X-ray Beamline Design 1

X-ray Monochromator

Shunji Goto
SPring-8/JASRI
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2. Light source
3. X-ray Monochromator
   Fundamental of Bragg reflection
   Dynamical theory
   DuMond diagram ~ extraction of x-rays from SR
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Beamline structure

 Beamline = “Bridge” between light source & experimental station

→ Light source
  Bending magnet
  Insertion device

→ Front-end
  Exp. hall
  SR
  Ring tunnel

→ Experimental station
  Shielding hutch

→ Transport and processing of photons
  photon energy, energy resolution,
  beam size, beam divergence, polarization,..

→ Vacuum
  protection of ring vacuum and beamline vacuum

→ Radiation safety
  Shielding and interlock

→ Optics & transport
  Monochromator, mirror
  shutter, slit
  pump,..
Light sources & X-ray optics

Check points to be considered for your SR application:

- White or monochromatic
- Energy range
- Energy resolution
- Flux & flux density
- Beam size at sample (micro beam?,...)
- Beam divergence/convergence at sample (Resolution in k-space)
- Higher order elimination w/ mirror
- Polarization conversion
- Spatial coherency

→ Light source, monochromator, mirror,
and other optical devices and components
BL classification (energy region)

Photon energy (eV) →

- **Bending magnet**: IR
- **Wiggler**: SX
- **Undulator**: HX

Energy regions:
- IR
- Visible ~ UV
- SX
- HX

Techniques:
- SX-PES
- HX-PES
- SX-MCD
- PEEM
- SAXS
- XAFS
- Powder XRD
- PX
- HP/HT
- NRS
- SAXS
- Inelastic
- XRD
- HX

Energy ranges:
- \(10^0\) to \(10^1\)
- \(10^2\) to \(10^3\)
- \(10^4\) to \(10^5\)
BL classification (energy resolution)

Energy resolution ($\Delta E/E$) →

- 10^{-7}
- 10^{-5}
- 10^{-3}
- White

Bending magnet
- XAFS
- SAXS
- Single crystal XRD
- PX
- Powder XRD
- Topograph
- Imaging
- Topograph
- Earth,.. HP/HT

Wiggler
- Inelastic

Undulator
- Inelastic
- XAFS
- Surface - interface
- XRF
- Microbeam, imaging
- XMCD
- HX-PES
- PX
- HP/HT XRD
- Powder XRD
Light sources (1)

Bending magnet or insertion devices?

Bending magnet:
for wide energy range, continuous spectrum
for wide beam application for large samples

Undulator (major part of 3GLS beamline):
for high-brilliance beam
for micro-/ nano-focusing beam

Wiggler:
for higher energy X-rays > 100 keV.

Power, brilliance, flux density, partial flux,..
can be calculated using code.

e.g. “SPECTRA” by T. Tanaka & H. Kitamura
Light sources (2)

Angular divergence and band width

→ Core part we need

Bending magnet

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

Undulator

\[ \sigma_r \approx \sqrt{\frac{\lambda_n}{2N\lambda_u}} = \frac{1}{2\gamma} \sqrt{\frac{1+K^2/2}{nN}} \]

\[ \frac{\Delta E}{E} \approx \frac{1}{nN} \]
Light sources (3)

Kilowatt of SR power $\rightarrow$ mostly eliminated before/by monochromator

Bending magnet

Power distribution

\[
\begin{aligned}
\psi_v & \approx 1/\gamma \\
\psi_h & \approx \text{const}
\end{aligned}
\]

Total power

\[
P_{\text{tot}}[\text{kW}] = 1.27 E^2 [\text{GeV}] B^2 [\text{T}] R [\text{m}] \phi [\text{rad}] I [\text{A}]
\]

\[
E = 8 \text{ GeV}, \ I = 0.1 \text{ A}, \ B = 0.68 \text{ T}, \ R = 39.3 \text{ m} \\
\Rightarrow P_{\text{tot}} = 0.15 \text{ kW/mrad}
\]

Undulator

\[
\begin{aligned}
\psi_v & \approx 1/\gamma \\
\psi_h & \approx K/\gamma
\end{aligned}
\]

K: deflection parameter

\(K = 0.5 \sim 2.5\)

Total power

\[
P_{\text{tot}}[\text{kW}] = 1.27 E^2 [\text{GeV}] \frac{1}{2} B_0^2 [\text{T}] L [\text{m}] I [\text{A}]
\]

\[
B_0 = 0.87 \text{ T}, \ L = 4.5 \text{ m} \\
\Rightarrow P_{\text{tot}} = 14 \text{ kW}
\]
**X-ray Monochromator**

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

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Bragg reflection

Bragg’s law in real space

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

Laue condition (Kinematical) in reciprocal space

\[ Q = K_s - K_0 = h \]

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

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

Scattering vector \( Q \)

Reciprocal lattice vector \( h \)

Incident wave \( K_0 \)

Scattered wave \( K_s \)

net plane (spacing \( d \))
Ewald sphere:

-Ewald sphere:

Radius = \(1/\lambda = K_0\)

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

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

$a = 5.431 \text{ Å}$

$\text{d-spacing}$

- (400) : 1.3578 Å
- (111) : 3.1356 Å
- (311) : 1.6375 Å
- (511) : 1.0452 Å

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

**Structure factor** ➞ Sum of atomic scattering with phase shift in the unit cell

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

Atomic scattering factor

\[ F(h) = \sum_j f_j(h, E) \exp\{2\pi i (hx_j + ky_j + lz_j)\} \]

For diamond structure

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

\[
\begin{align*}
\begin{cases}
  h + k + l &= 4m & F &= 8f & \leftarrow 8 \text{ atoms in phase} \\
  h + k + l &= 4m \pm 1 & F &= 4(1 \pm i)f & \leftarrow \text{Half contribute with phase shift } \pm \pi/2 \\
  h + k + l &= 4m \pm 2 & F &= 0 & \leftarrow \text{Half cancel with } \pi
\end{cases}
\end{align*}
\]

Position of atoms in the unit cell for diamond structure

\[ (x_j, y_j, z_j) = \]

1. \((0, 0, 0)\)
2. \((1/4, 1/4, 1/4)\)
3. \((1/2, 1/2, 0)\)
4. \((3/4, 3/4, 1/4)\)
5. \((0, 1/2, 1/2)\)
6. \((1/4, 3/4, 3/4)\)
7. \((1/2, 0, 1/2)\)
8. \((3/4, 1/4, 3/4)\)
Crystal structure factor for diamond structure

(400), (220),...
All in phase
⇒ \( F = 8f \)

(111), (311),...
Half contribute with phase shift ± \( \pi /2 \)
⇒ \( F = 4(1 ± i)f \)

(011), (200),...
Half cancel with \( \pi \)
⇒ Forbidden reflection
\( F = 0 \)
X-ray monochromator using perfect crystal

→ Perfect single crystal: silicon, diamond,..

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

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

![Graph showing photon energy tuning with Bragg angles for Si 111, Si 311, and Si 511 reflections.]

e.g. for SPring-8 standard DCM

Bragg angle: 3~27°
Kinematical X-ray diffraction

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

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

Peak intensity $\frac{\sin^2(\pi N_x h)}{\sin^2(\pi h)}$

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

Crystal size becomes larger $\Rightarrow$ narrower & higher, approaching delta function
Dynamical theory
Two-beam approximation
“Large & perfect” single crystal:
1) Multiple scattering w/ h & -h reflection
2) Extinction
   (Diffraction by “finite” number of net planes)

Kinematical diffraction is invalid
⇒ Dynamical theory must be applied.
Fundamental equation

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

\[
\frac{k_h^2 - K_0^2}{K_0^2} E_h = \sum_g \chi_{h-g} (e_h \cdot e_g) E_g
\]

- \( h, g, \ldots \) : Reciprocal lattice points
- \( E_h, E_g \) : Fourier components of electric field
- \( K_0 \) : Incident wave vector in vacuum
- \( k_h \) : Wave vectors in the crystal
- \( \chi_h \) : Fourier components of the polarizability (Negative values, 10^{-6} \sim 10^{-5})
- \( P = (e_h \cdot e_g) \) : Polarization factor between \( h \) and \( g \) waves
- \( k_h = k_0 + h \) : Momentum conservation
Two-beam approximation

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

\[
\frac{k_h^2 - K_0^2}{K_0^2} E_h = \sum_g \chi_{h-g} (\mathbf{e}_h \cdot \mathbf{e}_g) E_g
\]

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

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

\(\chi_0, \chi_h, \chi_{-h}\): Fourier components of the polarizability

(Negative values, 10^{-6}~10^{-5})

\(P = (\mathbf{e}_0 \cdot \mathbf{e}_h)\): Polarization factor (\(\sigma: P = 1, \pi: P = \cos 2\theta_B\))
Two-beam approximation

Using two equations, we obtain following secular equation:

(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

\[ (k_0^2 - k^2)(k_h^2 - k^2) = \chi_h \chi_{-h} P^2 K_0^4 \]

\[ k^2 = (1 + \chi_0) K_0^2 \]

\( k \): Mean wave number in the crystal

Scheme of self-consistent wave field
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.

Tangential component of wave vector must be continuous.

- Incident wave in vacuum
  - Refracted wave in the crystal
  - Bragg reflection in the crystal
  - Reflected wave in the crystal
  - Reflected wave in vacuum
Laue case and Bragg case

Laue case
(Transmission geometry)

Bragg case
(Reflection geometry)
Asymmetry ratio

\[
\begin{align*}
\gamma_0 &= \hat{K}_0 \cdot n \\
\gamma_h &= \hat{K}_h \cdot n
\end{align*}
\]

\[b = \frac{\gamma_0}{\gamma_h}\]

Laue case: \(b > 0\)

Symmetric Laue case: \(b = 1\)

Bragg case: \(b < 0\)

Symmetric Bragg case: \(b = -1\)

\(n\): normal vector to the surface
Dispersion surface

\[
\left( k_0^2 - k^2 \right) \left( k_h^2 - k^2 \right) = \chi_h \chi_{-h} P^2 K_0^4
\]

Secular equation is quartic equation, and it gives four-point solution on the \( n \)-vector, producing the dispersion surfaces.

Two dispersion surfaces show the gap near Bragg condition.
Deviation from Bragg condition

Excitation error

⇒ Geometrical deviation $\zeta_0$ from Bragg condition:

Distance between Ewald sphere and the reciprocal lattice point.

$\zeta_0$ is positive when H is inside the Ewald sphere (by S. Miyake).

\[
\zeta_0 \approx -\frac{2(K_0 \cdot h) + h^2}{2K_0}
\]
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.

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

$\zeta_0$ \[\downarrow\]

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

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

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

For symmetric Bragg case, sigma polarization:

\[
W = \left\{ \Delta \theta \sin 2\bar{\theta}_{BK} + 2 \frac{\Delta E}{E} \sin^2 \bar{\theta}_{BK} + \frac{\chi_{0r}}{2} \right\} \frac{1}{|\chi_{hr}|}
\]
**Sign of deviation parameter $W$**

Angle deviation at fixed energy

$\Rightarrow$ direction change of wave vector

Energy deviation at fixed angle

$\Rightarrow$ length change of wave vector
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

\( \chi_h \): Fourier component of polarizability \( \rightarrow \) proportional to the structure factor

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

\( v_c \): 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

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

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

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

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

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

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

\[ h = k = l = 0 \]

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

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

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

For Bragg case, no absorption, and thick crystal:

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

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

*Angular deviation*

*Energy deviation*

*Refraction*

Geometry for symmetrical Bragg case: 

- **\(K_0\)**
- **\(K_h\)**
- Surface
- Net plane
- \(\theta_B\)
- \(\theta_B + \Delta \theta\)
Darwin curve

For Bragg case, no absorption, and thick crystal:
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 \( g = 0, \kappa = 0 \) \( \Rightarrow \) \( R \rightarrow \text{Darwin curve} \)
Reflectivity curve for silicon

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

Si 111 refl., 10 keV

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

Si 333 refl., 30 keV

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

- Width of 0.1 ~ 100 µrad
- Peak ~1 with small absorption
DuMond (angle-energy) diagram

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

Angular width (Darwin width)

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

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

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

Darwin width

- Shift by refraction
- Slope: $-\cot \theta_B$
- Kinematical Bragg condition

Effective band width

- Light source divergence
- Energy resolution

Light source
Source divergence and diffraction width

Divergence of undulator radiation $\sim$ diffraction width

**Bending magnet**

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

**Undulator**

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

For SPring-8 case:

- **Bending magnet**

  $\sigma_r \approx 60 \, \mu\text{rad}$

- **Undulator ($N=140$)**

  $\sigma_r \approx 5 \, \mu\text{rad}$

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: $E = E_0 / \left(1 + K^2/2 + \gamma^2 \phi^2 \right)$

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

SPring-8 standard undulator + 20 μrad slit + Si 111 DCM
10-keV photons \( \Rightarrow 1.3 \times 10^{-4} \)
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 \( \pi/2 \) 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

ΔE/E = 5x10^-5

40 μrad
Improvement of energy resolution

(D) HR monochromator of $\sim\pi/2$ reflection ($\sim$meV) ➔ Inelastic scattering

Si 111 DCM

Si $nnn$ back-scattering mono.

Si 999 refl. for 17.8 keV

FWHM= 2.0 meV

Si 11 11 11 refl. for 21.7 keV

FWHM= 0.87 meV

$\Delta E/E = 5\times10^{-7}$

20 $\mu$rad
Photon flux after monochromator can be estimated using effective band width:

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

Throughput is estimated by overlapped area.

Note difference from energy resolution.
Effective band width

Starting with Darwin width in the energy axis

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

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

Neglecting anomalous scattering factor \( f' \)

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

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

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

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

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

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

\[= \left\lfloor \frac{8}{3} \right\rfloor \frac{|\chi_{hr}|}{2 \sin^2 \theta_B}
\]

↑ For no absorption

For double-crystal monochromator

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

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

↑ For no absorption

Effective band-width is obtained by integration of reflection curve.

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>
</tr>
</thead>
<tbody>
<tr>
<td>Si 111 DCM (6 keV)</td>
<td>1.0045x10^{-4}</td>
</tr>
<tr>
<td>Si 111 DCM (8 keV)</td>
<td>1.1399x10^{-4}</td>
</tr>
<tr>
<td>Si 111 DCM (10 keV)</td>
<td>1.2216x10^{-4}</td>
</tr>
<tr>
<td>Si 111 DCM (12 keV)</td>
<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>
</tr>
</tbody>
</table>

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

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

This approach is valid.
Photon flux at undulator beamline

We can obtain photon flux of $10^{13} \sim 10^{14}$ 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

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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
e.g. Double-crystal monochromator

\[ \theta_1 + \text{translation} + \theta_2 \text{ computer link} \]

1st crystal
\[ \theta \text{-stage} \]
2nd crystal

\[ h = 100 \text{ mm}, \]
\[ \theta_B = 5.7\text{~}72^\circ \text{ (for lower energy range)} \]

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

\[ h = 25 \text{ mm}, \theta_B = 5\text{~}70^\circ \]

KEK-PF BL-4C
Matsushita et al., NIM A246 (1986)

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

\[ \theta \text{-stage} \]
1st crystal
\[ \theta \text{rotation center} \]
2nd crystal
\[ Y_1 \text{ stage} \]
Z-cam stage

Offset \( h = 30 \text{ mm} \)
=3~27° for higher energy range

SPring-8 std. DCM

Crystal cooling

**Why crystal cooling?**

Q_{in} (Heat load by SR) = Q_{out} (Cooling + Radiation,..)
→ with temperature rise ΔT
→ αΔT = Δd (d-spacing change)

α: thermal expansion coefficient
or → Δθ (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: α,
- Thermal conductivity in crystal: κ,
- Heat transfer to coolant and crystal holder.

**Solutions:**
(S-1) κ/α → 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>κ (W/m/K)</td>
<td>150</td>
<td>1000</td>
<td>2000</td>
</tr>
<tr>
<td>α (1/K)</td>
<td>2.5x10^{-6}</td>
<td>-5x10^{-7}</td>
<td>1x10^{-6}</td>
</tr>
<tr>
<td>κ/α x10^{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, \( N = 140, \lambda u = 32 \text{ mm} \)
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) **I1a diamond with indirect water cooling** - (S1)
Summary

Key issues on the x-ray monochromator were shown, 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, · · · 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

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

R. W. James
“The Dynamical Theory of X-Ray Diffraction”
Solod State Physics 15, (1963) 53-220.

B. W. Batterman & H. Cole
“Dynamical Diffraction of X-Rays by Perfect Crystals”

Oxford (2001)

Dover (1945)

References

For monochromator

[1] T. Matsushita & H. Hashizume, 
Handbook on Synchrotron Radiation Vol. 1, 


For atomic scattering factor

- For $f^0$

- For anomalous scattering factor $f’, f”$
  http://henke.lbl.gov/optical_constants/index.html,
  [7] Tables of NIST,
Thank you for your attention.