E_h$

Goal

$R = r^2 = \left( \frac{E_h}{E_0} \right)^2$

$FWHM = \Delta \theta_{Darwin}$

Reflectivity curve

Effective band width
#5

Dispersion surface

Using two equations, we obtain following secular equation:

\[(A) \quad \frac{k_0^2 - K_0^2}{K_0^2} E_0 = \chi_0 E_0 + P\chi_{-h} E_h\]

\[(B) \quad \frac{k_h^2 - K^2}{K^2} E_h = P\chi_h E_0 + \chi_0 E_h\]

\[\text{Secular equation}\]

\[ (k_0^2 - k^2)(k_h^2 - k^2) = \chi_h \chi_{-h} P^2 K^4 \]

\[k_h = k_0 + h\]

\[\chi_h = \chi_{-h} = 0\]

Not our goal!

Real space

Reciprocal space

Kinematical
Dispersion surface

(A) \[ \frac{k_0^2 - K_0^2}{K_0^2} E_0 = \chi_0 E_0 + P \chi_{-h} E_h \]

(B) \[ \frac{k_h^2 - K^2}{K^2} E_h = P \chi_h E_0 + \chi_0 E_h \]

Secular equation

\[ (k_0^2 - k^2)(k_h^2 - k^2) = \chi_h \chi_{-h} P^2 K^4 \]

\[ k_h = k_0 + h \]

\[ \chi_h \neq 0 \neq \chi_{-h} \]

Secular equation can be reduced to quadratic equation near Brillouin zone boundary.

Real space

Bragg case

Reciprocal space
Dispersion surface

(A) \[
\frac{k_0^2 - K_0^2}{K_0^2} E_0 = \chi_0 E_0 + P\chi_{-h} E_h
\]

(B) \[
\frac{k_h^2 - K^2}{K^2} E_h = P\chi_h E_0 + \chi_0 E_h
\]

Secular equation
\[
\left(k_0^2 - k^2\right)\left(k_h^2 - k^2\right) = \chi_h \chi_{-h} P^2 K^4
\]

\[k_h = k_0 + h\]
\[\chi_h \neq 0 \neq \chi_{-h}\]
Dispersion surface

(A) \( \frac{k_0^2 - K_0^2}{K_0^2} E_0 = \chi_0 E_0 + P \chi_{-h} E_h \)

(B) \( \frac{k_h^2 - K^2}{K^2} E_h = P \chi_h E_0 + \chi_0 E_h \)

Secular equation
\[
\left(k_0^2 - k^2\right)\left(k_h^2 - k^2\right) = \chi_h \chi_{-h} P^2 K^4
\]

\( k_h = k_0 + h \)
\( \chi_h \neq 0 \neq \chi_{-h} \)

In the gap between two dispersion surfaces, total reflection occurs for Bragg case.
Normalized deviation parameter $W$

Parameter $W$ is related to the gap between two dispersion surfaces and total reflection occurs at $-1 < W < 1$ for Bragg case.

$$W = -\frac{2(K_0 \cdot h) + h^2}{2K_0^2} \sqrt{\gamma_0 \left| \frac{1}{\gamma_h \cdot |P|} \right|} + \frac{\chi_{0r}}{2 \chi_{hr} \cdot |P|} \sqrt{\gamma_0 \left( 1 - \frac{\gamma_h}{\gamma_0} \right)}$$

$\Delta \theta$: Angle deviation for fixed photon energy,

$\Delta E$: Energy deviation for fixed incident angle

$$W = \left\{ \Delta \theta \sin 2\theta_{BK} + 2 \frac{\Delta E}{E} \sin^2 \theta_{BK} + \frac{\chi_{0r}}{2} \left( 1 - \frac{\gamma_h}{\gamma_0} \right) \right\} \sqrt{\gamma_0 \left| \frac{1}{\gamma_h \cdot \chi_{hr} \cdot |P|} \right|}$$

For symmetric Bragg case, sigma polarization:

$$W = \left\{ \Delta \theta \sin 2\theta_{BK} + 2 \frac{\Delta E}{E} \sin^2 \theta_{BK} + \chi_{0r} \right\} \frac{1}{\chi_{hr}}$$
Movement of tie point

Tie point moves by *changing the incident angle* at fixed photon energy (wavelength).

1. **Lower angle**
   \[ W < -1 \]

2. **Near Bragg condition**
   \[-1 < W < 1 \]

3. **Higher angle**
   \[ W > 1 \]

Total reflection

Dominant branch for thick Bragg-case crystal is close to O-sphere.
Calculation of polarizability

\[ \chi_h: \text{Fourier component of polarizability} \]

\[ \rightarrow \text{proportional to the structure factor} \]

\[ \chi_h = -\frac{r_e \lambda^2}{\pi v_c} F(h, E) \]

\[ v_c: \text{unit cell volume} \]

\[ \chi_h = \chi_{hr} + i\chi_{hi} \]

\[ \chi_{hr} \leftrightarrow f^0(h) + f'(E) \]

Atomic form factor
+ real part of anomalous factor

\[ \chi_{hi} \leftrightarrow f''(E) \]

Imaginary part of anomalous factor

For diamond structure

\[ h + k + l = 4m \]

\[ \chi_{hr} = -\frac{r_e \lambda^2}{\pi v_c} 8(f^0 + f')e^{-M} \]

\[ \chi_{hi} = -\frac{r_e \lambda^2}{\pi v_c} 8f''e^{-M} \]

\[ h + k + l = 4m \pm 1 \]

\[ \chi_{hr} = -\frac{r_e \lambda^2}{\pi v_c} 4(1 + i)(f^0 + f')e^{-M} \]

\[ \chi_{hi} = -\frac{r_e \lambda^2}{\pi v_c} 4(1 + i)f''e^{-M} \]

\[ h = k = l = 0 \]

\[ \chi_{0r} = -\frac{r_e \lambda^2}{\pi v_c} 8(Z + f') \]

\[ \chi_{0i} = -\frac{r_e \lambda^2}{\pi v_c} 8f'' \]
Amplitude ratio

From the solution of the fundamental equations, we obtain the ratio \( r = \frac{E_h}{E_0} \) (reflection coefficient) as a function of parameter \( W \).

For Bragg case, no absorption, and thick crystal:

\[
\begin{align*}
  r &= \frac{E_h}{E_0} = -\frac{\sqrt[\gamma_0]{|\chi_{hr}|P}}{\gamma_h |\chi_{-h}|P} (W + \sqrt{W^2 - 1}) & (W < -1) \\
  r &= \frac{E_h}{E_0} = -\frac{\sqrt[\gamma_0]{|\chi_{hr}|P}}{\gamma_h |\chi_{-h}|P} (W + i\sqrt{1-W^2}) & (-1 \leq W \leq 1) \quad \text{Total reflection} \\
  r &= \frac{E_h}{E_0} = -\frac{\sqrt[\gamma_0]{|\chi_{hr}|P}}{\gamma_h |\chi_{-h}|P} (W - \sqrt{W^2 - 1}) & (W > 1)
\end{align*}
\]

\[ R = r^2 \]
#10

**Reflectivity (Darwin curve)**

*Darwin curve* (intrinsic reflection curve for monochromatic plane wave) for Bragg case, no absorption, and thick crystal:

\[
R = \begin{cases} 
(W + \sqrt{W^2 - 1})^2 & (W < -1) \\
1 & (-1 \leq W \leq 1) \quad \leftarrow \text{Total reflection region} \\
(W - \sqrt{W^2 - 1})^2 & (W > 1)
\end{cases}
\]

\(W\): deviation parameter for s-polarization, symmetrical Bragg case

\[
W = \left( \frac{\Delta \theta \sin 2\theta_B + 2 \sin^2 \theta_B \frac{\Delta E}{E} + \chi_0}{\chi_h} \right) \frac{1}{|\chi_h|}
\]

**Geometry for symmetrical Bragg case**

\[\theta_B, \theta_B\]

\[K_0, K_h\]

\[\text{Surface net plane}\]

\[\theta_B + \Delta \theta, \theta_B + \Delta \theta\]
Darwin curve

For Bragg case, no absorption, and thick crystal:

\[ R = 1 \quad (-1 \leq W \leq 1) \]

\[ \Delta \theta_{\text{Darwin}} = \frac{2|\chi_{hr}|}{\sin 2\theta_B} \propto |F(h)| \]
Reflectivity with absorption

Reflectivity

- symmetrical Bragg case,
- s-polarization,
- thick crystal

\[
R = L - \sqrt{L^2 - 1}
\]

\[
L = \frac{\left\{ W^2 + g^2 + \sqrt{ \left( W^2 - g^2 - 1 + \kappa^2 \right)^2 + 4(gW - \kappa)^2 } \right\}}{1 + \kappa^2}
\]

\[
W = \left( \Delta \theta \sin 2\bar{\theta}_B + 2\sin^2 \bar{\theta}_B \frac{\Delta E}{E} + \chi_{0r} \right) \frac{1}{|\chi_{hr}|}
\]

\[
g = \frac{\chi_{0i}}{|\chi_{hr}|}, \quad \kappa = \frac{|\chi_{hi}|}{|\chi_{hr}|}
\]

Note: No absorption \( g = 0, \kappa = 0 \) \( \Rightarrow \) \( R \to \text{Darwin curve} \)
Reflectivity curve for silicon

Examples for symmetrical Bragg case, with absorption, s-polarization and thick crystal:

Si 111 refl., 10 keV
\[
\chi_{0r} = -9.78 \times 10^{-6} \\
\chi_{0i} = -1.48 \times 10^{-7} \\
\chi_{111r} = -3.66 \times 10^{-6}(1+i) \\
\chi_{111i} = -7.30 \times 10^{-8}(1+i)
\]

Si 333 refl., 30 keV
\[
\chi_{0r} = -1.07 \times 10^{-6} \\
\chi_{0i} = -1.75 \times 10^{-9} \\
\chi_{333r} = -2.24 \times 10^{-7}(1+i) \\
\chi_{333i} = -7.87 \times 10^{-10}(1+i)
\]

- Width of \(0.1 \sim 100 \ \mu\text{rad}\)
- Peak \(\sim 1\) with small absorption
Tailoring x-rays to application

\[ \downarrow \]

X-ray monochromator

- Principle
  - Introduction of diffraction theory
  - Dynamical theory
  - DuMond diagram

- Engineering
DuMond (angle-energy) diagram

The diagram helps to understand how we can extract x-rays from SR source.

Angular width (Darwin width)

$$\Delta \theta_{\text{Darwin}} = \frac{2|\chi_{hr}|}{\sin 2\theta_B} \propto |F(h)|$$

$$\Delta W = 2$$

Energy resolution

$$\frac{\Delta E}{E} = \cot \theta_B \sqrt{\Omega^2 + \Delta \theta_{\text{Darwin}}^2}$$

Effective band width

$$\frac{\Delta E}{E} \approx \frac{|\chi_{hr}|}{\sin^2 \theta_B}$$

Gaussian approximation for both light source and reflection curve

Relative energy

$$\Delta E/E = W = -1 \quad W = 1$$

Angular width (Darwin width)

Shift by refraction

Slope: $-\cot \theta_B$

Kinematical Bragg condition

Light source

Effective band width

Energy resolution
Source divergence and diffraction width

\[ \sigma_r \approx 0.597 \frac{1}{\gamma} \sqrt{\frac{\lambda}{\lambda_c}} \propto \sqrt{\frac{1}{\hbar \omega}} \]

- Bending magnet

\[ \sigma_r \approx \sqrt{\frac{\lambda}{2N\lambda_u}} \propto \sqrt{\frac{1}{\hbar \omega}} \]

- Undulator

\[ \sigma_r \approx 60 \mu \text{rad} \]

- Undulator (N= 140)

\[ \sigma_r \approx 5 \mu \text{rad} \]

For SPring-8 case:

Divergence of undulator radiation \sim diffraction width
Energy resolution

\[
\frac{\Delta E}{E} = \cot \theta_B \sqrt{\Omega^2 + \omega^2}
\]

\(\Omega\): source divergence,
\(\omega\): diffraction width

Angle-energy diagram
(DuMond diagram)

For usual beamline: \(\Delta E/E = 10^{-5} \sim 10^{-3}\)
DuMond diagram: undulator & DCM

SPring-8 standard undulator
($\lambda u = 32 \text{ mm}, N = 140, K = 1.34, E_{1st} = 10 \text{ keV}$)
+ DCM (Si 111 refl.)

**Intensity distribution of undulator**

**Acceptance by crystal**

**Undulator radiation:**
\[ E = \frac{E_0}{\left(1 + \frac{K^2}{2} + \gamma^2 \phi^2 \right)} \]

**Wider slit increases unused photons (power) on the monochromator!**
DuMond diagram: undulator & DCM

Undulator radiation

Acceptance by Si 111 DCM

ΔE/E = 5x10^{-4}

100 μrad

FWHM = 1.3 eV

SPring-8 standard undulator + 20 μrad slit + Si 111 DCM
10-keV photons → 1.3x10^{-4}
Improvement of energy resolution

(A) Collimation using slit

(B) Collimation using pre-optics w/ collimation mirror, CRL,..

(C) Additional crystal w/ (+,+) setting

(D) HR monochromator of π/2 reflection (~meV)

(B)~(D): restriction on photon energy
Improvement of energy resolution

(C) Additional crystal w/ (+,+) setting

⇒ HXPES

Si 111 DCM

Si nnn channel-cut mono.

Si 333 refl. for 6 keV

FWHM = 45 meV

Si 555 refl. for 10 keV

FWHM = 18 meV

Photon energy → Resolution

Angle →

ΔE/E = 5×10^{-5}

40 μrad
Improvement of energy resolution

(D) HR monochromator of \( \sim \pi/2 \) reflection (~meV) → Inelastic scattering

Si 111 DCM

Si \textit{nnn} back-scattering mono.

Si 999 refl. for 17.8 keV

Si 111 11 refl. for 21.7 keV

\[ \Delta E/E = 5 \times 10^{-7} \]

\[ 20 \mu \text{rad} \]

FWHM = 2.0 meV

FWHM = 0.87 meV
Photon flux after monochromator

Photon flux (throughput) after monochromator can be estimated using effective band width:

Photon flux (ph/s) =

Photon flux from light source (ph/s/0.1%bw) × 1000 × Effective band width of monochromator

Energy resolution

Throughput is estimated by overlapped area.

Note difference from energy resolution.
Effective band width

Starting with Darwin width in the energy axis

\[ \frac{\Delta E}{E} \approx \frac{|\chi_{hr}|}{\sin^2 \theta_B} \]

\[ \chi_{hr} \propto \lambda^2 \left\{ f^0(d_{hkl}) + f'(\lambda) \right\} \]

Neglecting anomalous scattering factor \( f' \)

\[ \chi_{hr} \propto \lambda^2 f^0(d_{hkl}) \]

\[ \frac{\Delta E}{E} = -\frac{\Delta \lambda}{\lambda} \approx \frac{|\chi_{hr}|}{\sin^2 \theta_B} \]

\[ = 4d_{hkl}^2 \frac{|\chi_{hr}|}{\lambda^2} \]

\[ \frac{\Delta E}{E} = -\frac{\Delta \lambda}{\lambda} \propto d_{hkl}^2 f^0(d_{hkl}) \]

\[ \text{e.g. for Si 111 refl. DCM case} \]

Note relative energy width is constant.

Independent of photon energy
Effective band width (Integrated intensity)

For single-bounce monochromator

\[
\frac{\Delta E}{E} = \left| \chi_{hr} \right| \frac{\int R(W) dW}{2 \sin^2 \theta_B}
\]

\[
\approx \frac{8}{3} \left| \chi_{hr} \right| \left[ \frac{1}{2 \sin^2 \theta_B} \right]
\]

↑ For no absorption

For double-crystal monochromator

\[
\frac{\Delta E}{E} = \left| \chi_{hr} \right| \frac{\int R(W)^2 dW}{2 \sin^2 \theta_B}
\]

\[
\approx \frac{32}{15} \left| \chi_{hr} \right| \left[ \frac{1}{2 \sin^2 \theta_B} \right] = \approx 2
\]

↑ For no absorption

When you need flux → Lower order (Si 111 refl.,..)

When you need resolution → Higher order (Si 311, Si 511 refl.,..)
Photon flux estimation

Effective band width

<table>
<thead>
<tr>
<th>Reflection (nominal energy)</th>
<th>Effective band width</th>
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<tbody>
<tr>
<td>Si 111 DCM (6 keV)</td>
<td>1.0045x10^{-4}</td>
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<td>Si 111 DCM (8 keV)</td>
<td>1.1399x10^{-4}</td>
</tr>
<tr>
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<td>1.2216x10^{-4}</td>
</tr>
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<td>1.2710x10^{-4}</td>
</tr>
<tr>
<td>Si 111 DCM (14 keV)</td>
<td>1.3021x10^{-4}</td>
</tr>
<tr>
<td>Si 333 DCM (14 keV)</td>
<td>8.0996x10^{-6}</td>
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Photon flux \((\text{ph/s/100mA/20 \text{ \mu rad(H)}})\)

\(\text{(A) SPECTRA} \times \text{Effective band width} \Leftrightarrow \text{(B) SPECTRA} \times \text{DuMond}\)

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<th>Reflection</th>
<th>Flux (A)</th>
<th>Flux (B)</th>
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<tr>
<td>Si 111 DCM (6 keV)</td>
<td>5.68x10^{13}</td>
<td>5.70x10^{13}</td>
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<td>Si 111 DCM (8 keV)</td>
<td>6.14x10^{13}</td>
<td>6.15x10^{13}</td>
</tr>
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<td>Si 111 DCM (10 keV)</td>
<td>6.01x10^{13}</td>
<td>6.02x10^{13}</td>
</tr>
<tr>
<td>Si 111 DCM (12 keV)</td>
<td>5.28x10^{13}</td>
<td>5.29x10^{13}</td>
</tr>
<tr>
<td>Si 111 DCM (14 keV)</td>
<td>4.20x10^{13}</td>
<td>4.20x10^{13}</td>
</tr>
<tr>
<td>Si 333 DCM (14 keV)</td>
<td>2.62x10^{12}</td>
<td>2.61x10^{12}</td>
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### Photon flux estimation

#### Effective band width

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Photon flux (throughput) after monochromator can be estimated using effective band width:

\[
\text{Photon flux (ph/s)} = \text{Photon flux from light source (ph/s/0.1%bw)} \times 1000 \times \text{Effective band width of monochromator}
\]

This approach is valid.
We can obtain photon flux of $10^{13}$ to $10^{14}$ ph/s/100 mA/mm² using standard undulator sources and Si 111 reflections at SPring-8 beamlines.

Higher harmonics elimination more $\Rightarrow$ mirror or detuning of DCM
Tailoring x-rays to application

↓

X-ray monochromator

Principle

✓ Introduction of diffraction theory
✓ Dynamical theory
✓ DuMond diagram

Engineering
Double-crystal monochromator

✓ Fixed-exit operation for usability at experimental station.

✓ Choose suitable mechanism for energy range (Bragg angle range).

✓ Precision, stability, rigidity,...

\[ y = AB = \frac{h}{2 \sin \theta_B} \]
\[ z = OB = \frac{h}{2 \cos \theta_B} \]

Fixed-exit operation using rotation (\(\theta\)) + two translation mechanism
Double-crystal monochromator

$\theta_1 + \text{translation} + \theta_2$ computer link

$\theta$-stage

1st crystal

2nd crystal

Translation stage

$h = 100 \text{ mm},$

$\theta_B = 5.7^\circ - 72^\circ$ (for lower energy range)

$\theta + \text{two translation (1 cam)}$

$\theta$-stage

1st crystal

2nd crystal

$\theta$ rotation center

$Y_1$ stage

Z-cam stage

$h = 30 \text{ mm}$

$\theta_B = 3^\circ - 27^\circ$ for higher energy range

$SPring-8 \text{ std. DCM}$

$Matsushita \ et \ al., \ NIM \ A246 \ (1986)$

$SPring-8 \ BL15XU$

$Yabashi \ et \ al., \ Proc. \ SPIE \ 3773, \ 2 \ (1999)$

$\theta + \text{two translation (2 cams)}$

$h = 25 \text{ mm}, \ \theta_B = 5^\circ - 70^\circ$

$KEK-PF \ BL-4C$

$h = 100 \text{ mm}, \ \theta_B = 5.7^\circ - 72^\circ$ (for lower energy range)
Crystal cooling

Why crystal cooling?
Q_{in} (Heat load by SR) = Q_{out} (Cooling + Radiation,..)
→ with temperature rise $\Delta T$
→ $\alpha \Delta T = \Delta d$ (d-spacing change)
$\alpha$: thermal expansion coefficient
or $\to \Delta \theta$ (bump of lattice due to heat load)

Miss-matching between 1st and 2nd crystals occurs:
→ Thermal drift, loss of intensity, broadening of beam, loss of brightness
→ Melting or limit of thermal strain → Broken!

We must consider:
- Thermal expansion of crystal: $\alpha$,
- Thermal conductivity in crystal: $\kappa$,
- Heat transfer to coolant and crystal holder.

Solutions:
(S-1) $\kappa/\alpha \to$ Larger
(S-2) Contact area between crystal and coolant/holder
→ larger
(S-3) Irradiation area → Larger,
and power density → smaller

Figure of merit

<table>
<thead>
<tr>
<th></th>
<th>Silicon</th>
<th>Silicon</th>
<th>Diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\kappa$ (W/m/K)</td>
<td>150</td>
<td>1000</td>
<td>2000</td>
</tr>
<tr>
<td>$\alpha$ (1/K)</td>
<td>2.5x10^{-6}</td>
<td>-5x10^{-7}</td>
<td>1x10^{-6}</td>
</tr>
<tr>
<td>$\kappa/\alpha \times 10^6$</td>
<td>60</td>
<td>2000</td>
<td>2000</td>
</tr>
</tbody>
</table>

Figure of merit of cooling:
Good for silicon (80 K) and diamond (300 K)
**Crystal cooling at SPring-8**

**<Bending magnet beamline>**

Power & power density:
\~100 W, \~1 W/mm²

- **Fin crystal direct-cooling - (S2)**

**<Undulator beamline>**

Linear undulator, \( N = 140, \lambda_u = 32 \) mm

Power & power density: 300\~500 W , 300\~500 W/mm²

- **a) Direct cooling of silicon pin-post crystal – (S2) & (S3)**

- **b) Silicon cryogenic cooling - (S1)**

- **c) Ila diamond with indirect water cooling - (S1)**
Improvement of stability of DCM

Turbulence suppressing flexible tube for LN2

Precise temp. control of 1st & 2nd crystals

Radiation shield

1st crystal

2nd crystal

X-ray

Thermal Isolation
Improvement of stability of DCM

Measured Intensity fluctuation of 1 Å x-rays at BL13XU
  Average time : 1 ms ⋯ very sensitive
  Measurement frequency : 1 kHz
  Δθ1 stage : 0.2” stepping at a time interval of 5 s

Angular fluctuation between the crystals : 1” → 0.15”
Intensity fluctuation of 1 Å x-rays : 5% → 2%
Key issues of X-ray monochromator

Introducing the **dynamical x-ray diffraction** for **large & perfect crystal**, w/ several important points:

1) Total reflection occurs at the gap between dispersion surfaces.

2) Normalized deviation parameter $W$ is related to the gap.

3) $W$ is parameter of angular deviation and energy (wavelength) deviation.

   It gives **DuMond diagram** as a band of $|W|<1$.

4) By combination of light source and monochromator crystals, photon energy, energy resolution, photon flux, etc. can be controlled / tuned.

Double-crystal monochromator w/ crystal cooling is needed for practical use at the SR beamline.

By understanding these, you will be approaching to good design/use of the beamline for your SR science.
Text books following Laue’s dynamical theory

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**Ergebnisse der Exakt Naturwiss.**  
**10** (1931) 133-158.

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R. W. James  
“The Dynamical Theory of X-Ray Diffraction”  

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B. W. Batterman & H. Cole  
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- For $f^0$

- For anomalous scattering factor $f'$, $f''$
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  [7] Tables of NIST,
Acknowledgment

Thank you for your kind attention.

Enjoy Cheiron school
Enjoy SPring-8
and
Enjoy Japan!