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Cheiron School 2012

X-ray Beamline Design 1

X-ray Monochromator

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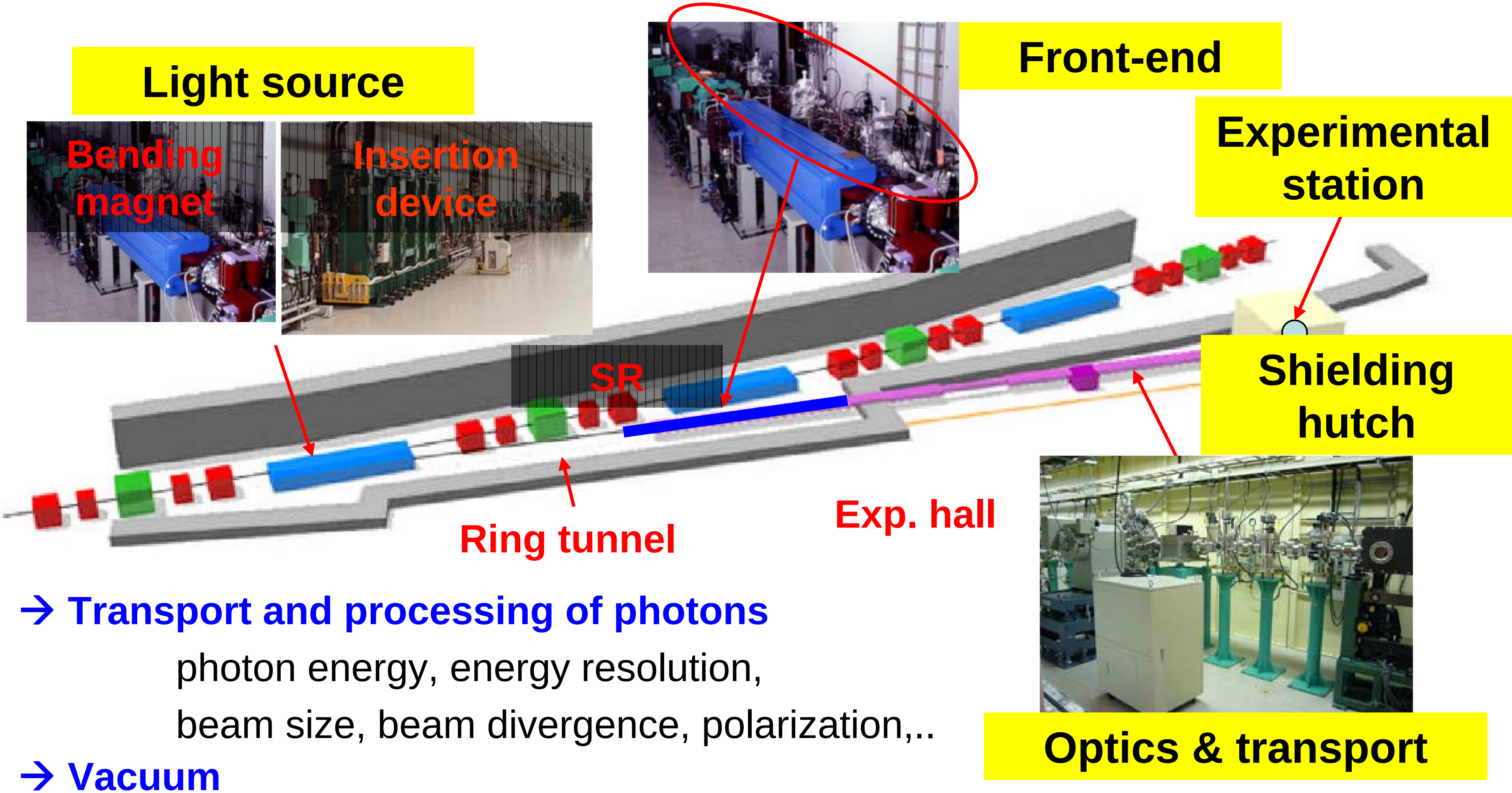
SPring-8/JASRI

Outline

1. Introduction
2. Light source
3. X-ray Monochromator
   - Fundamental of Bragg reflection
   - Dynamical theory
   - DuMond diagram ~ extraction of x-rays from SR
   - Double crystal monochromator
   - Crystal cooling
4. Example of beamlines at SPring-8
5. Summary

Beamline structure

Beamline = "Bridge" between light source & experimental station



→ **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

Monochromator, mirror

shutter, slit

pump,..

Light sources & X-ray optics

Check points to be considered for your SR application:

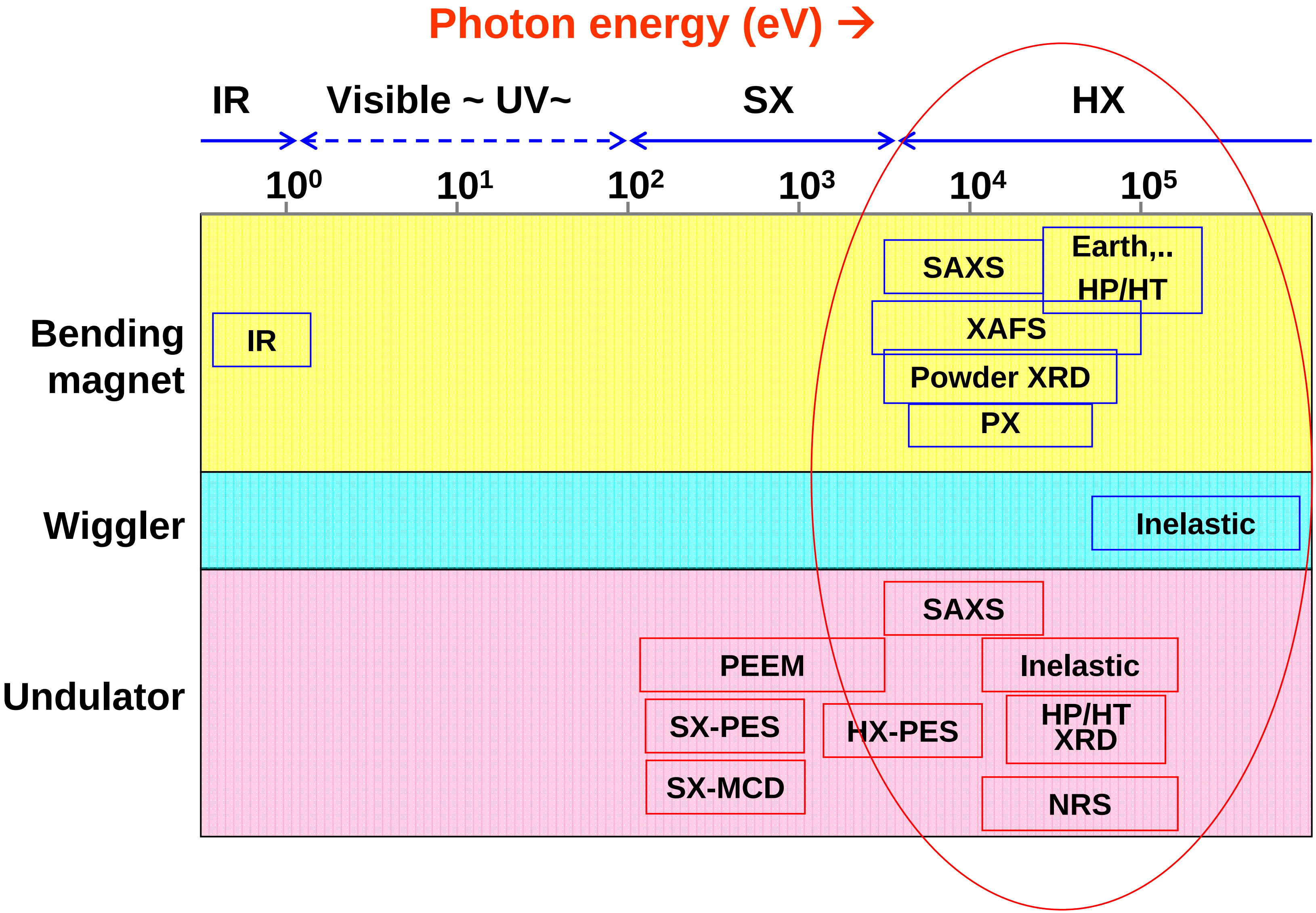
- White or monochromatic
- Energy range
- Energy resolution
- Flux & flux density
- Beam size at sample (micro beam?,...)
- Beam divergence/convergence at sample (Resolution in k-space)
- Higher order elimination w/ mirror
- Polarization conversion
- Spatial coherency

....

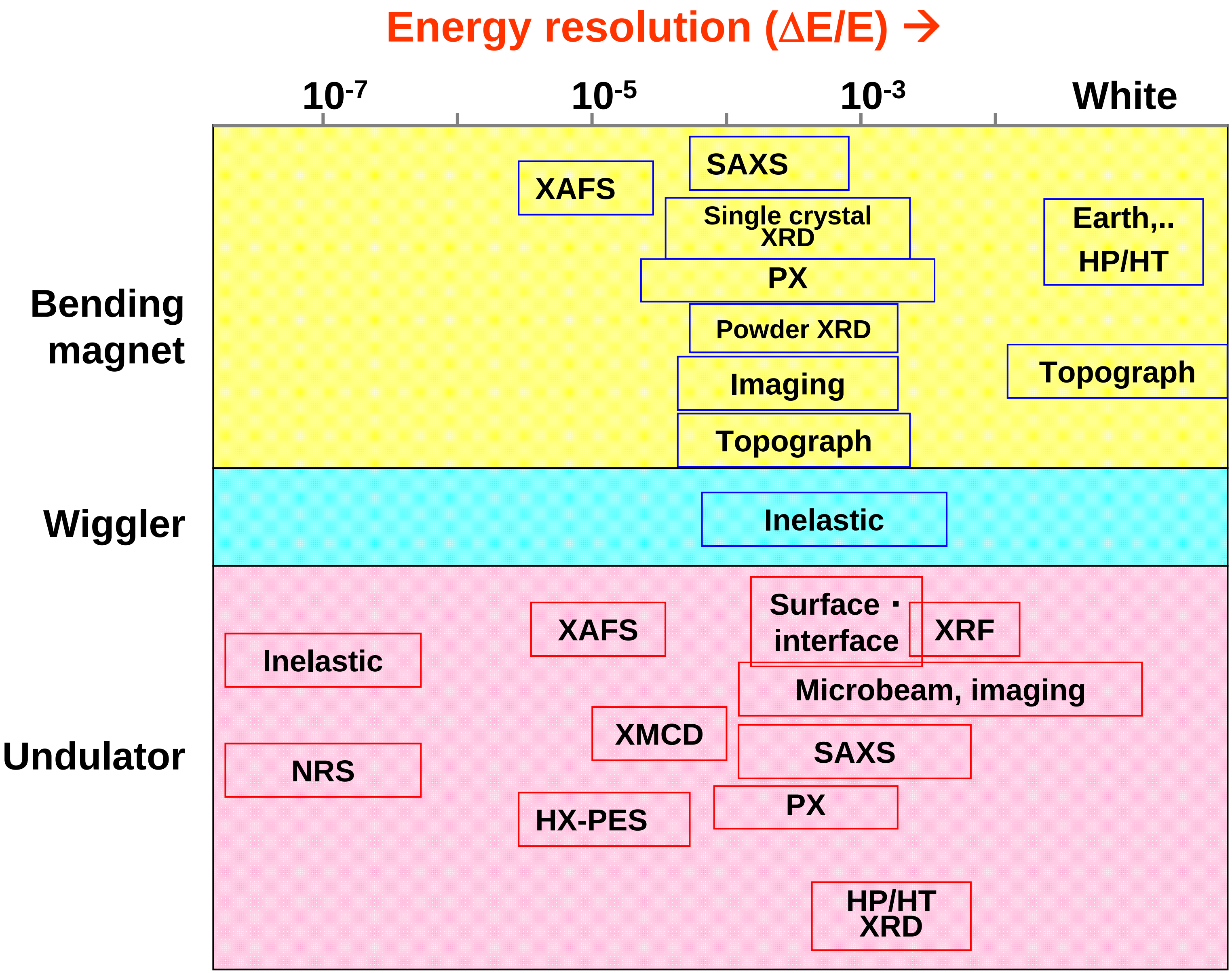
→ Light source, monochromator, mirror,

and other optical devices and components

BL classification (energy region)



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

Imaging

Topograph

Earth,..

HP/HT

Topograph

Wiggler

Inelastic

Undulator

Inelastic

NRS

XAFS

XMCD

HX-PES

Surface · interface

XRF

Microbeam, imaging

SAXS

PX

HP/HT XRD

Light sources (1)

Bending magnet or insertion devices ?

Bending magnet:

for wide energy range, continuous spectrum

for wide beam application for large samples

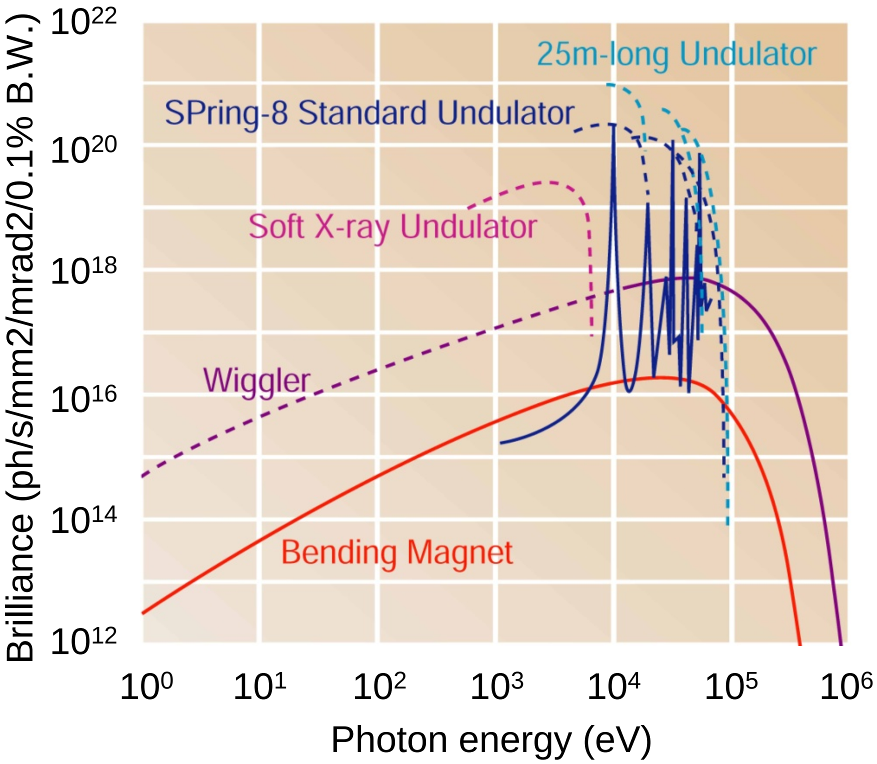
Undulator (major part of 3GLS beamline):

for high-brilliance beam

for micro-/ nano-focusing beam

Wiggler:

for higher energy X-rays > 100 keV.



Brilliance for SPring-8 case

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

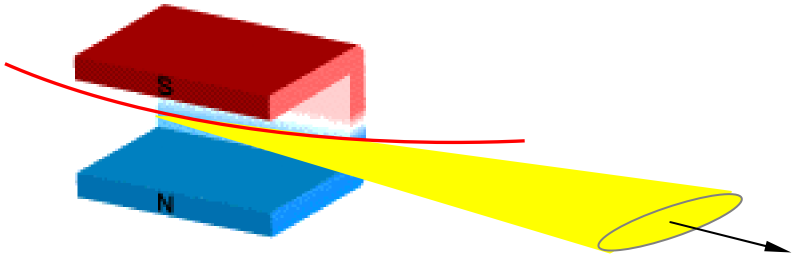
Bending magnet

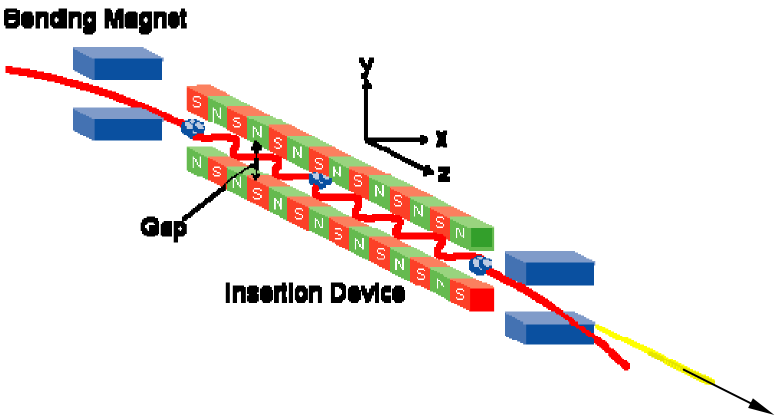
$$\sigma_{r'} \approx 0.597 \frac{1}{\gamma}\sqrt{\frac{\lambda}{\lambda_c}}$$

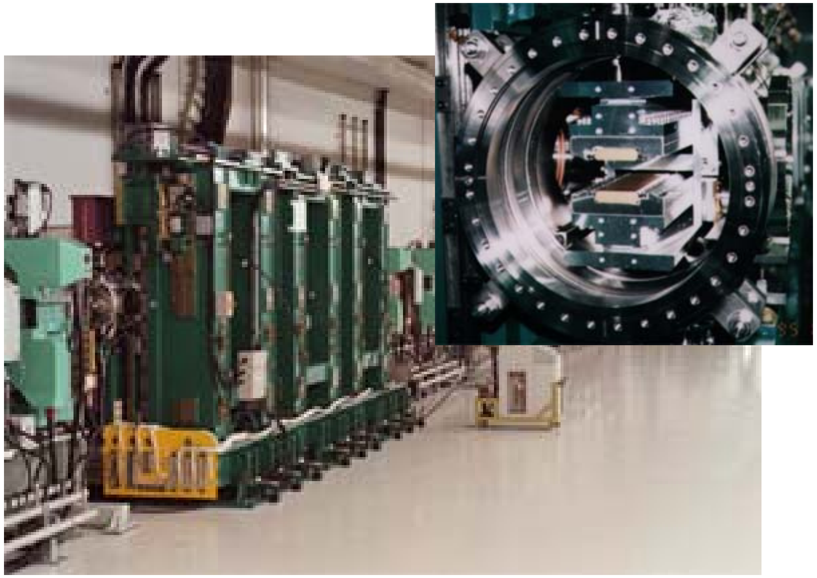
Undulator

$$\sigma_{r'} \approx \sqrt{\frac{\lambda_n}{2N\lambda_u}} = \frac{1}{2\gamma}\sqrt{\frac{1+K^2/2}{nN}}$$

$$\frac{\Delta E}{E} \approx \frac{1}{nN}$$





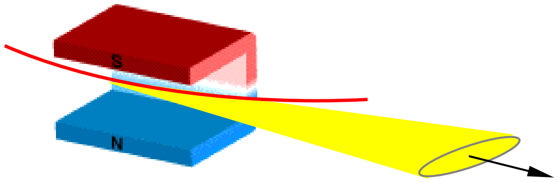


SPring-8 in-vacuum undulator

Light sources (3)

Kilowatt of SR power → mostly eliminated before/by monochromator

Bending magnet



Power distribution

$$\begin{cases} \psi_v \approx 1/\gamma \\ \psi_h \approx const \end{cases}$$

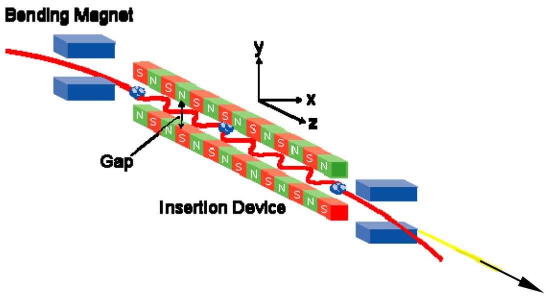
Total power

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

E= 8 GeV, I= 0.1 A, B= 0.68 T, R= 39.3 m

→ P_{tot}= 0.15 kW/mrad

Undulator



$$\begin{cases} \psi_v \approx 1/\gamma \\ \psi_h \approx K/\gamma \end{cases}$$

K: deflection parameter

(K= 0.5~2.5)

$$P_{\text{tot}}[\text{kW}] = 1.27E^2[\text{GeV}]\overbrace{\frac{1}{2}B_0{}^2}^{\left\langle B_0{}^2 \sin^2\left(2\pi z/\lambda_u\right)\right\rangle}[\text{T}]L[\text{m}]I[\text{A}]$$

B_0= 0.87 T, L= 4.5 m

→ P_{tot}= 14 kW

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 ← Bragg's law

Energy resolution ← source divergence, Darwin width,..

Flux (throughput) ← related to Darwin width

➔ Understanding the dynamical theory for large & perfect crystal

Practical of the monochromator

- Double-crystal monochromator for fixed-exit

Single-bounce monochromator is for limited case

- Crystal cooling

High heat load depending on light source

➔ Mechanical engineering issues

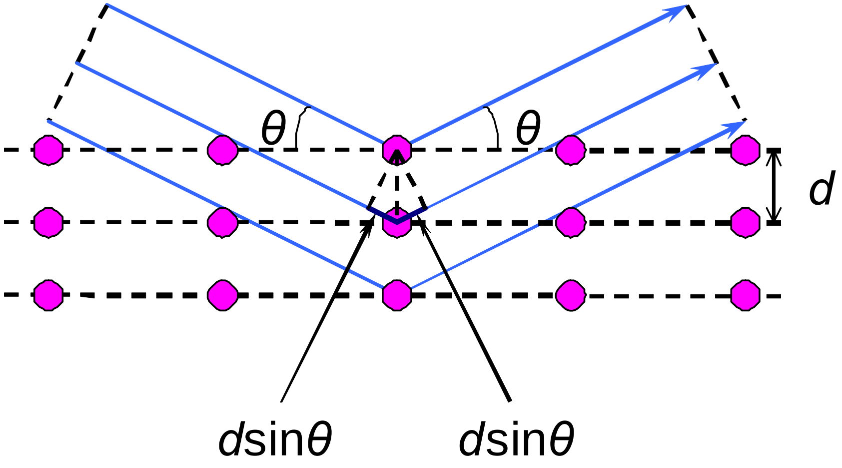
Bragg reflection

Bragg’s law in real space

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

2) Phase matching between net planes.

$$\boxed{2d\sin\theta_{\mathrm{B}} = m\lambda}$$

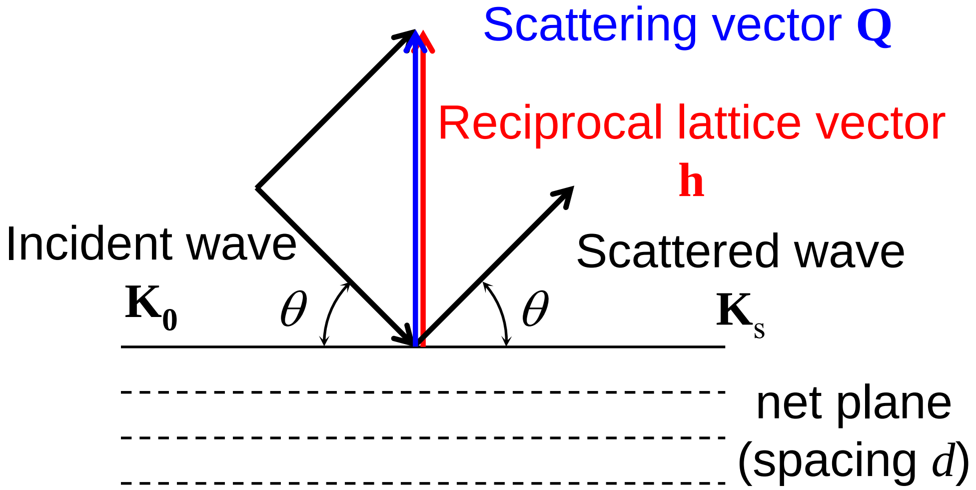


Laue condition (Kinematical) in reciprocal space

$$\boxed{\mathbf{Q} = \mathbf{K}_{\mathrm{s}} - \mathbf{K}_{0} = \mathbf{h}}$$

Reciprocal lattice vector $\mathbf{h}$

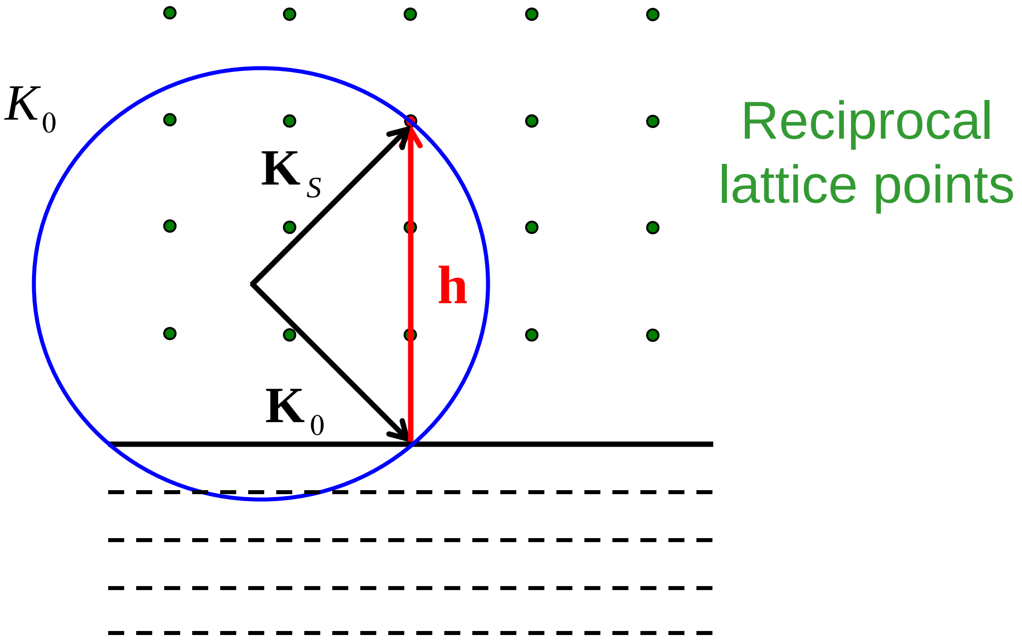
- Normal to net plane
- Length = $1/d$



Ewald sphere

Ewald sphere:

$$Radius = 1/\lambda = K_0$$

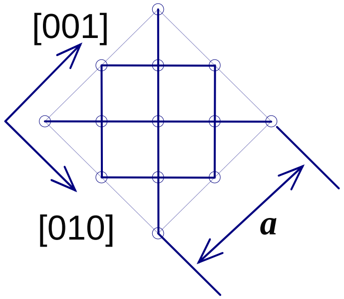


➔ When a reciprocal lattice point is on the Ewald sphere, Bragg reflection occurs.

Miller indices and *d*-spacing for silicon

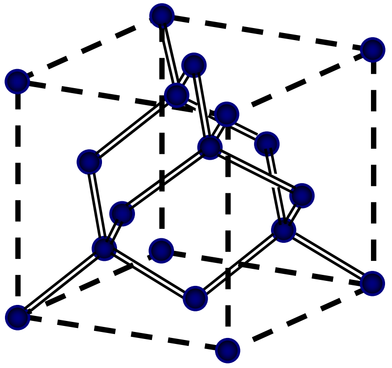
$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Top view

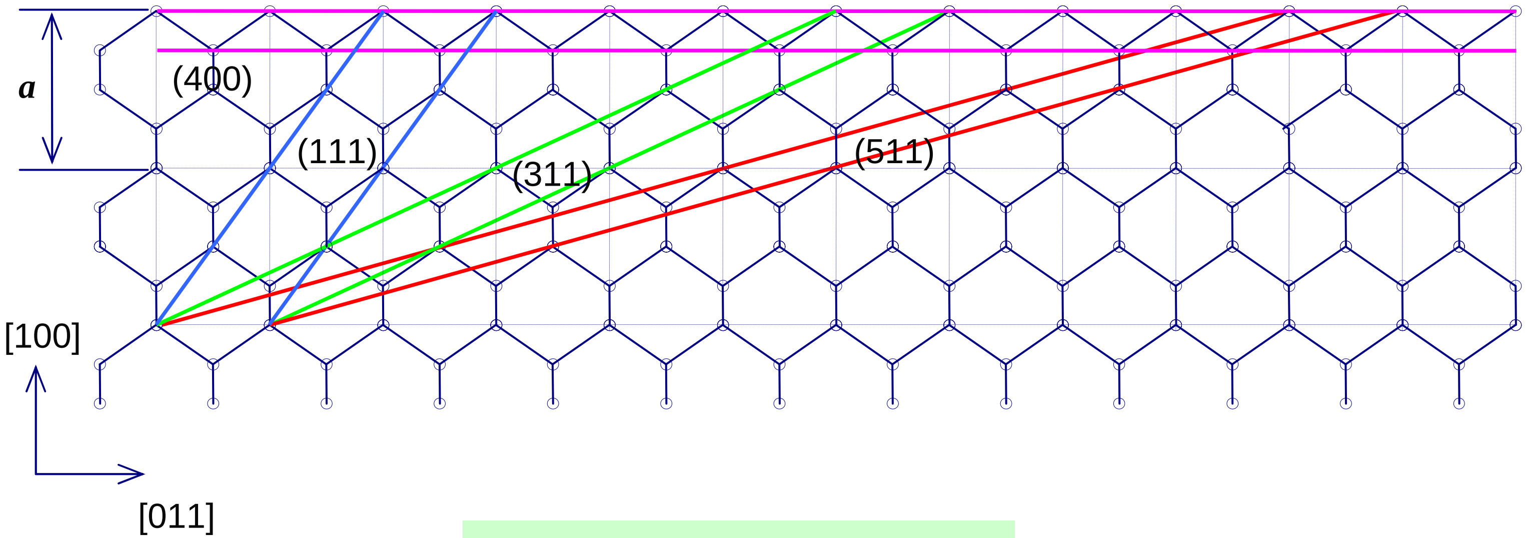


$a = 5.431$ Å

d-spacing (400) : 1.3578 Ǻ
(111) : 3.1356 Ǻ
(311) : 1.6375 Ǻ
(511) : 1.0452 Ǻ



Side view



Diamond : $a = 3.567$ Å

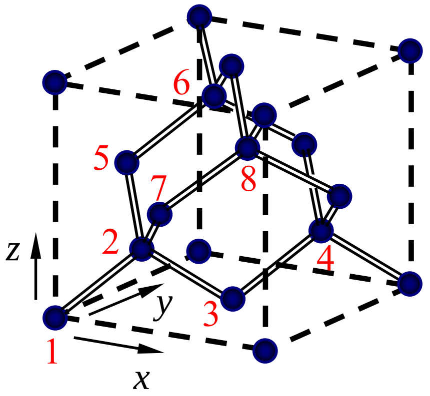
Crystal structure factor for diamond structure

Structure facrtor ➔ Sum of atomic scattering with phase shift in the unit cell

$$F(\mathbf{h}) = \sum_j \underline{\underline{f_j(\mathbf{h}, E)}} \exp(2\pi i \mathbf{h} \cdot \mathbf{r}_j)$$

Atomic scattering factor

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



Position of atoms in the unit cell for diamond structure

$(x_j, y_j, z_j) =$

$(0, 0, 0)_1$, $(1/4, 1/4, 1/4)_2$,

$(1/2, 1/2, 0)_3$, $(3/4, 3/4, 1/4)_4$,

$(0, 1/2, 1/2)_5$, $(1/4, 3/4, 3/4)_6$,

$(1/2, 0, 1/2)_7$, $(3/4, 1/4, 3/4)_8$

For diamond structure

h, k, l Mixture of odd and even numbers

$$F = 0$$

h, k, l All odd, or, all even numbers, and m: integer,

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

← 8 atoms in phase

← Half contribute with phase shift $\pm\pi/2$

← Half cancel with π

Crystal structure factor for diamond structure

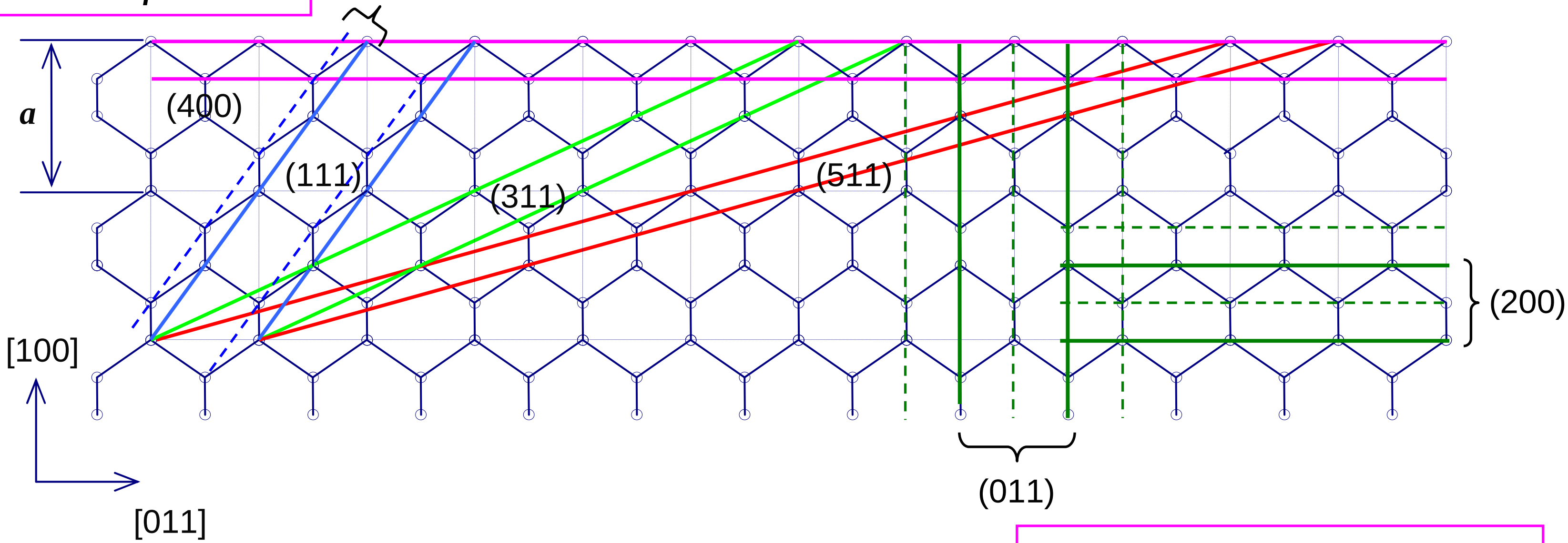
(400), (220),...

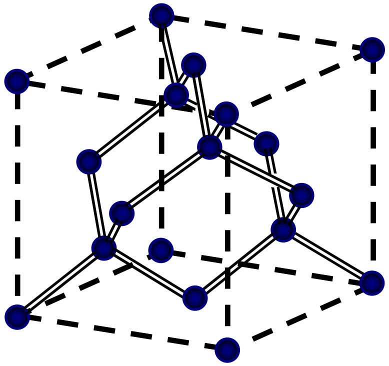
All in phase

➔ $F = 8f$

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

➔ $F = 4(1 \pm i) f$





(011), (200),...

Half cancel with π

➔ Forbidden reflection
$F = 0$

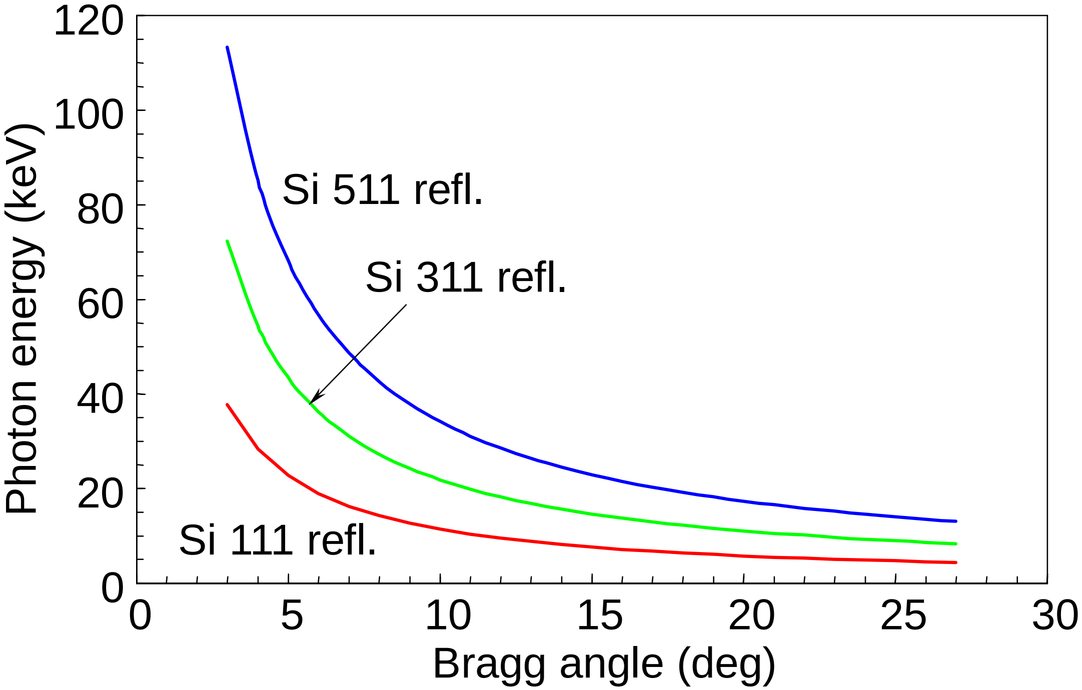
X-ray monochromator using perfect crystal

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

Photon energy tuning:

- ➢ Crystal & lattice plane
- ➢ Bragg angle range

$$E\ [\mathrm{keV}] = \frac{12.3984}{2d_{hkl}\,[\mathrm{\AA}]\sin\theta_{\mathrm{B}}}$$



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:

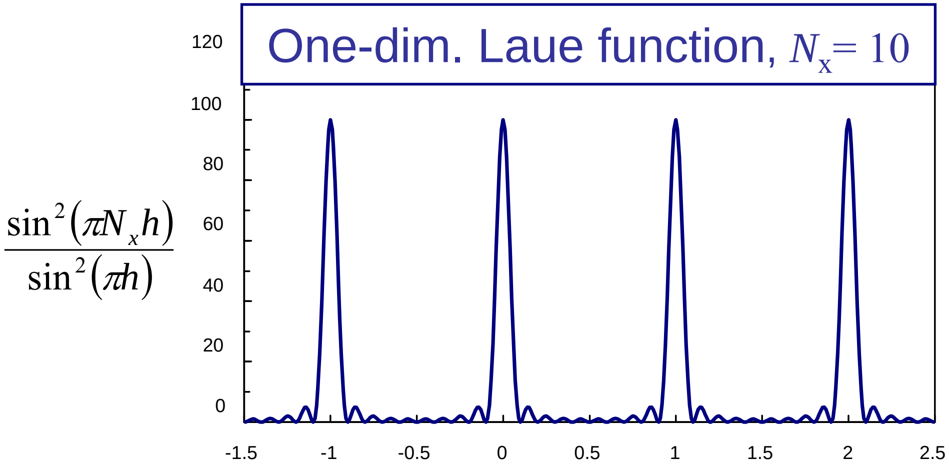
$$I = I_e \left|F(\mathbf{Q})\right|^2 \cdot \left|G(\mathbf{Q})\right|^2$$

Laue function: $\left|G(\mathbf{Q})\right|^2 = \frac{\sin^2(\pi N_x h)}{\sin^2(\pi h)} \cdot \frac{\sin^2(\pi N_y k)}{\sin^2(\pi k)} \cdot \frac{\sin^2(\pi N_z l)}{\sin^2(\pi l)}$

← 3-dim. Periodic structure

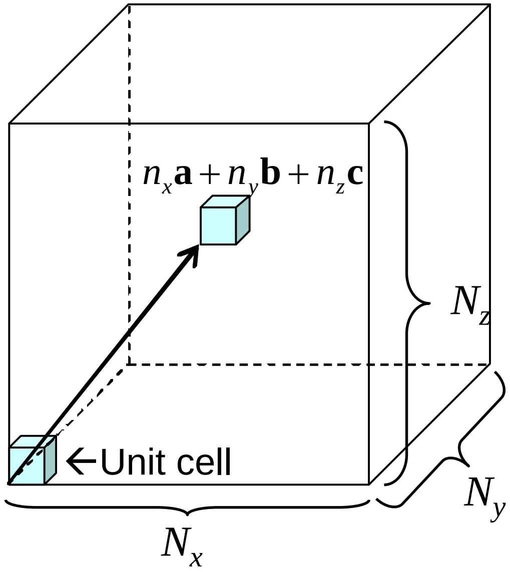
h, k, l: integer→ Intense peaks

➔ (hkl) reflection



Peak intensity N_x^{2}

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



Crystal size becomes larger ➔ narrower & higher, approaching delta function

Dynamical theory

Two-wave approximation

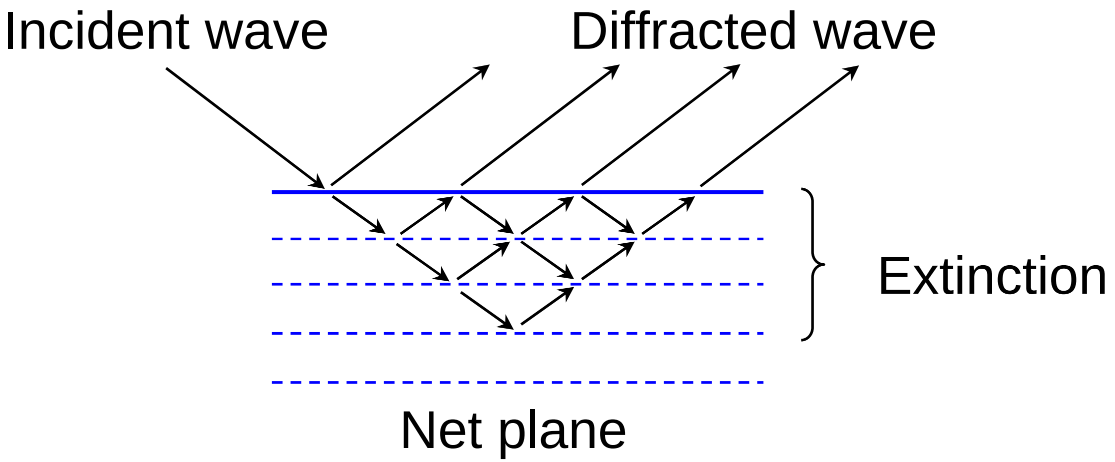
Kinematical to dynamical theory

“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):

$$\boxed{\frac{k_h{}^2 - K_0{}^2}{K_0{}^2} E_h = \sum_g \chi_{h-g} \left(\mathbf{e}_h \cdot \mathbf{e}_g \right) E_g}$$

$h, g, \ldots$: Reciprocal lattice points

E_h, E_g : Fourier components of electric field

$\boldsymbol{K}_0$: Incident wave vector in vacuum

$\boldsymbol{k}_h$: Wave vectors in the crystal

χ_h : Fourier components of the polarizability (Negative values, 10^{-6}~10^{-5})

$P = (\mathbf{e}_h \cdot \mathbf{e}_g)$: Polarization factor between ***h*** and ***g*** waves

$k_h = k_0 + h$: Momentum conservation

Two-wave approximation

Fundamental equation is reduced to the equation for

two waves of incidence and “one” intense diffraction

$$\boxed{\frac{k_h{}^2 - K_0{}^2}{K_0{}^2} E_h = \sum_g \chi_{h-g} \left(\mathbf{e}_h \cdot \mathbf{e}_g\right) E_g}$$

$$\Longrightarrow$$

$$\boxed{\begin{aligned} &(\mathrm{A}) \quad \frac{k_0{}^2 - K_0{}^2}{K_0{}^2} E_0 = \chi_0 E_0 + P\chi_{-h} E_h \\ &(\mathrm{B}) \quad \frac{k_h{}^2 - K^2}{K^2} E_h = P\chi_h E_0 + \chi_0 E_h \end{aligned}}$$

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

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

$P = \left(\mathbf{e}_0 \cdot \mathbf{e}_h\right)$: Polarization factor ($\sigma : P = 1, \ \pi : P = \cos 2\theta_B$)

Two-wave approximation

Using two equations, we obtain following secular equation:

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

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

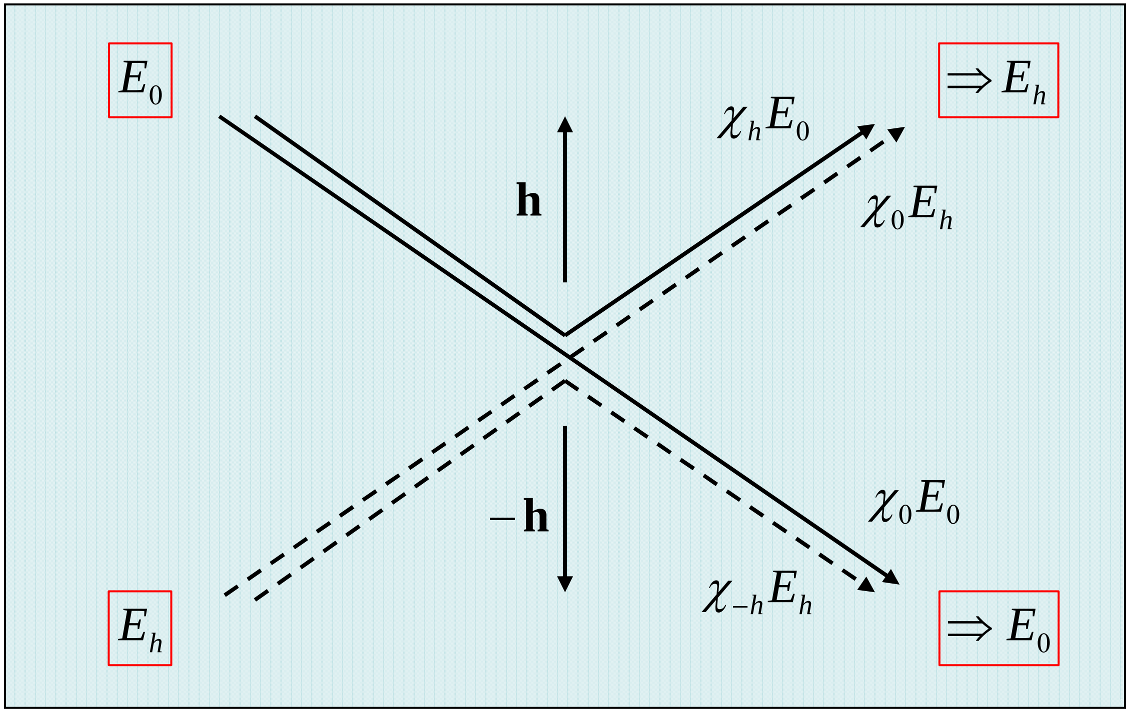
$\Rightarrow$

Secular equation

$$\boxed{\left(\mathbf{k}_0{}^2 - k^2\right)\left(\mathbf{k}_h{}^2 - k^2\right) = \chi_h\chi_{-h}P^2K_0{}^4}$$

$$k^2 = \left(1+\chi_0\right)K_0{}^2$$

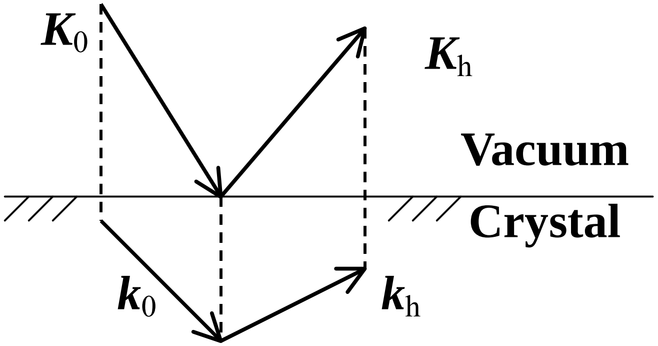
k : Mean wave number in the crystal



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

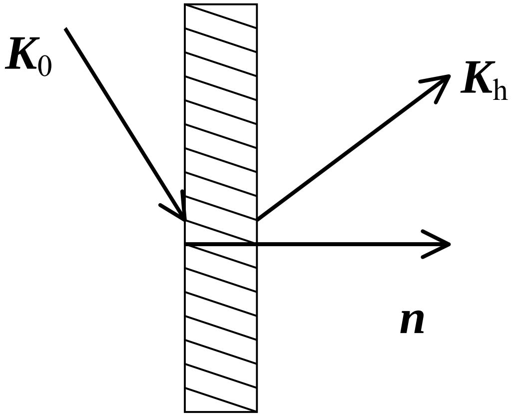
→ Refracted wave in the crystal

→ Bragg reflection in the crystal

→ Reflected wave in the crystal

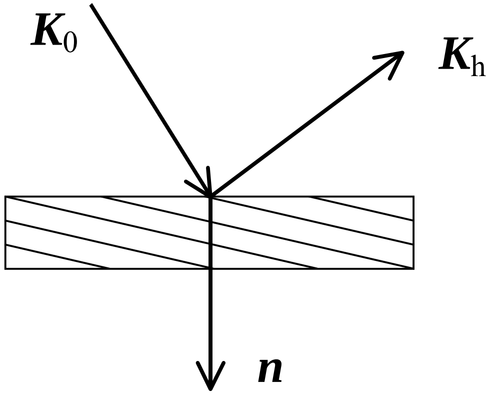
→ Reflected wave in vacuum

Laue case and Bragg case



Laue case

(Transmission geometry)

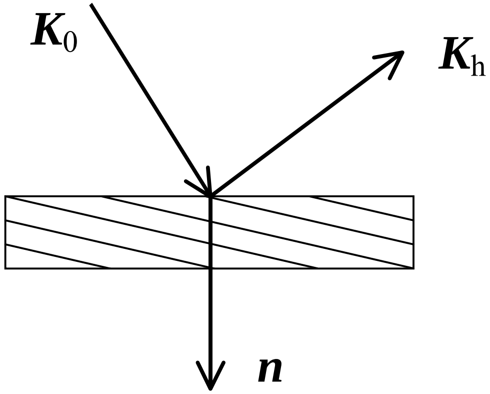


Bragg case

(Reflection geometry)

Asymmetry ratio

$$\begin{cases} \gamma_0 = \hat{K}_0 \cdot n \\ \gamma_h = \hat{K}_h \cdot n \end{cases} \qquad b = \frac{\gamma_0}{\gamma_h}$$



Laue case: *b*>0

Symmetric Laue case: *b*= 1

Bragg case: *b*< 0

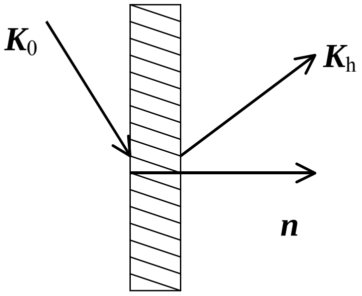
Symmetric Bragg case: *b*= -1

n: normal vector to the surface

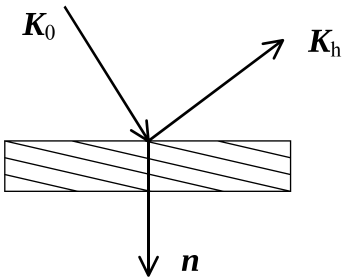
Dispersion surface

$$\left(\mathbf{k}_0{}^2 - k^2\right)\left(\mathbf{k}_h{}^2 - k^2\right) = \chi_h \chi_{-h} P^2 K_0{}^4$$

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

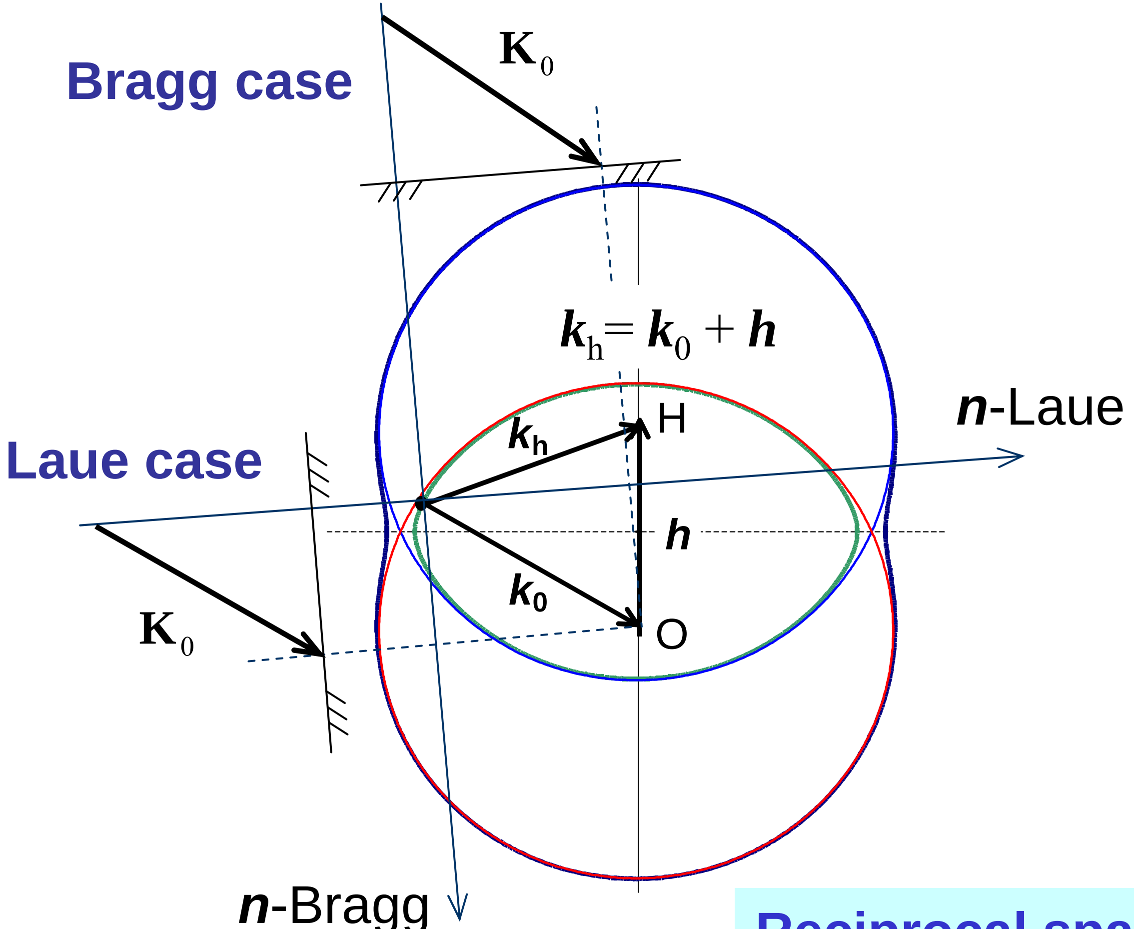


Laue case



Bragg case

Real space



Reciprocal space

Two dispersion surfaces show the gap near Bragg condition.

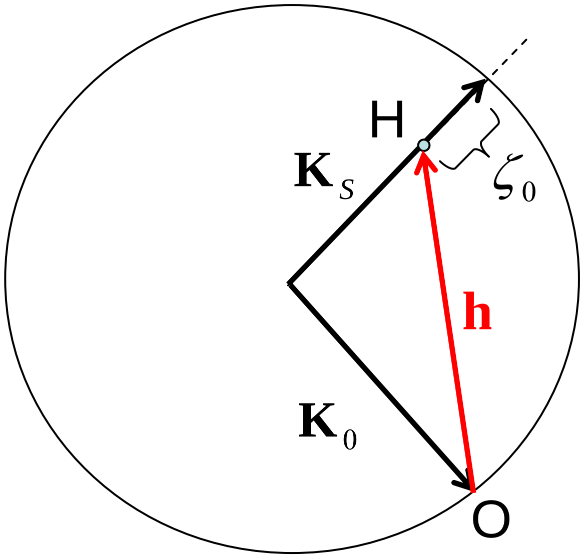
Deviation from Bragg condition

Excitation error

➔ Geometrical deviation ζ_0 from Bragg condition:

Distance between Ewald sphere and the reciprocal lattice point.

ζ_0 is positive when H is inside the Ewald sphere (by S. Miyake).



$$\varsigma_0 \approx -\frac{2(\mathbf{K}_0 \cdot \mathbf{h}) + h^2}{2K_0}$$

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.

$$W = -\underbrace{\frac{2(\mathbf{K}_0 \cdot \mathbf{h}) + h^2}{2K_0^{\ 2}}}_{\zeta_0} \sqrt{\frac{\gamma_0}{|\gamma_h|}} \frac{1}{|\chi_{hr}| \cdot |P|} + \frac{\chi_{0r}}{2|\chi_{hr}| \cdot |P|} \sqrt{\frac{\gamma_0}{|\gamma_h|}} \left(1 - \frac{\gamma_h}{\gamma_0}\right)$$

Δθ: Angle deviation for fixed photon energy,

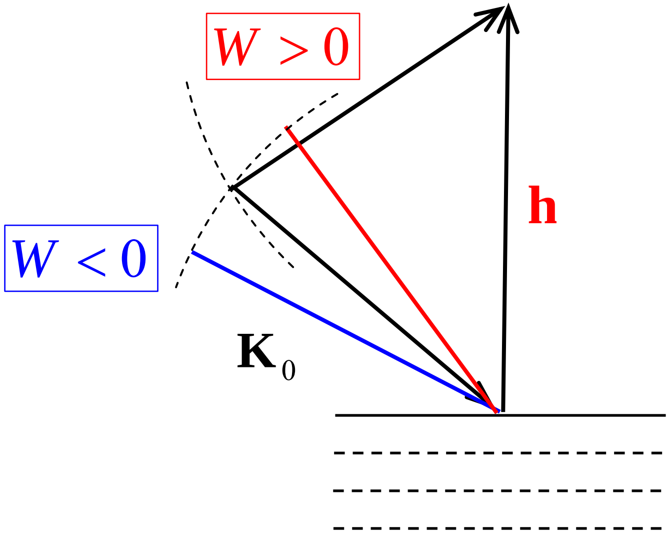
Δ*E*: Energy deviation for fixed incident angle

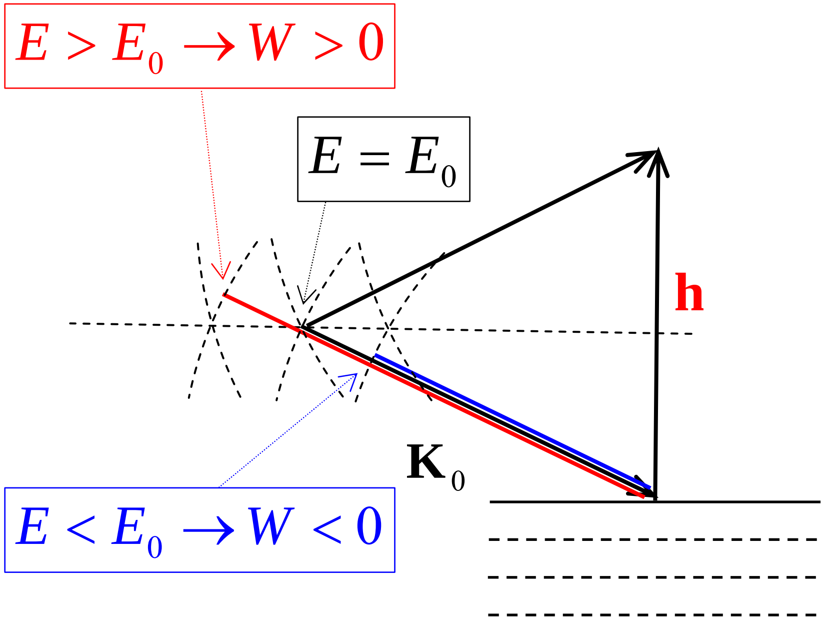
$$W = \left\{ \Delta\theta \sin 2\bar{\theta}_{BK} + \frac{\Delta E}{E} \sin^2 \bar{\theta}_{BK} + \frac{\chi_{0r}}{2} \left(1 - \frac{\gamma_h}{\gamma_0}\right) \right\} \sqrt{\frac{\gamma_0}{|\gamma_h|}} \frac{1}{|\chi_{hr}| \cdot |P|}$$

For symmetric Bragg case, sigma polarization:

$$W = \left\{ \Delta\theta \sin 2\bar{\theta}_{BK} + \frac{\Delta E}{E} \sin^2 \bar{\theta}_{BK} + \chi_{0r} \right\} \frac{1}{|\chi_{hr}|}$$

Sign of deviation parameter *W*





Angle deviation at fixed energy

➔ direction change of wave vector

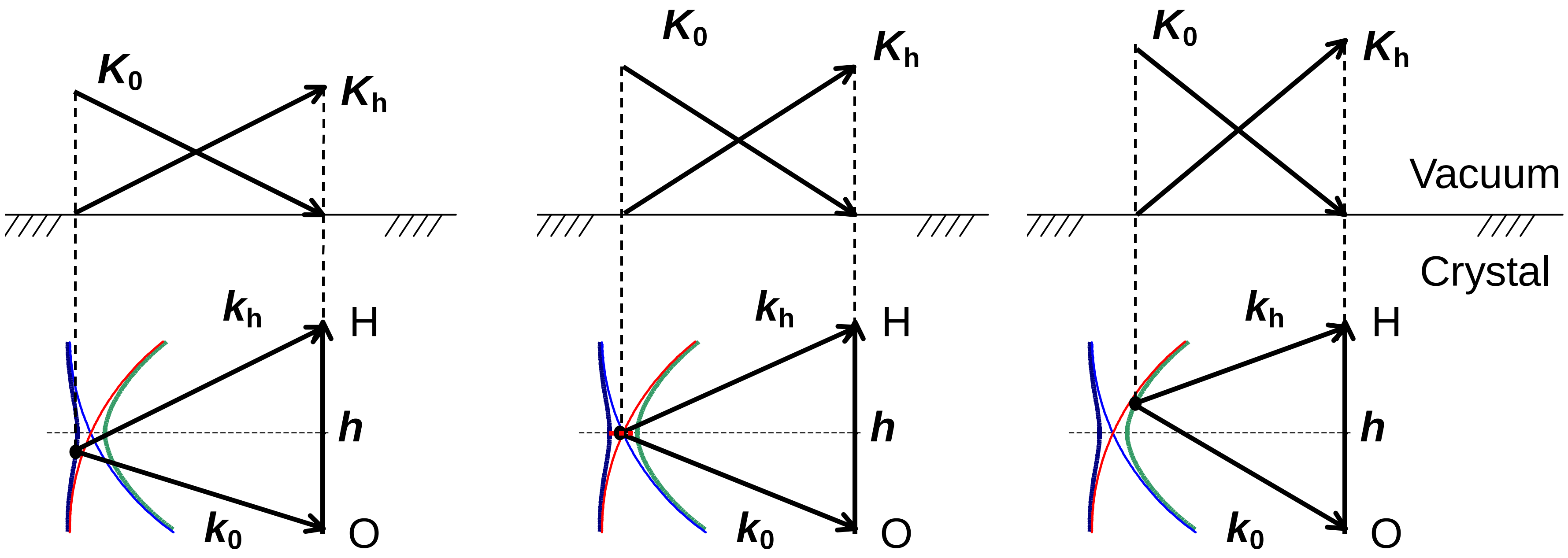
Energy deviation at fixed angle

➔ 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

χ_h: Fourier component of polarizability

→ proportional to the structure factor

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

v_c: unit cell volume

$$\chi_h = \chi_{hr} + \chi_{hi}$$

$$\chi_{hr} \Leftrightarrow f^0(\mathbf{h}) + f'(E)$$

Atomic form factor
+ real part of anomalous factor

$$\chi_{hi} \Leftrightarrow f''(E)$$

Imaginary part of
anomalous factor

For diamond structure

$$\boxed{h + k + l = 4m}$$

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

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

$$\boxed{h + k + l = 4m \pm 1}$$

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

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

$$\boxed{h = k = l = 0}$$

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

$$\chi_{0i} = -\frac{r_e \lambda^2}{\pi v_c} 8 f''$$

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:

$$
\begin{cases}
r = \dfrac{E_h}{E_0} = -\sqrt{\dfrac{\gamma_0}{|\gamma_h|}}\dfrac{|\chi_{hr}|}{\chi_{-h}}\dfrac{|P|}{P}\left(W + \sqrt{W^2 - 1}\right) \quad (W < -1) \\[2em]
r = \dfrac{E_h}{E_0} = -\sqrt{\dfrac{\gamma_0}{|\gamma_h|}}\dfrac{|\chi_{hr}|}{\chi_{-h}}\dfrac{|P|}{P}\left(W + i\sqrt{1 - W^2}\right) \quad (-1 \le W \le 1) \quad \leftarrow \textbf{Total reflection} \\[2em]
r = \dfrac{E_h}{E_0} = -\sqrt{\dfrac{\gamma_0}{|\gamma_h|}}\dfrac{|\chi_{hr}|}{\chi_{-h}}\dfrac{|P|}{P}\left(W - \sqrt{W^2 - 1}\right) \quad (W > 1)
\end{cases}
$$

Reflectivity (Darwin curve)

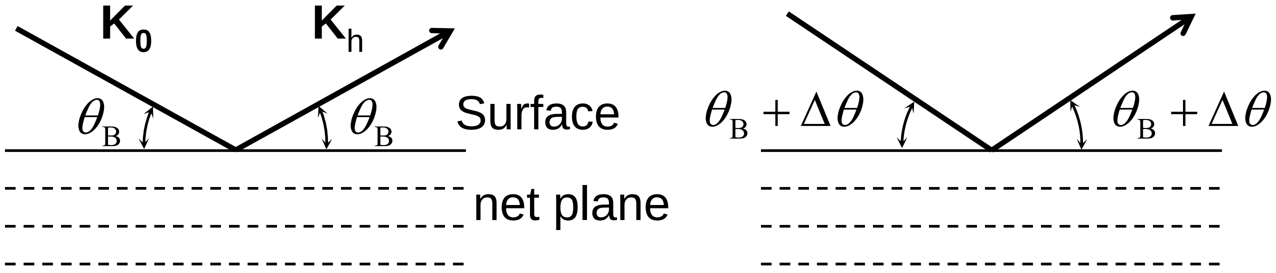
Darwin curve (intrinsic reflection curve for monochromatic plane wave) for Bragg case, no absorption, and thick crystal:

$$
\begin{cases}
R = \left(W + \sqrt{W^2 - 1}\right)^2 & (W < -1) \\
R = 1 \quad (-1 \le W \le 1) & \leftarrow \text{Total reflection region} \\
R = \left(W - \sqrt{W^2 - 1}\right)^2 & (W > 1)
\end{cases}
$$

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

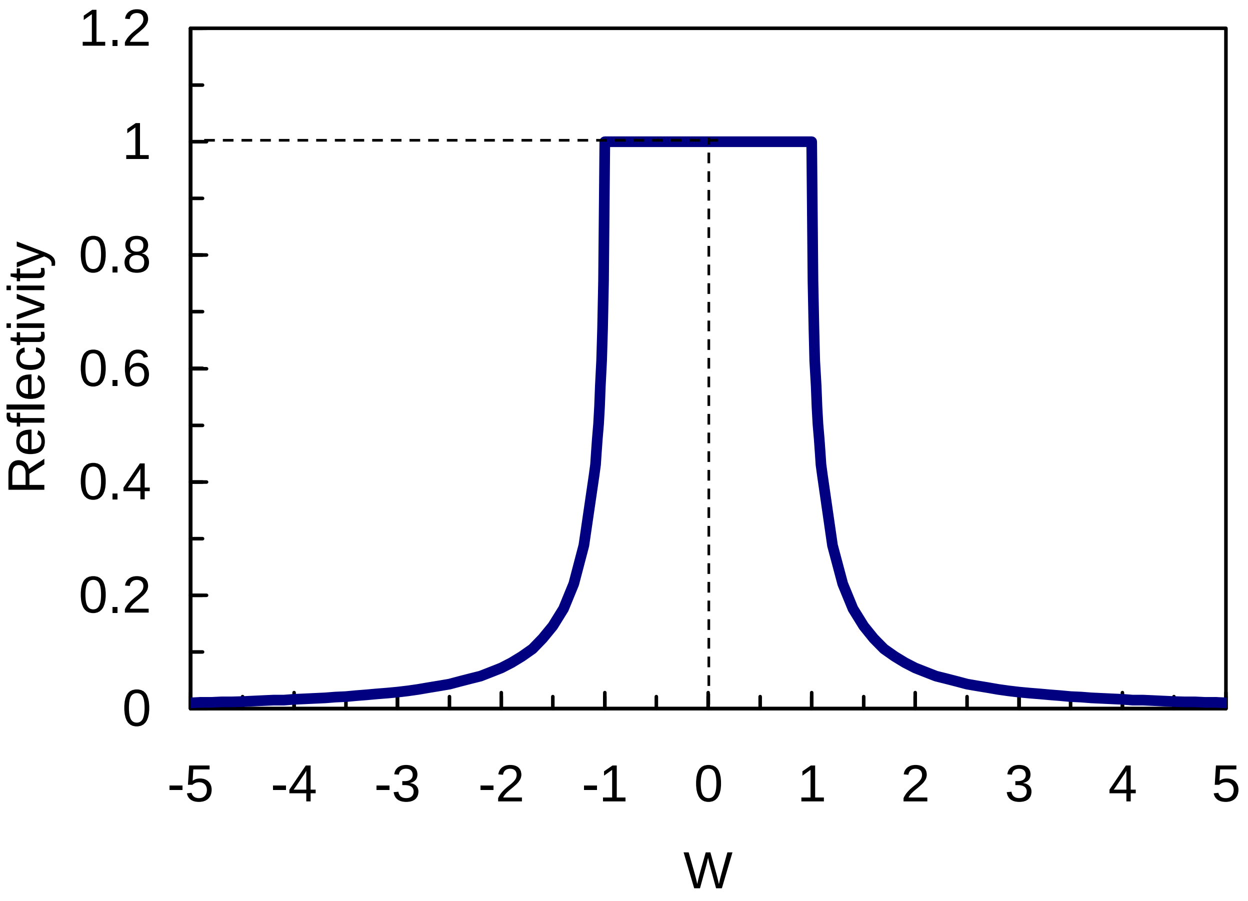
$$
\boxed{W = \left(\underbrace{\Delta\theta \sin 2\theta_{\mathrm{B}}}_{\text{Angular deviation}} + \underbrace{2\sin^2\theta_{\mathrm{B}}\frac{\Delta E}{E}}_{\text{Energy deviation}} + \underbrace{\chi_0}_{\text{Refraction}}\right)\frac{1}{|\chi_h|}}
$$

Geometry for symmetrical Bragg case



Darwin curve

For Bragg case, no absorption, and thick crystal:



Reflectivity with absorption

Reflectivity

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

$$\boxed{R = L - \sqrt{L^2 - 1}}$$

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

$$W = \left(\Delta\theta \sin 2\overline{\theta}_{\mathrm{B}} + 2\sin^2 \overline{\theta}_{\mathrm{B}} \frac{\Delta E}{E} + \chi_{0r}\right)\frac{1}{\left|\chi_{hr}\right|}$$

$$g = \frac{\chi_{0i}}{\left|\chi_{hr}\right|}, \quad \kappa = \frac{\left|\chi_{hi}\right|}{\left|\chi_{hr}\right|}$$

Note: No absorption $g = 0, \kappa = 0 \;\Rightarrow\; R \rightarrow Darwin\ curve$

Reflectivity curve for silicon

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

Si 111 refl., 10 keV

$$\chi_{0r} = -9.78\times10^{-6}$$

$$\chi_{0i} = -1.48\times10^{-7}$$

$$\chi_{111\_r} = -3.66\times10^{-6}(1+i)$$

$$\chi_{111\_i} = -7.30\times10^{-8}(1+i)$$

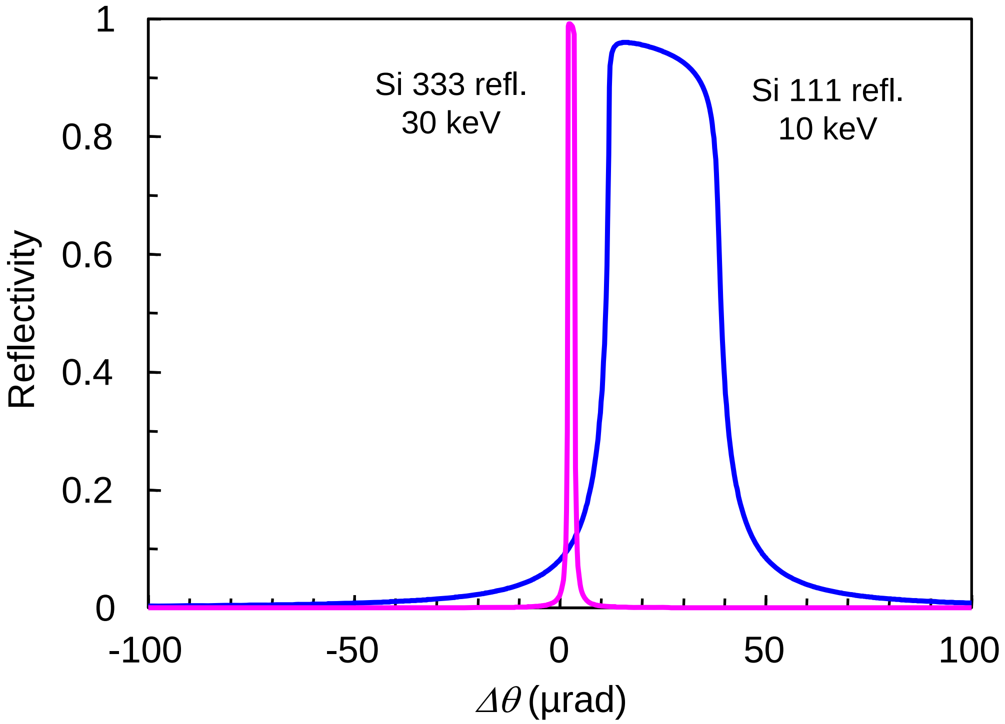
Si 333 refl., 30 keV

$$\chi_{0r} = -1.07\times10^{-6}$$

$$\chi_{0i} = -1.75\times10^{-9}$$

$$\chi_{333\_r} = -2.24\times10^{-7}(1+i)$$

$$\chi_{333\_i} = -7.87\times10^{-10}(1+i)$$



- 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)

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

← ΔW= 2

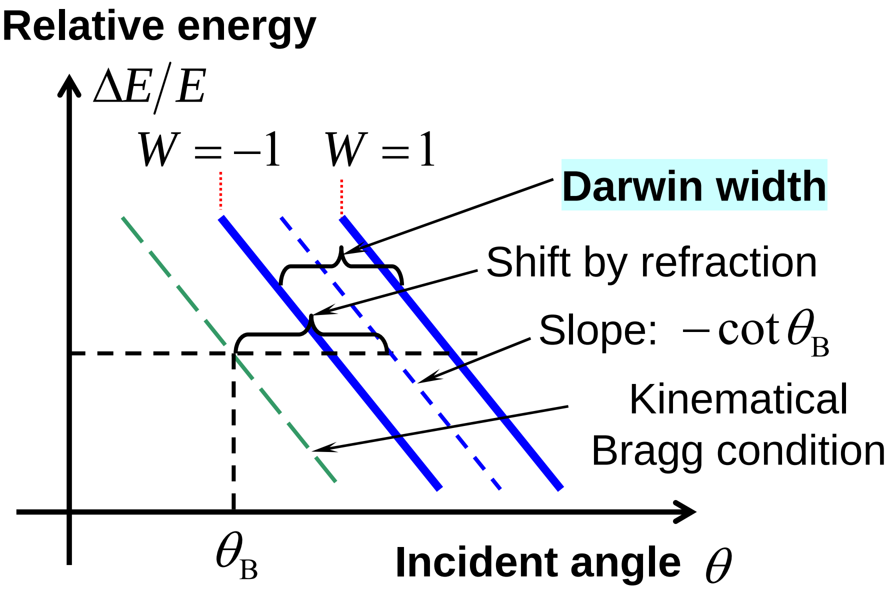
Energy resolution

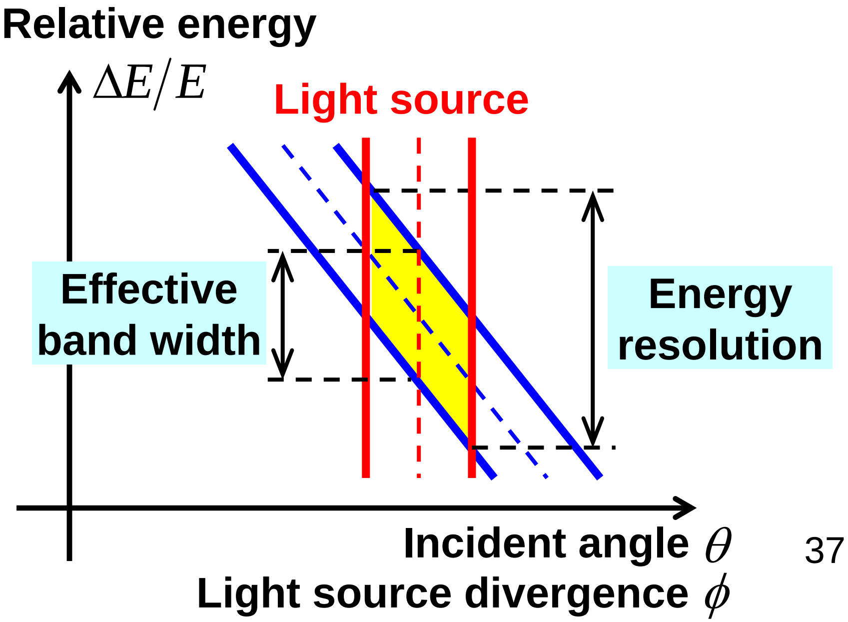
$$\frac{\Delta E}{E} = \cot\theta_{\text{B}}\sqrt{\Omega^2 + \Delta\theta_{\text{Darwin}}{}^2}$$

← Gaussian approximation for both light source and reflection curve

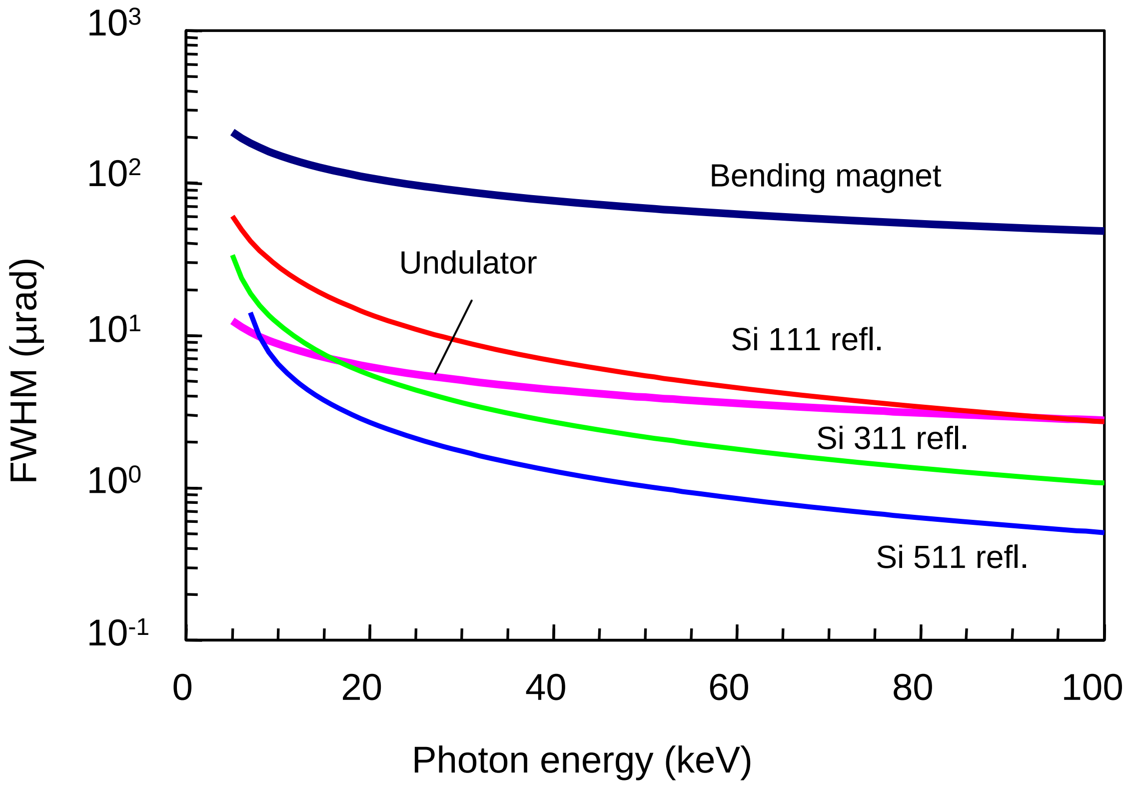
Effective band width

$$\frac{\Delta E}{E} \approx \frac{\left|\chi_{hr}\right|}{\sin^2\theta_{\text{B}}}$$





Source divergence and diffraction width



Natural divergence

- 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)

$$\sigma_{\mathrm{r}'} \approx 5\,\mu\text{rad}$$

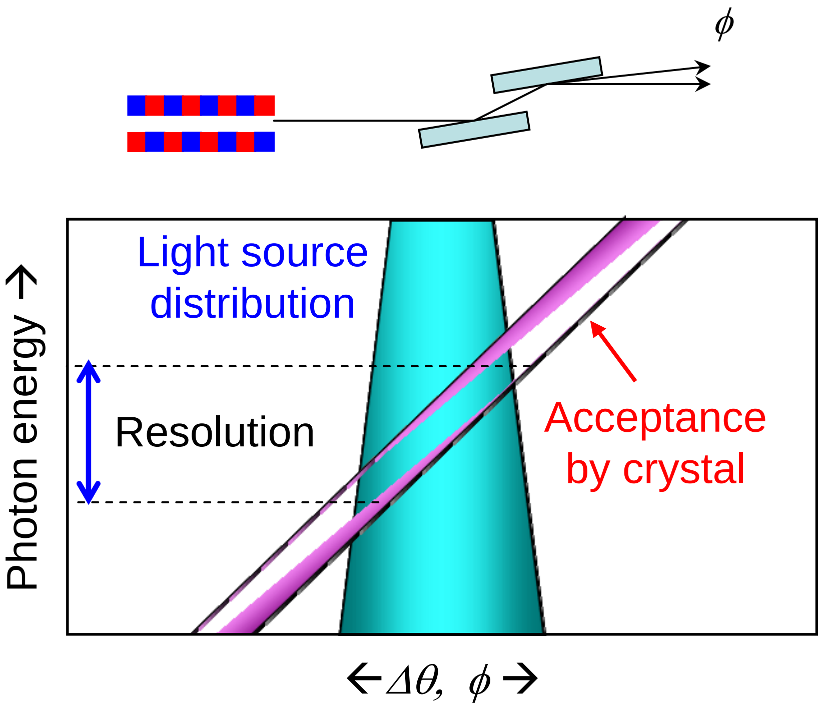
Divergence of undulator radiation ~ diffraction width

Energy resolution

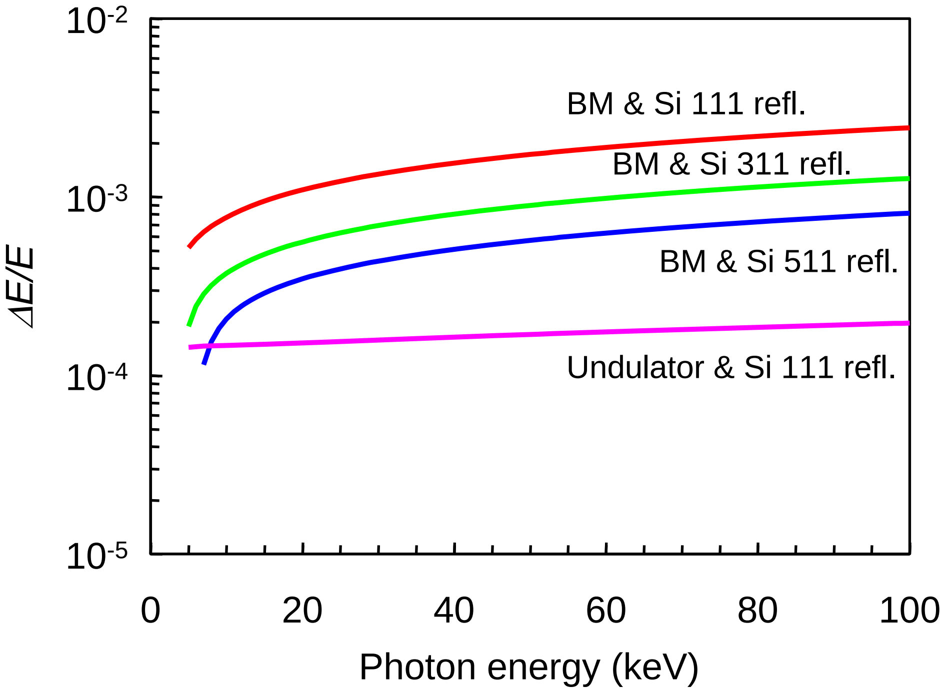
$$\frac{\Delta E}{E} = \cot\theta_{\mathrm{B}}\sqrt{\Omega^2 + \omega^2}$$

Ω: source divergence,

ω: diffraction width

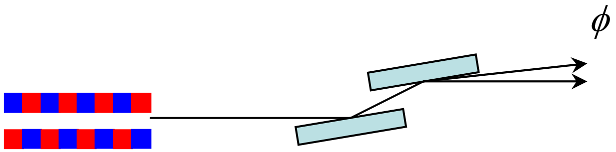


Angle-energy diagram (DuMond diagram)



For usual beamline : $\Delta E/E = 10^{-5} \sim 10^{-3}$

DuMond diagram: undulator & DCM



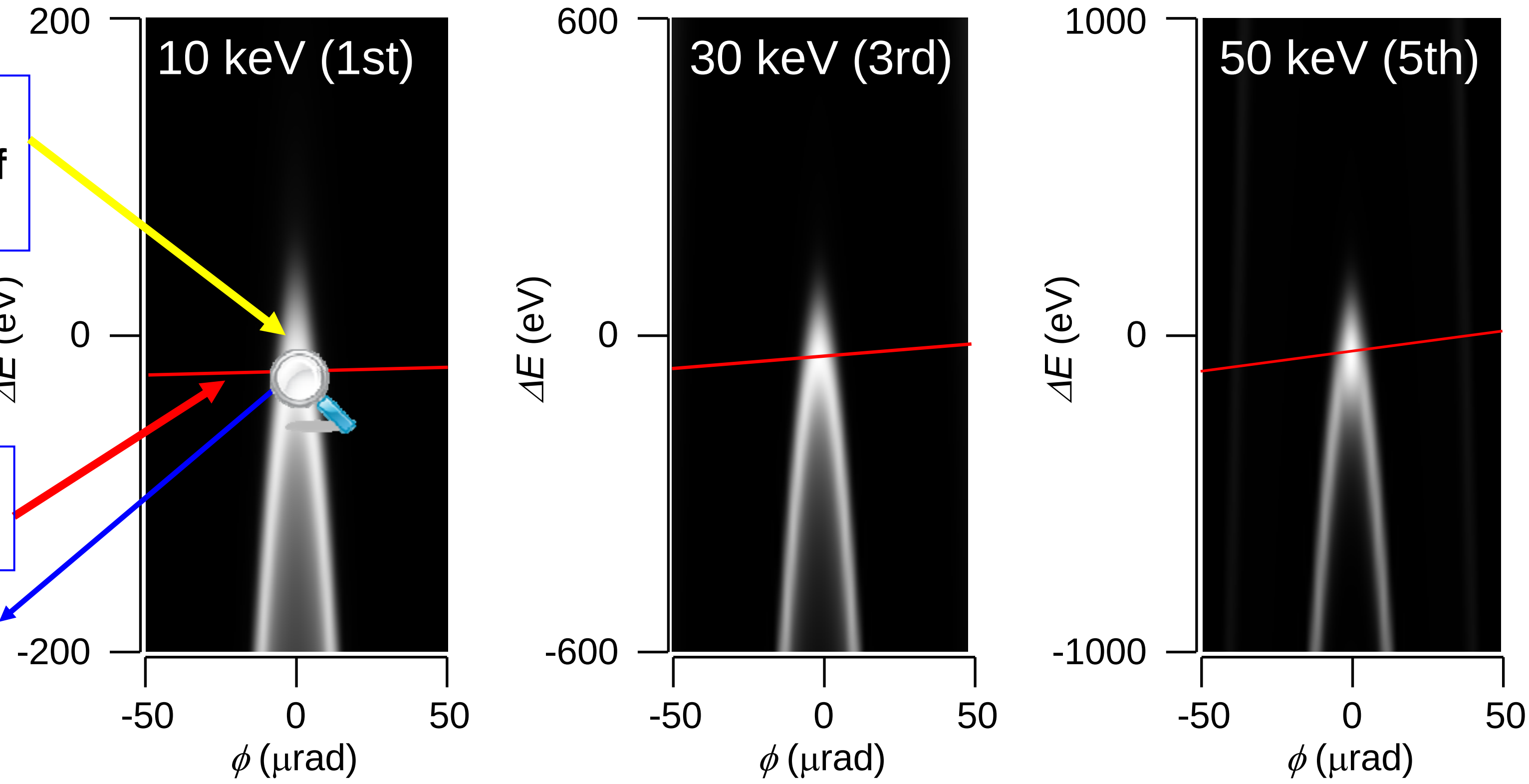
SPring-8 standard undulator

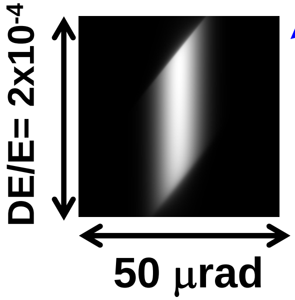
(λu= 32 mm, N= 140, K= 1.34, E_{1st}= 10 keV)

+ DCM (Si 111 refl.)

Intensity distribution of undulator

Acceptance by crystal



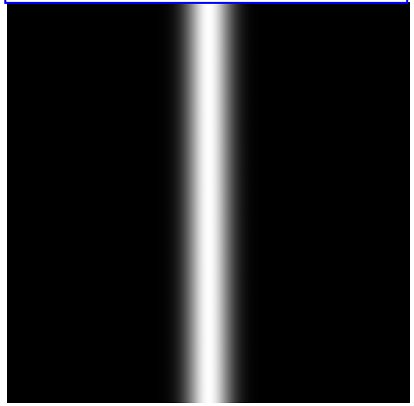


Undulator radiation: $\boxed{E = E_0 \Big/ \left(1 + K^2 / 2 + \gamma^2 \phi^2\right)}$

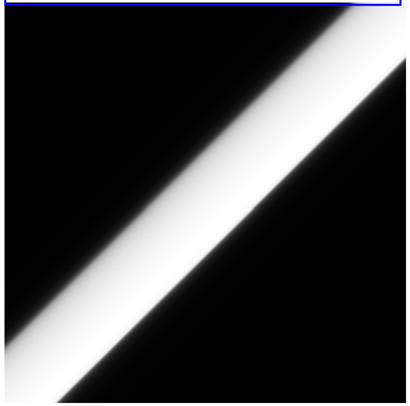
Wider slit increases unused photons (power) on the monochromator !

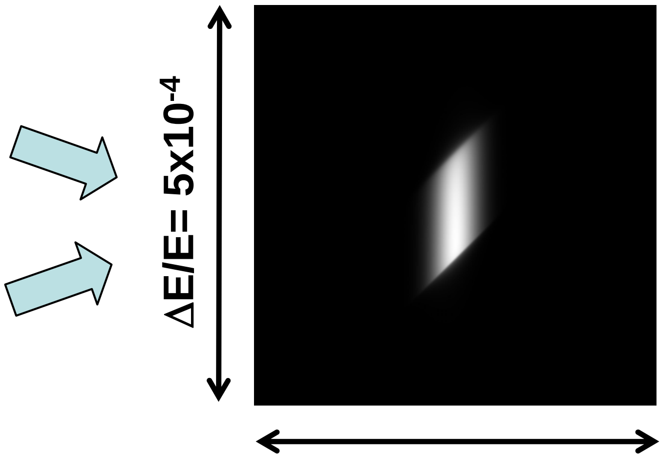
DuMond diagram: undulator & DCM

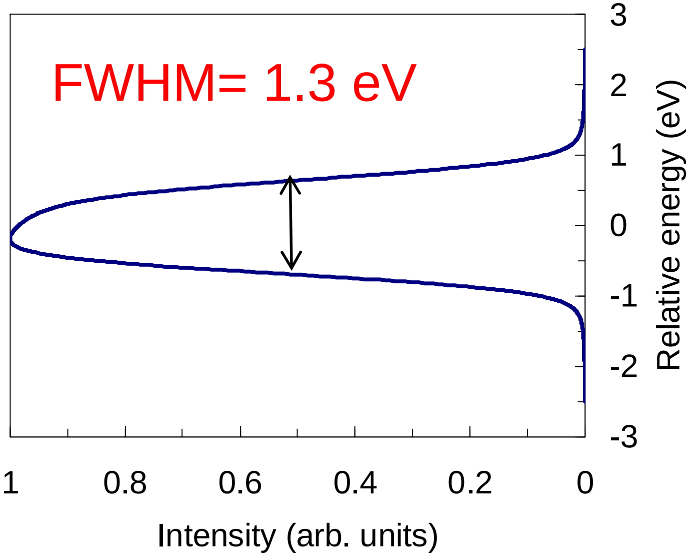
Undulator radiation



Acceptance by Si 111 DCM



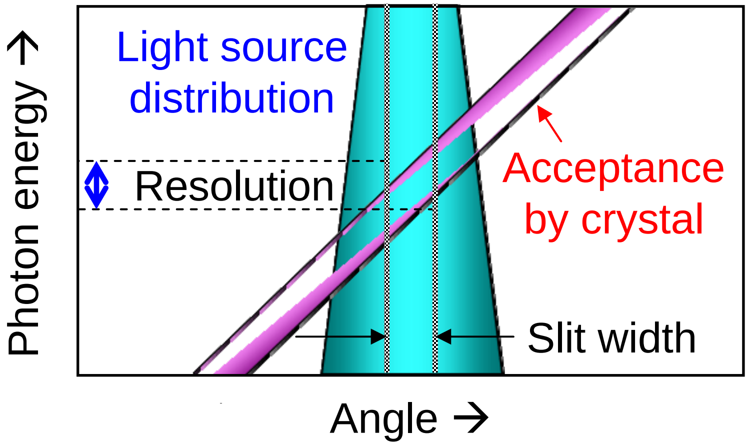




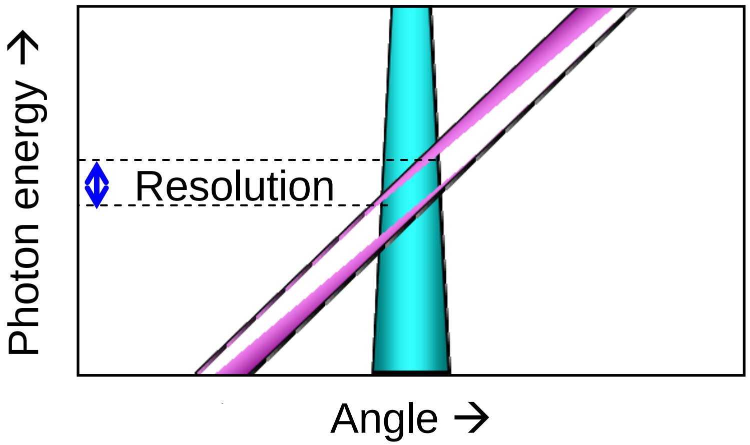
SPring-8 standard undulator + 20 μrad slit + Si 111 DCM

10-keV photons ➔ $1.3x10^{-4}$

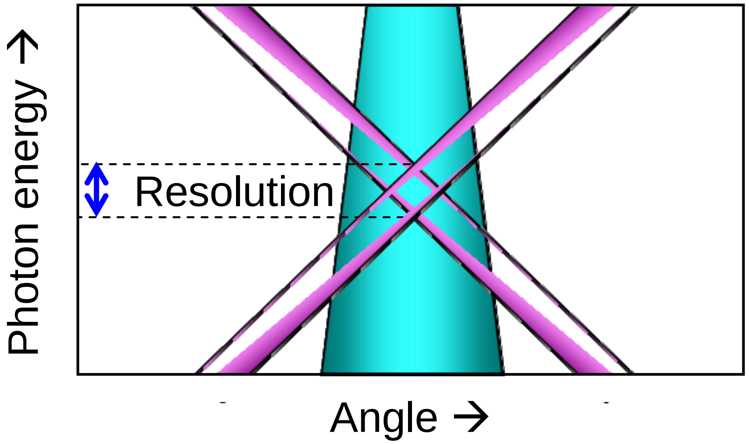
Improvement of energy resolution



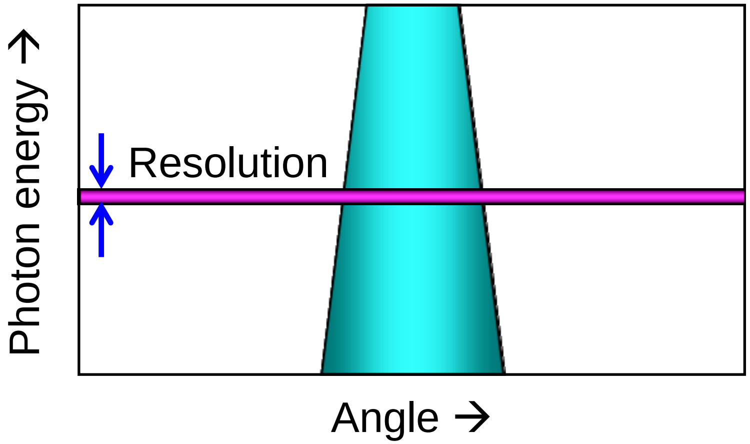
(A) Collimation using slit



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



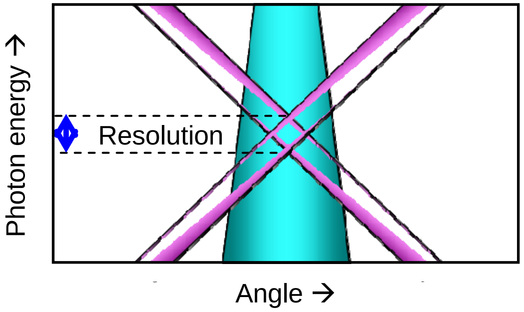
(C) Additional crystal w/ (+,+) setting



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

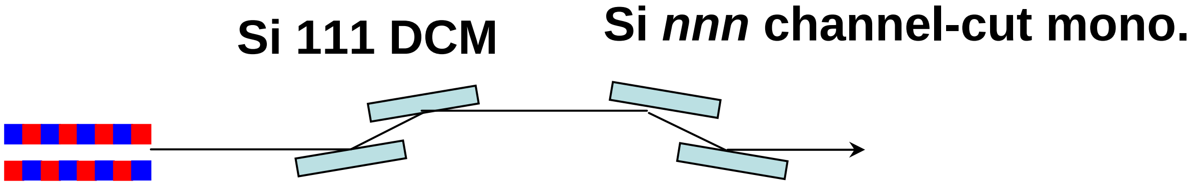
(B)~(D): restriction on photon energy

Improvement of energy resolution

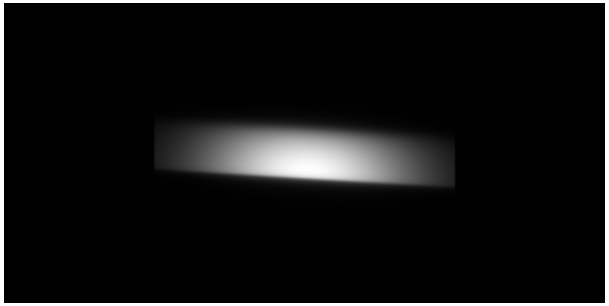


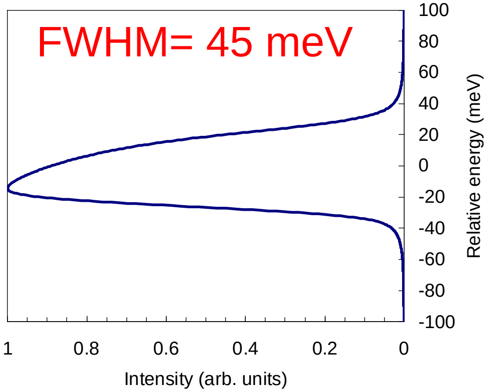
(C) Additional crystal w/ (+,+) setting

➔ HXPES

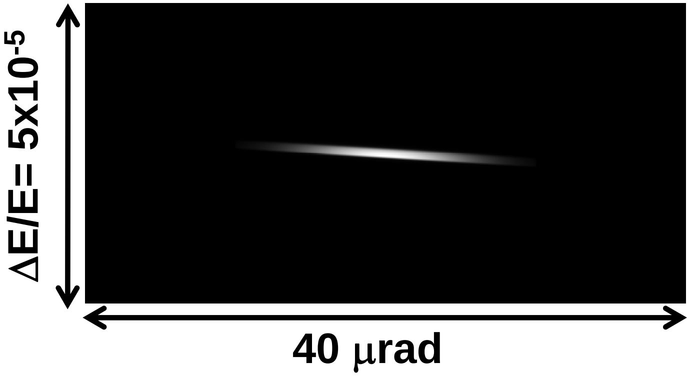


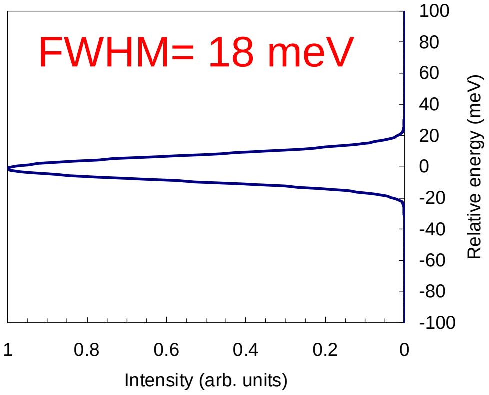
Si 333 refl. for 6 keV



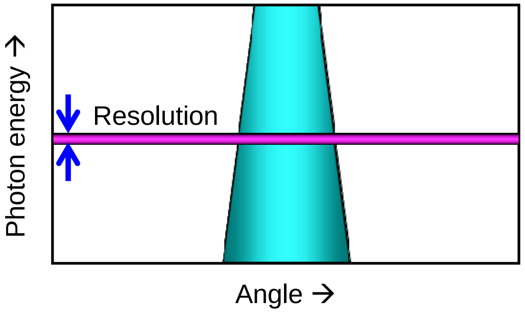


Si 555 refl. for 10 keV



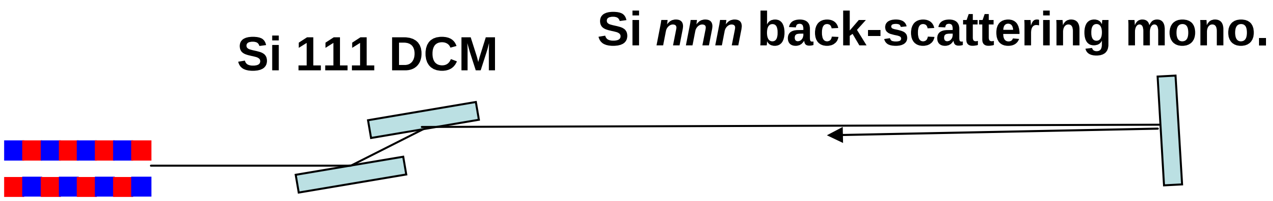


Improvement of energy resolution

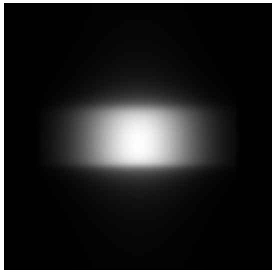


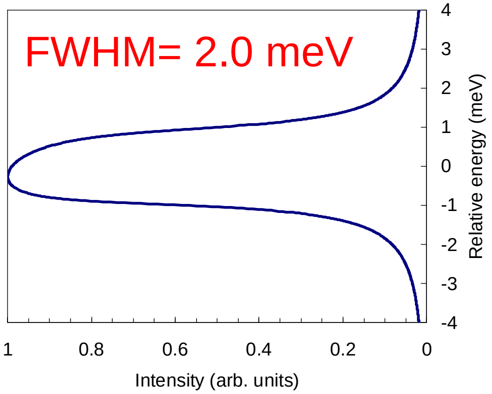
(D) HR monochromator of ~π/2 reflection (~meV)

➔ Inelastic scattering

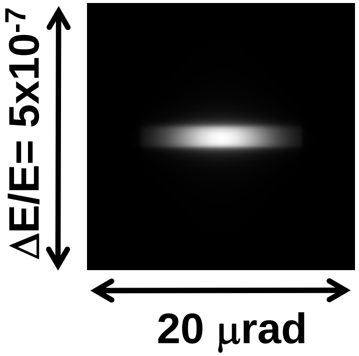


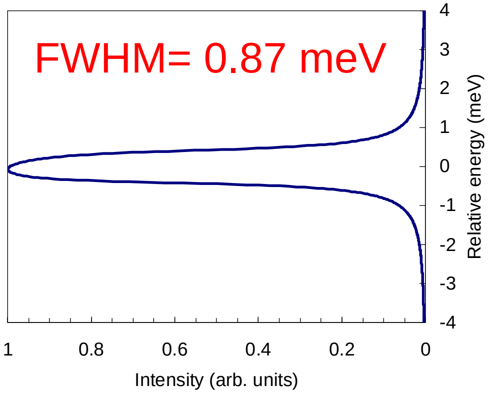
Si 999 refl. for 17.8 keV





Si 11 11 11 refl. for 21.7 keV





Photon flux after monochromator

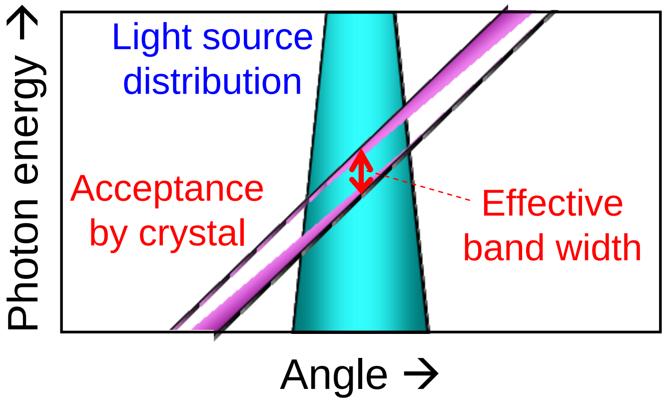
Photon flux (throughput) after monochromator can be estimated using effective band width:

Photon flux (ph/s) =

Photon flux from light source (ph/s/0.1%bw)

x 1000

x 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

$$\frac{\Delta E}{E} \approx \frac{\left|\chi_{hr}\right|}{\sin^2 \theta_{\mathrm{B}}}$$

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

Neglecting anomalous scattering factor *f’*

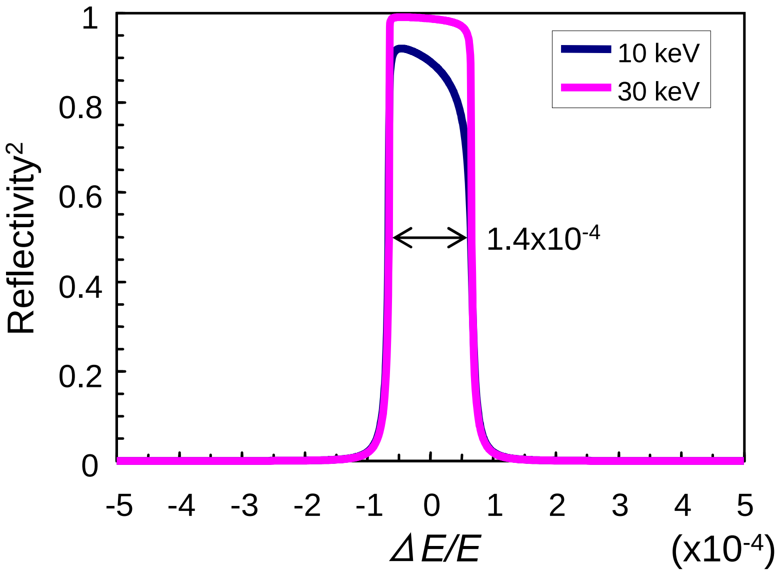
$$\chi_{hr} \propto \lambda^2 f^{\,0}(d_{hkl})$$

$$\frac{\Delta E}{E} = -\frac{\Delta \lambda}{\lambda} \approx \frac{\left|\chi_{hr}\right|}{\sin^2 \theta_{\mathrm{B}}}$$

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

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

Independent of photon energy



e.g. for Si 111 refl. DCM case

Note relative energy width is constant.

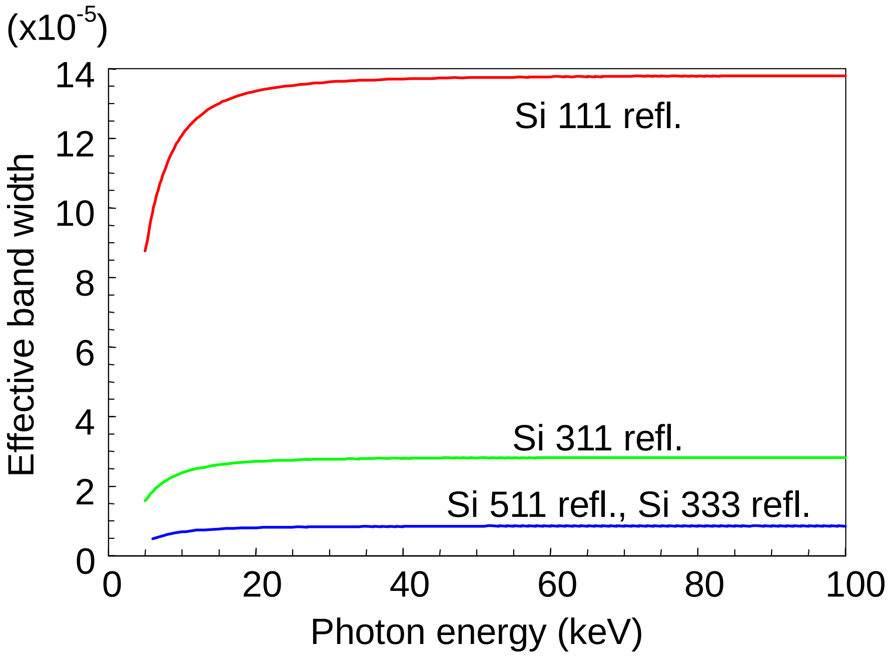
Effective band width (Integrated intensity)

For double-crystal monochromator

$$\frac{\Delta E}{E} = \frac{|\chi_{hr}|}{2\sin^2\theta_{\mathrm{B}}}\underline{\int R(W)^2\,dW}$$

$$\Uparrow$$

= ~2



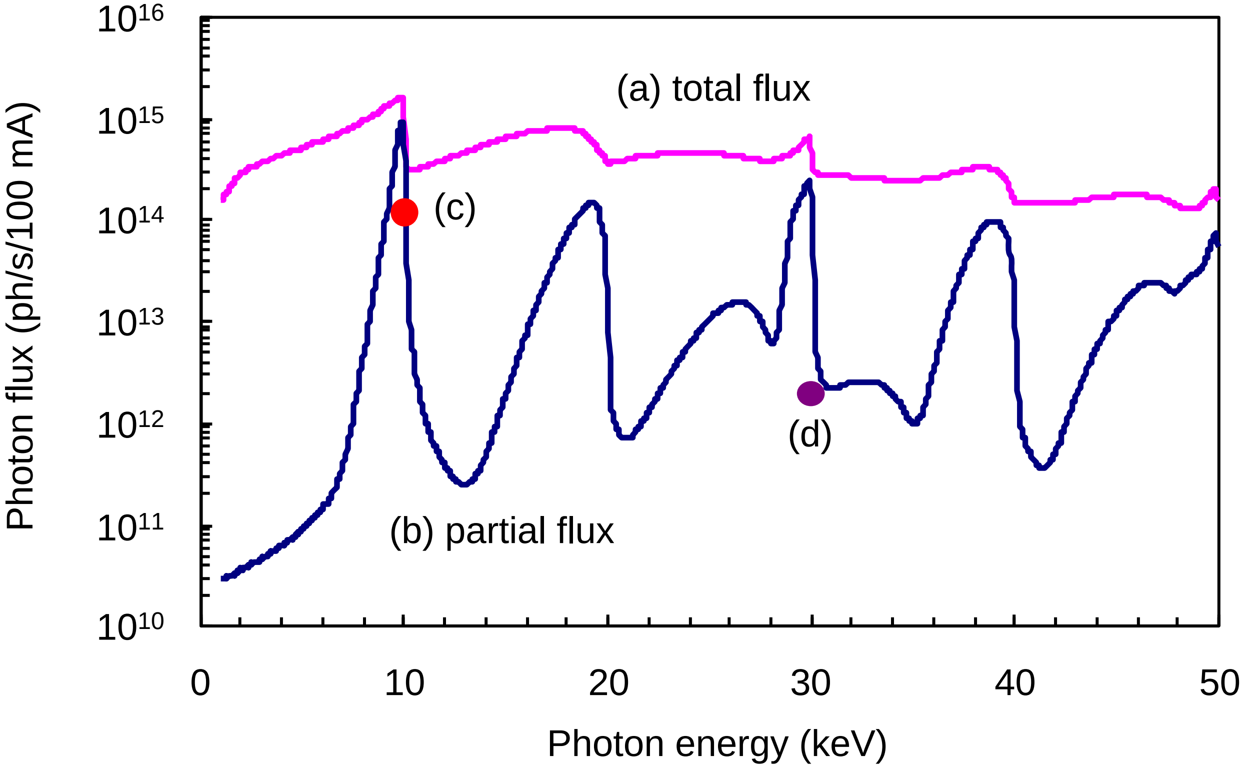
Effective band-width is obtained

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 at undulator beamline



(a) Total flux @ 0.1% b.w.
(b) After frontend slit
1 × 1 mm^2 @30 m
(c) Si 111 refl. @10 keV
Effective b.w. = 1.3x10^{-4}
(d) 3rd harmonics @30 keV
Effective b.w. = 8.0x10^{-6}

Higher harmonics elimination more → mirror or detuning of DCM

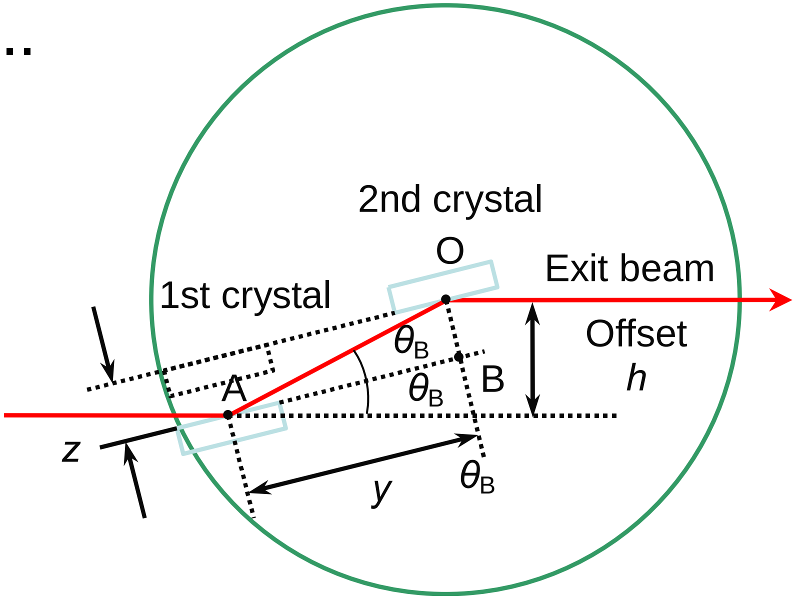
We can obtain photon flux of 10^{13}~10^{14} ph/s/100 mA/mm^2 using standard undulator sources and Si 111 reflections at SPring-8 beamlines.

Double-crystal monochromator

- Fixed-exit operation for usability at experimental station.
- Choose suitable mechanism for energy range (Bragg angle range).
- Precision, stability, rigidity,...

$$y = \mathrm{AB} = \frac{h}{2\sin\theta_B}$$

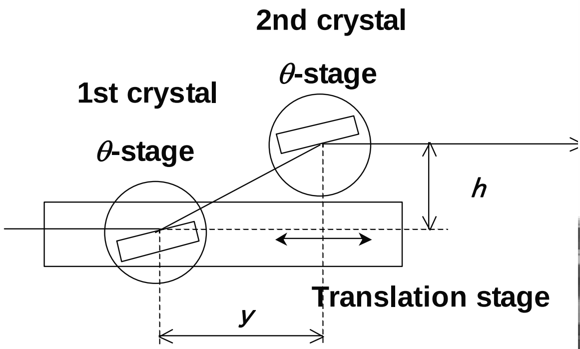
$$z = \mathrm{OB} = \frac{h}{2\cos\theta_B}$$

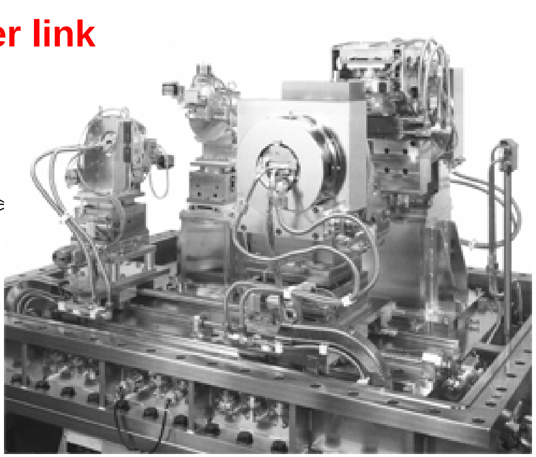


Fixed-exit operation using rotation (θ) + two translation mechanism

e.g. Double-crystal monochromator

θ1 + translation + θ2 computer link



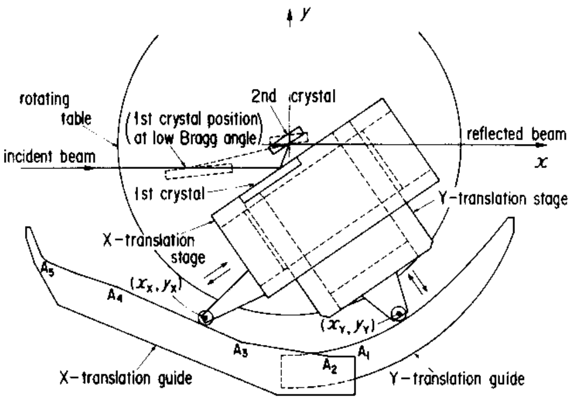


h= 100 mm,

SPring-8 BL15XU

θ_B= 5.7~72° (for lower energy range)

θ + two translation (2 cams)

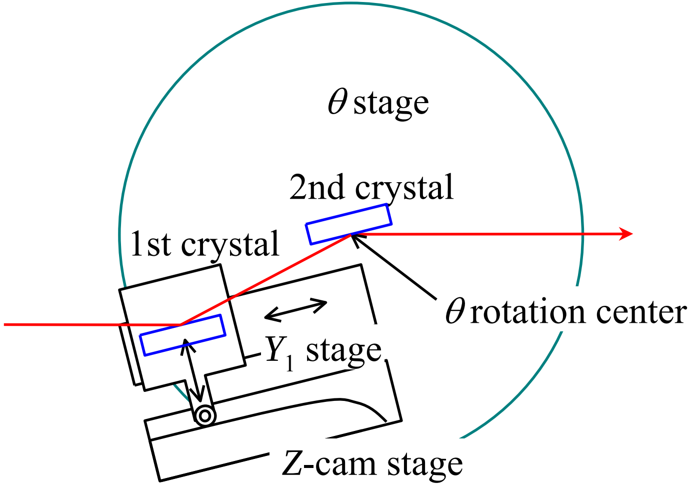


h= 25 mm, θ_B= 5~70°

KEK-PF BL-4C

Matsushita et al., NIM A246 (1986)

θ + two translation (1 cam)



Offset h= 30 mm

θ_B =3~27° for higher energy range

SPring-8 std. DCM

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

Crystal cooling

Why crystal cooling？

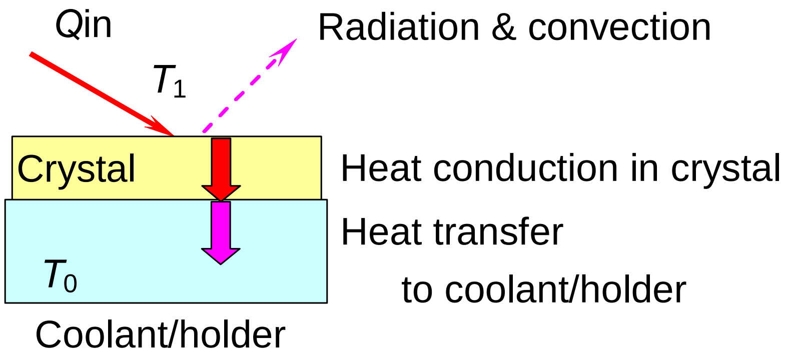
Qin (Heat load by SR) = Qout (Cooling + Radiation,..)

→ with temperature rise ΔT

→ $\alpha \Delta T = \Delta d$ (*d*-spacing change)

α: thermal expansion coefficient

or → $\Delta \theta$ (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: 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

	Silicon	Silicon	Diamond
	300 K	80 K	300 K
κ (W/m/K)	150	1000	2000
α (1/K)	$2.5\text{x}10^{-6}$	$-5\text{x}10^{-7}$	$1\text{x}10^{-6}$
κ / α x10^6	60	2000	2000

Figure of merit of cooling:
Good for silicon (80 k)
and diamond (300 K)

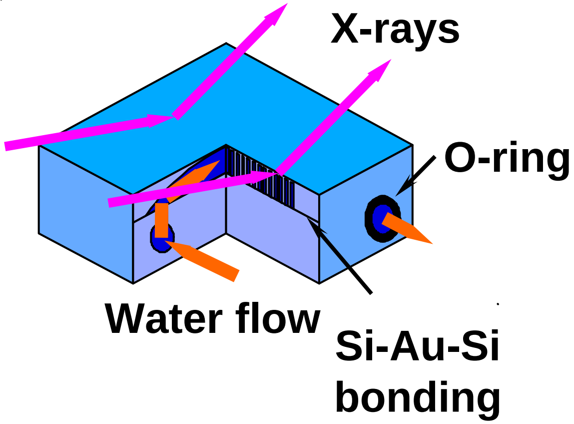
Crystal cooling at SPring-8

<Bending magnet beamline>

Power & power density:

~100 W, ~1 W/mm^2

Fin crystal direct-cooling - (S2)



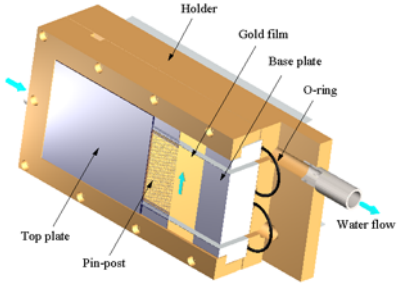
<Undulator beamline>

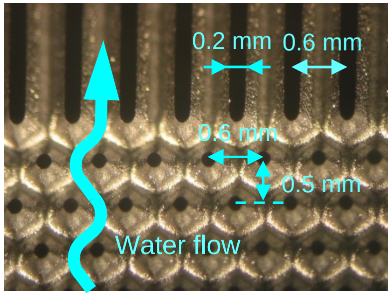
Linear undulator, *N*= 140, λu= 32 mm

Power & power density: 300~500 W ,

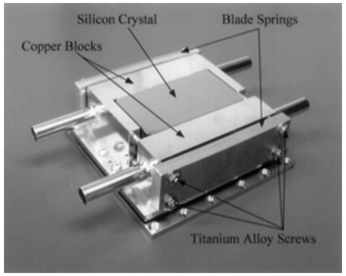
300~500 W/mm^2

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

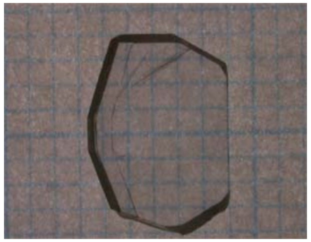


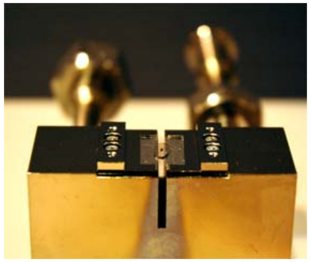


b) Silicon cryogenic cooling - (S1)



c) IIa diamond with indirect water cooling - (S1)



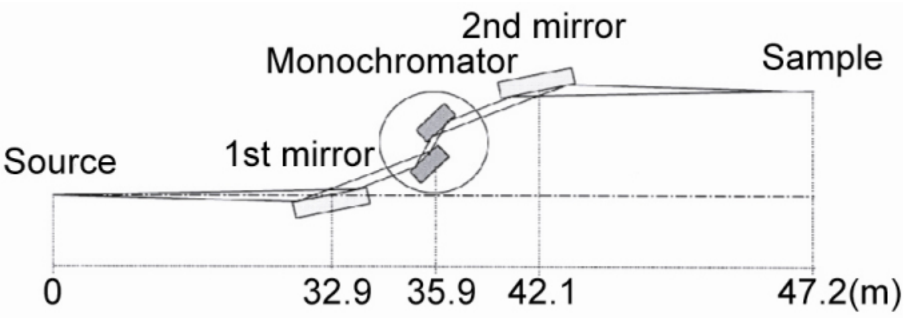


Example of x-ray beamline

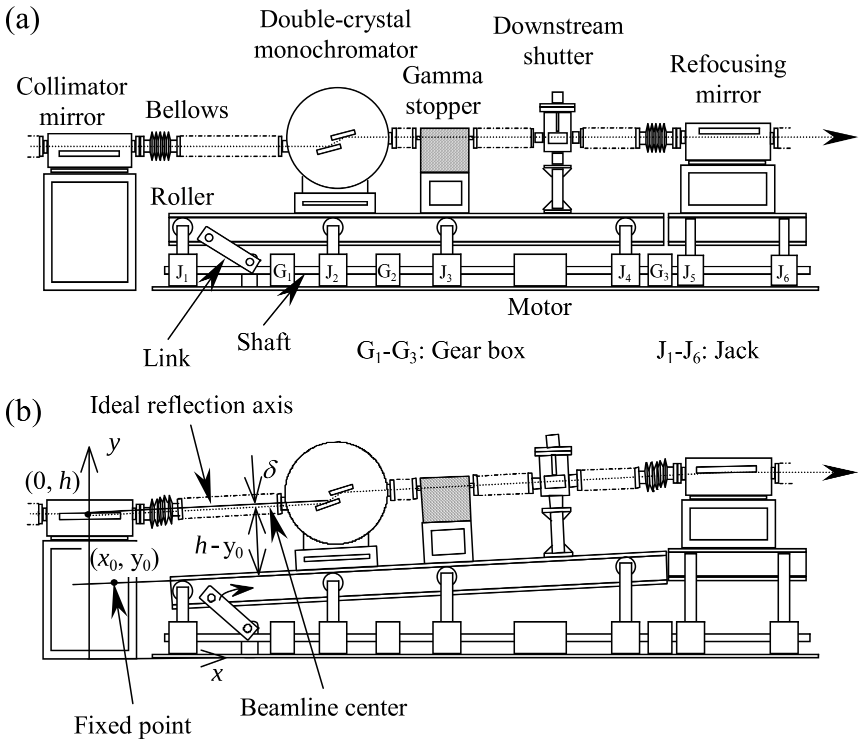
- SPring-8 case -

XAFS & single crystal diffraction

- Bending magnet
- Collimator mirror,
  + DCM,
  + refocusing mirror

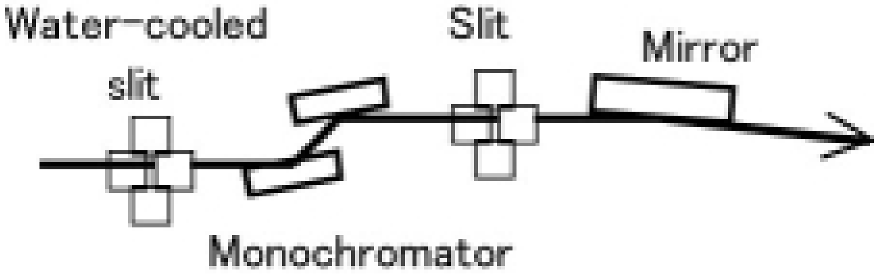


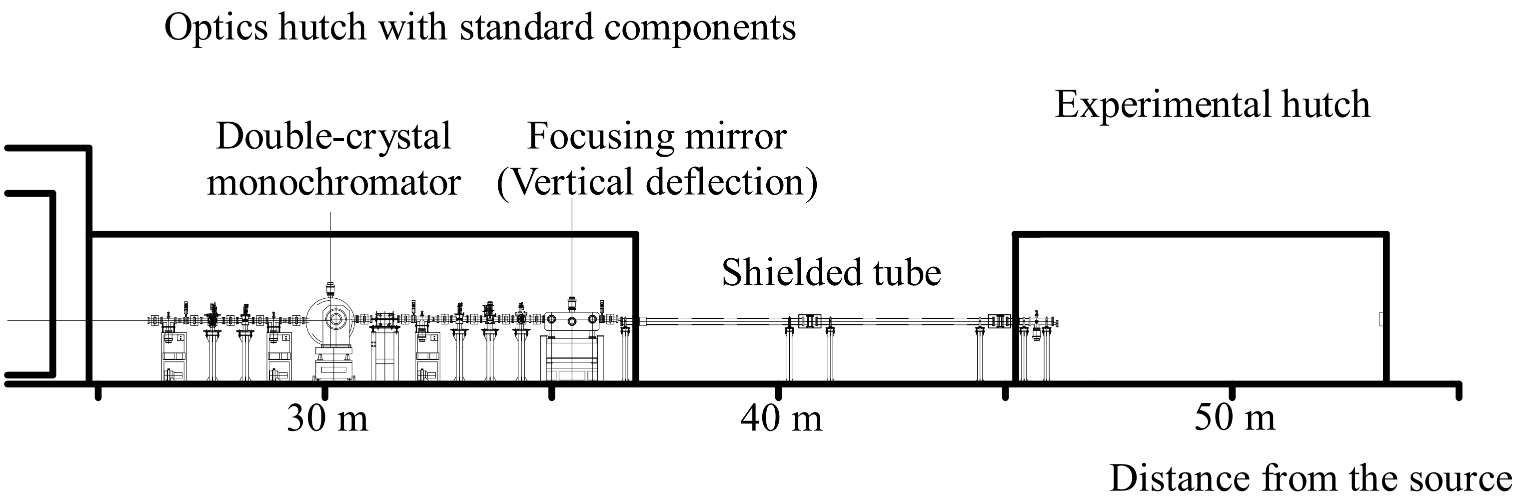
Optical layout for energy range less than 60 keV



Protein crystallography

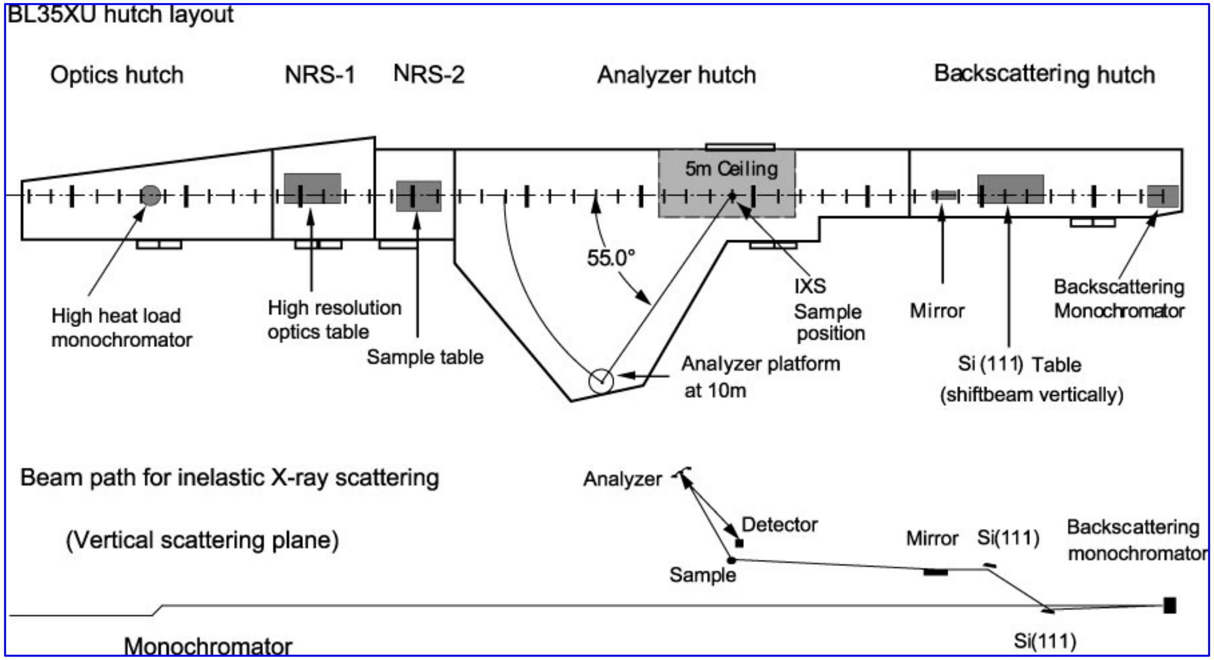
- Bending magnet
- DCM + focusing mirror

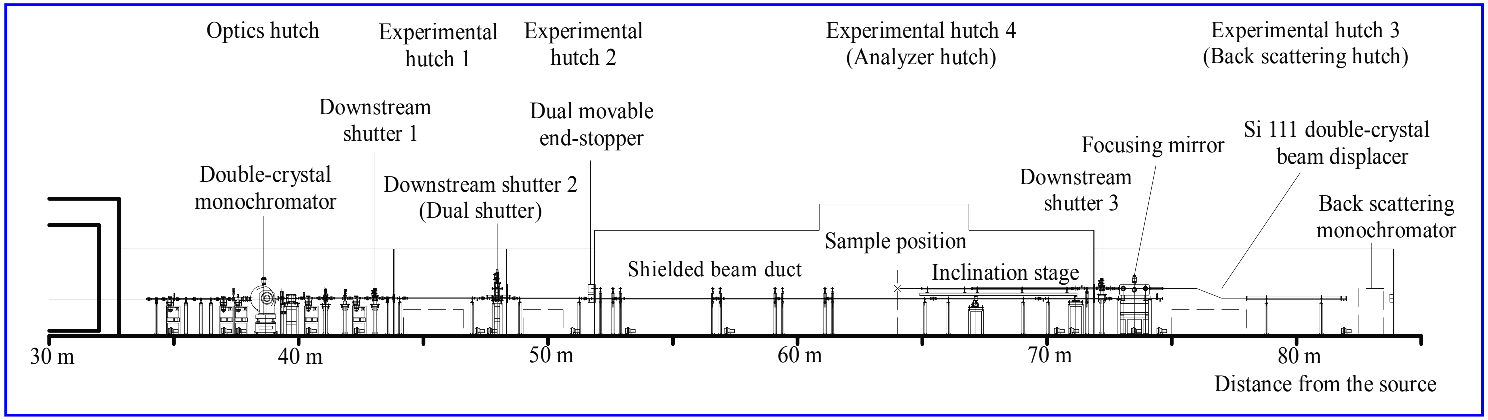




High resolution inelastic scattering

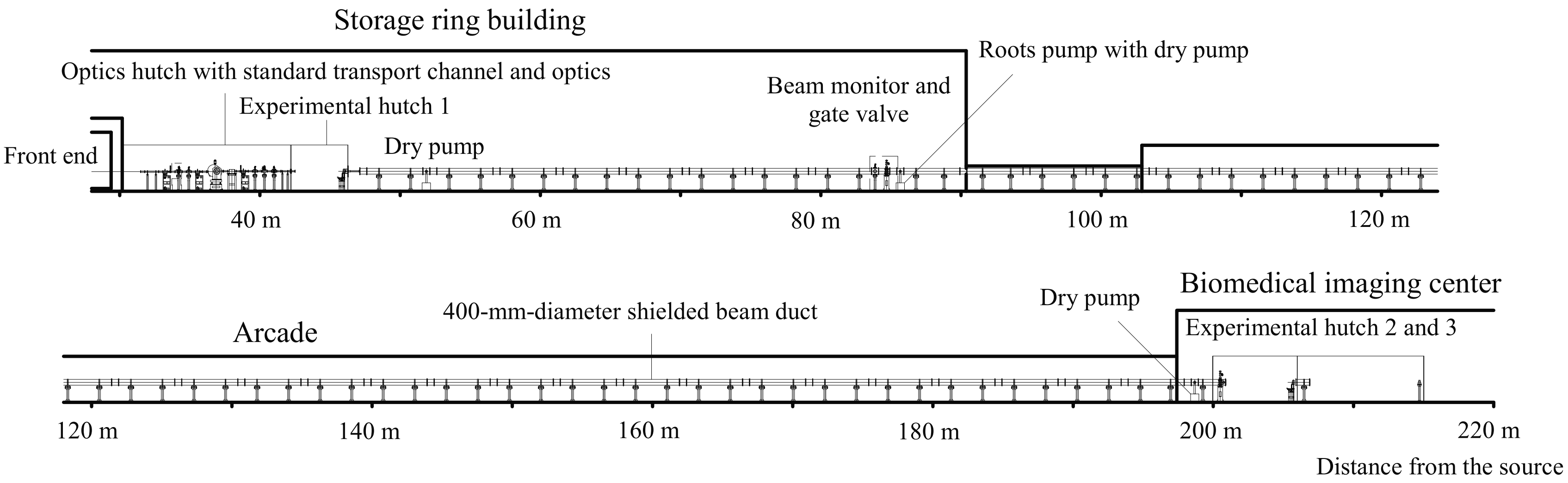
- Undulator
- DCM + back-reflection monochromator & analyzer (w/ ~meV resolution)

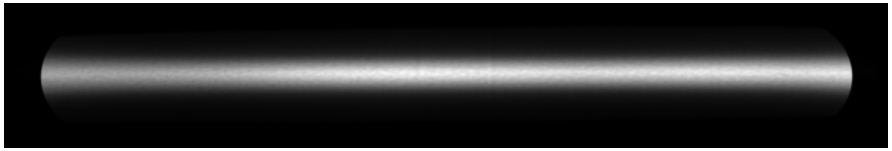




200-m-long beamline

- Bending magnet
- DCM





300-mm-wide beam at end-station

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.

Die dynamische Theorie der Röntgenstrahlinterferenzen in neuer Form.

Von **M. v. LAUE**, Berlin.

Mit 4 Abbildungen.

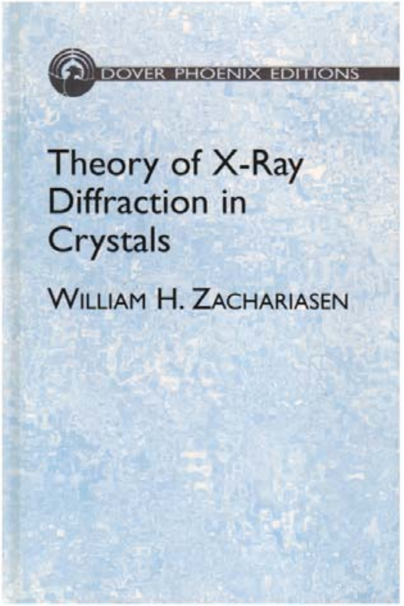
Inhaltsverzeichnis.

EWALDs dynamische Theorie der Röntgenstrahlinterferenzen[1] gehört nach unserer Ansicht auf alle Zeiten zu den Meisterwerken der mathematischen Physik. Sie bewältigte mit glänzenden Methoden ein zunächst schier unlösbares Problem, rechtfertigte eigentlich erst die elementare,
rein auf Phasenzusammensetzung beruhende Theorie,
Unzulänglichkeiten quantitativ abzuschätzen lehrte,
Verbundenheit mit der optischen Dispersionstheorie
Abweichungen von den Ergebnissen der älteren The
wenige Jahre später für die vollständige Deutung der
HJALMARs sowie für eine exakte Messung der Wellenlä
lich wurden. Aber wir glauben aussprechen zu dürfen,
denen, die ihre Resultate oft benutzen, nicht allzu
durchgearbeitet haben. Denn jene glänzenden mathematischen Methoden waren nicht nur schwierig zu finden, sie bereiten in manchen Teilen auch dem Leser Schwierigkeiten. Daran hat auch die Neubearbeitung durch WALLER[2] nicht viel geändert, welche im übrigen das Verdienst besitzt, zuerst Gitter mit Basis in die Rechnung einbezogen zu haben. Der Zweck der folgenden Seiten ist, der Theorie eine leichter verständliche Form zu geben. Daß wir trotz weitgehenden Verzichtes auf neue Ergebnisse die neue Form veröffentlichen, scheint uns durch die Wichtigkeit der Sache gerechtfertigt; ebenso, daß wir, um dem Leser das Zurückgreifen auf die genannten Arbeiten zu erleichtern, die geometrische Diskussion EWALDs nochmals zum Abdruck bringen, obwohl wir an ihr fast nichts zu ändern brauchen.

---

[1] EWALD, P. P.: Ann. Physik **54**, 519, 557 (1917); Z. Physik **2**, 332 (1920); **30**, 1 (1924).
[2] WALLER, J.: Uppsala Universitets Arsskrift 1925.

Dover (1945)



B. W. Batterman & H. Cole

“Dynamical Diffraction of X-Rays by Perfect Crystals”

Rev. Modern Phys. **36**,

(1964) 681-717.

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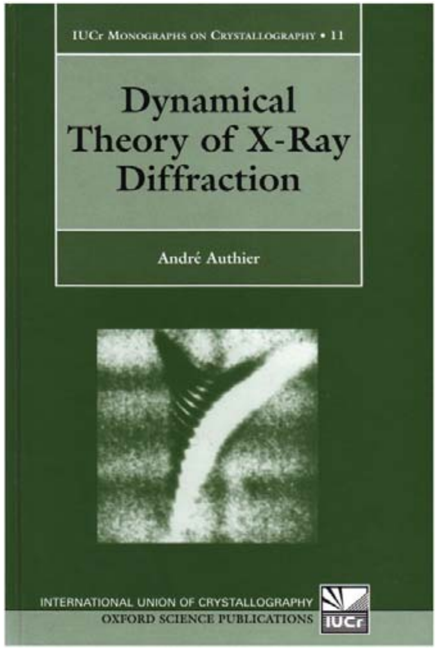
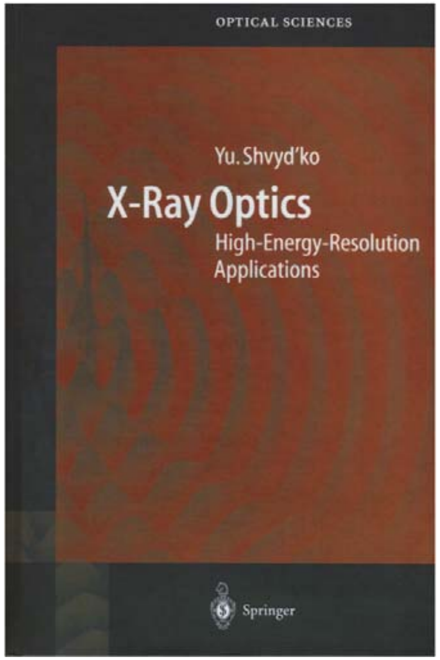


Springer (2004)



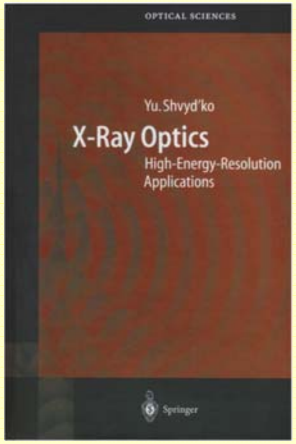
R. W. James

“The Dynamical Theory of X-Ray Diffraction”

Solod State Physics **15**, (1963) 53-220.

References

For monochromator



OPTICAL SCIENCES

Yu. Shvyd'ko

X-Ray Optics

High-Energy-Resolution Applications

Springer

[1] T. Matsushita & H. Hashizume,

Handbook on Synchrotron Radiation Vol. 1,

North-Holland (1983).

[2] Y. Shvyd’ko, Springer (2004), *for high energy resolution*

For atomic scattering factor

- For f^0

[3] International Tables for X-ray Crystallography (IUCr).
[4] Hubbell et al.: J. Phys. Chem. Ref. Data Vol. 4, No. 3, 1975.

- For anomalous scattering factor f', f''

[5] S. Sasaki, KEK report 88-14 (1989),
[6] Tables of LBNL (B. L. Henke et al.),
http://henke.lbl.gov/optical_constants/index.html,
[7] Tables of NIST,
http://physics.nist.gov/PhysRefData/FFast/html/form.htm

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Thank you for your attention.