September 27, 2011

Cheiron School 2011

X-ray Beamline Design 1
- X-ray Monochromator -

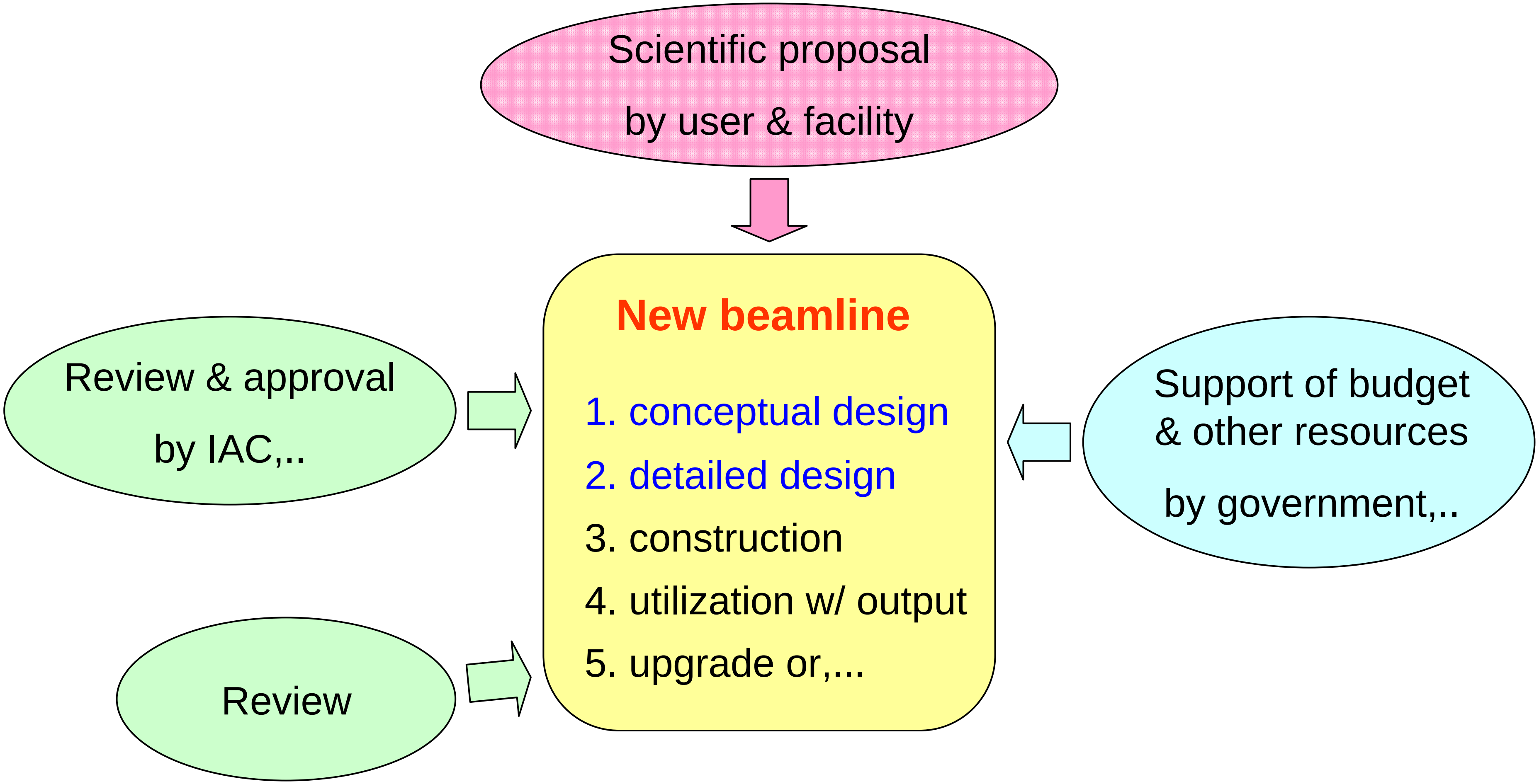
Shunji Goto

SPring-8/JASRI

Outline

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

Process of beamline construction



Scientific proposal

by user & facility

New beamline

1. conceptual design
2. detailed design
3. construction
4. utilization w/ output
5. upgrade or,...

Review & approval

by IAC,..

Review

Support of budget & other resources

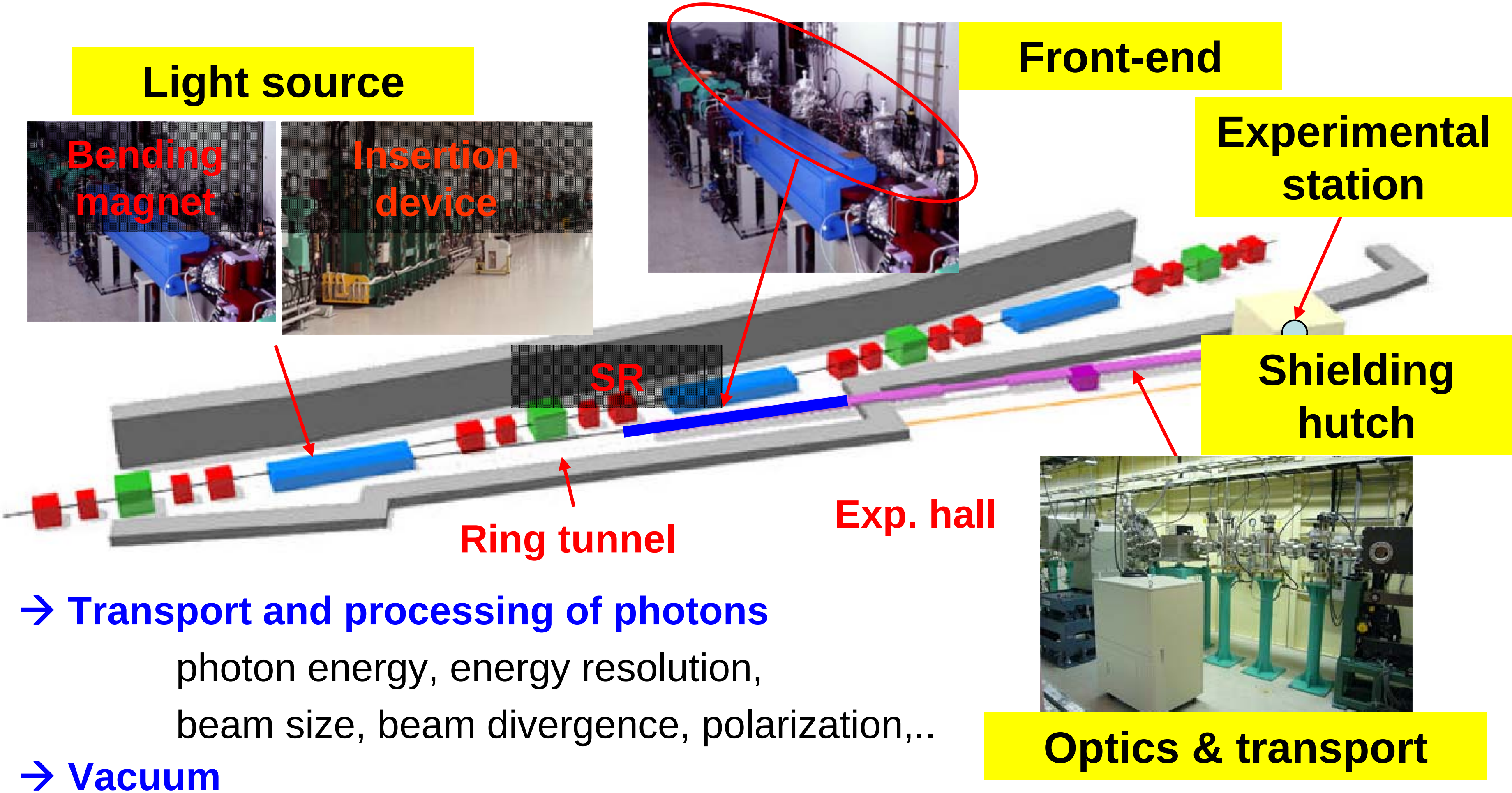
by government,..

Beamline design is first step and crucial for success of the beamline !

→ Fundamental of X-ray beamline; light source, monochromator, mirror,...

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 application:

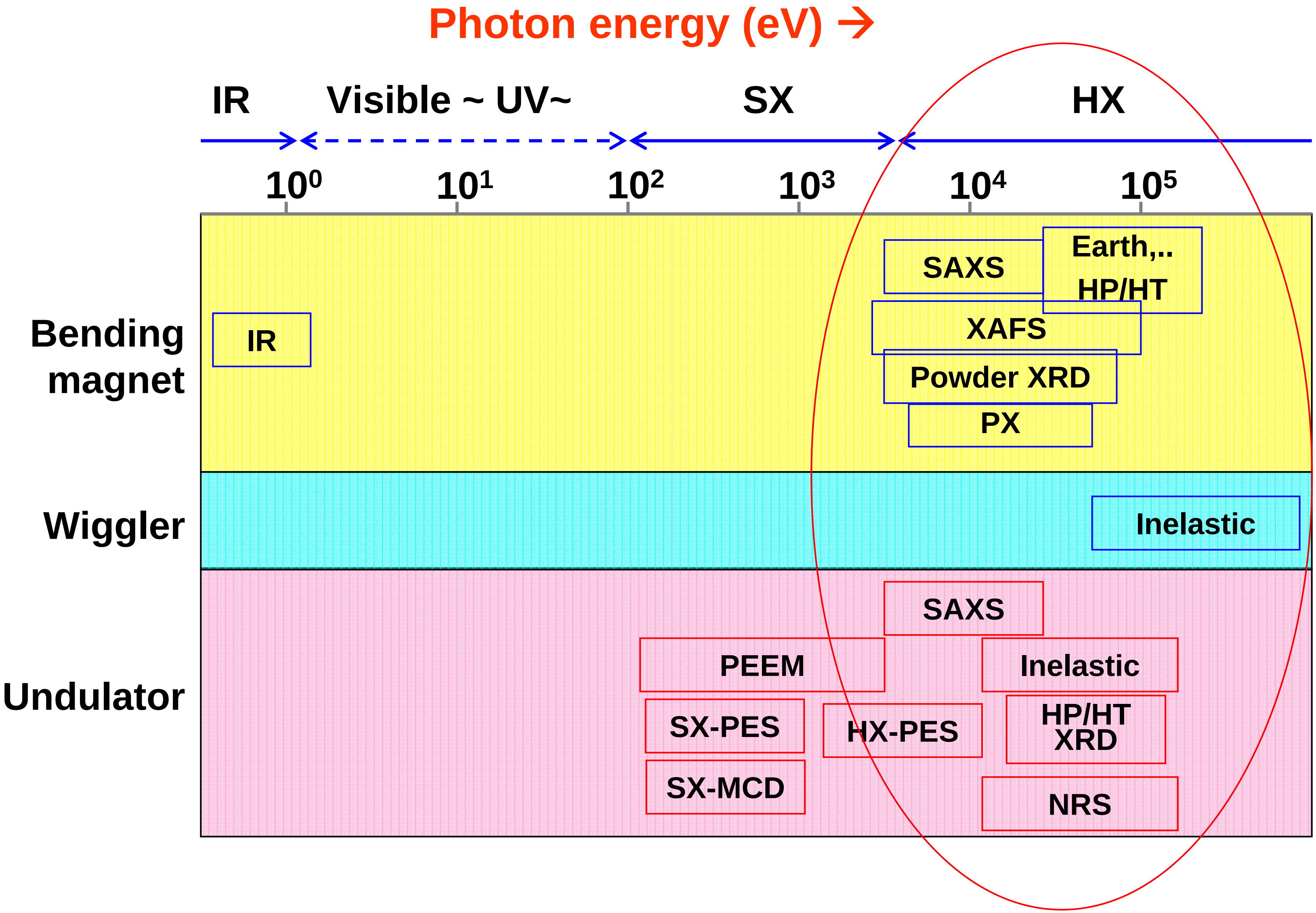
- White or monochromatic
- Energy range
- Energy resolution
- Flux & flux density
- Beam size at sample (micro beam?,...)
- Beam divergence/convergence at sample (Resolution in k-space)
- Higher order elimination w/ mirror
- Polarization conversion
- Spatial coherency

....

→ Light source, monochromator, mirror,

and other optical devices and components

BL classification (energy region)



Photon energy (eV) →

IR

Visible ~ UV~

SX

HX

10^0 10^1 10^2 10^3 10^4 10^5

Bending magnet

IR

SAXS

Earth,..

HP/HT

XAFS

Powder XRD

PX

Wiggler

Inelastic

Undulator

SAXS

PEEM

Inelastic

SX-PES

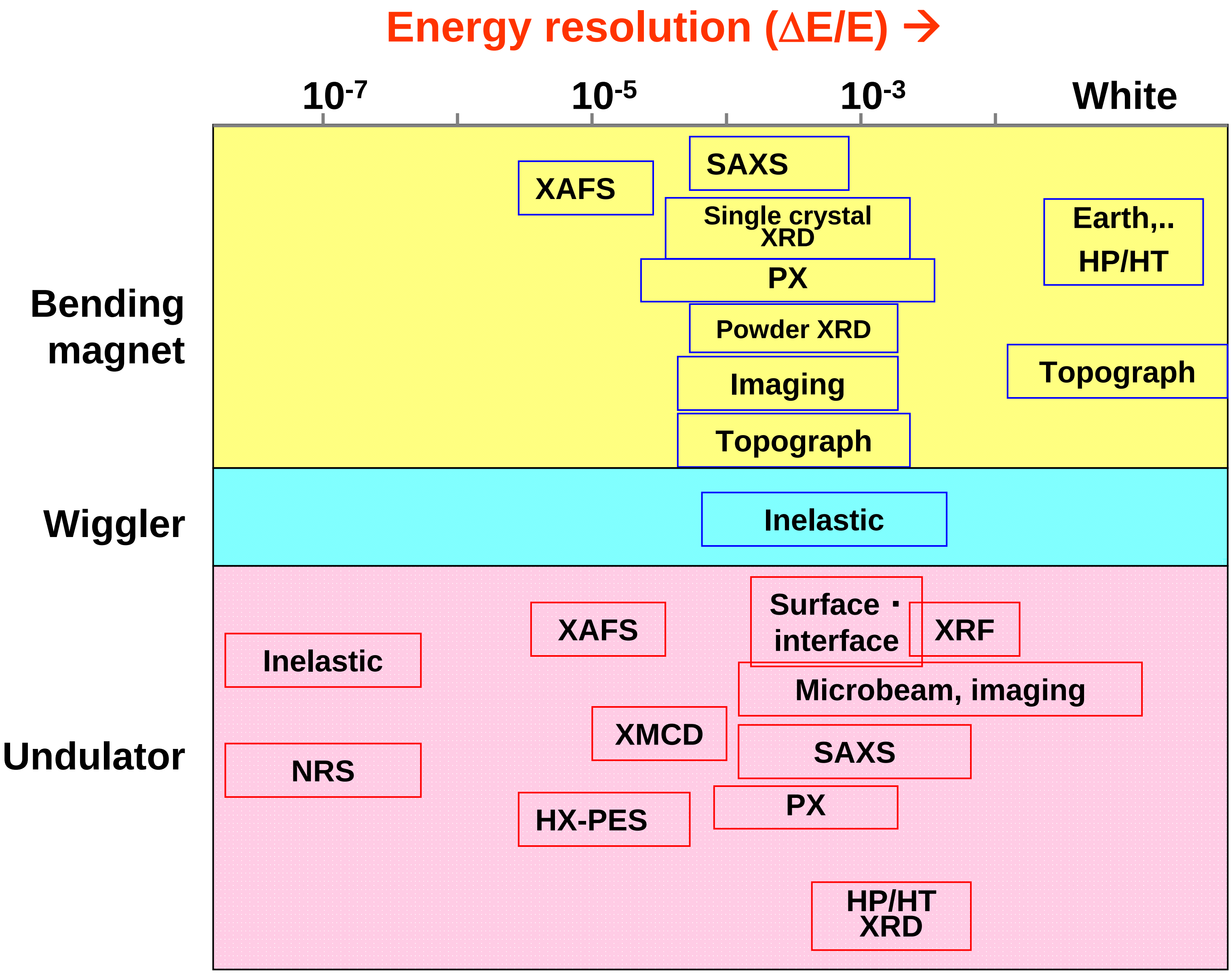
HX-PES

HP/HT XRD

SX-MCD

NRS

BL classification (energy resolution)



Energy resolution (ΔE/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

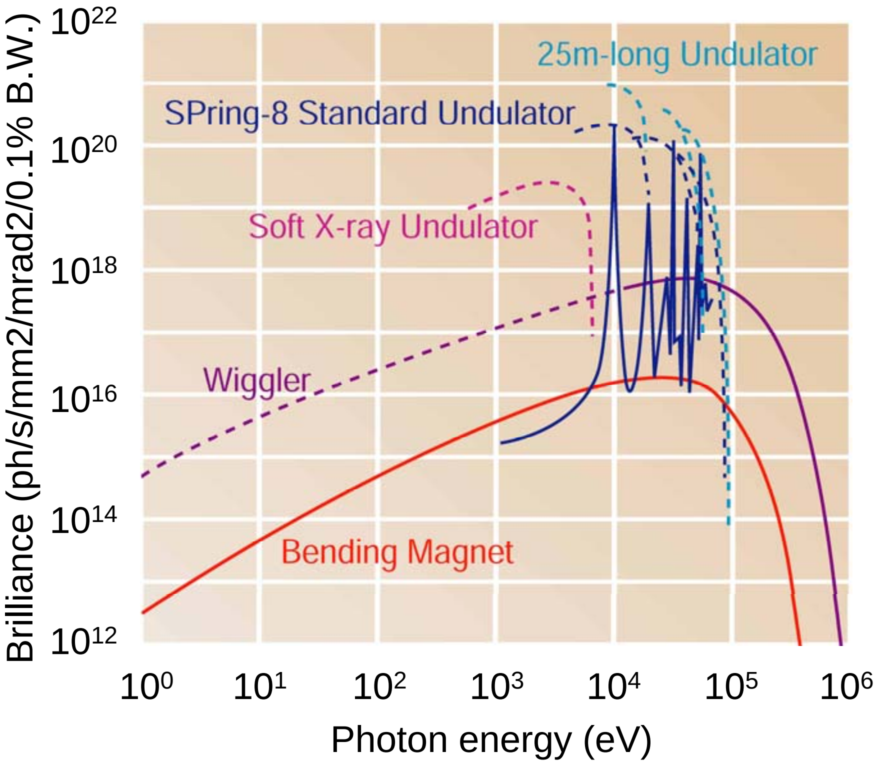
Undulator (major part of 3GLS beamline):

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

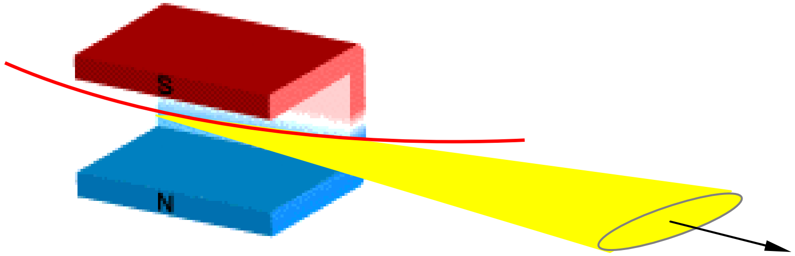
Light sources (2)

Angular divergence and band width

→ Core part we need

Bending magnet

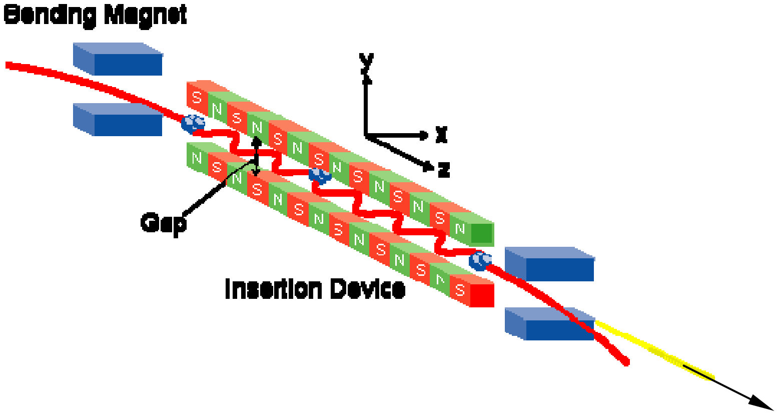
$$\sigma_{r'} \approx 0.597 \frac{1}{\gamma}\sqrt{\frac{\lambda}{\lambda_c}}$$

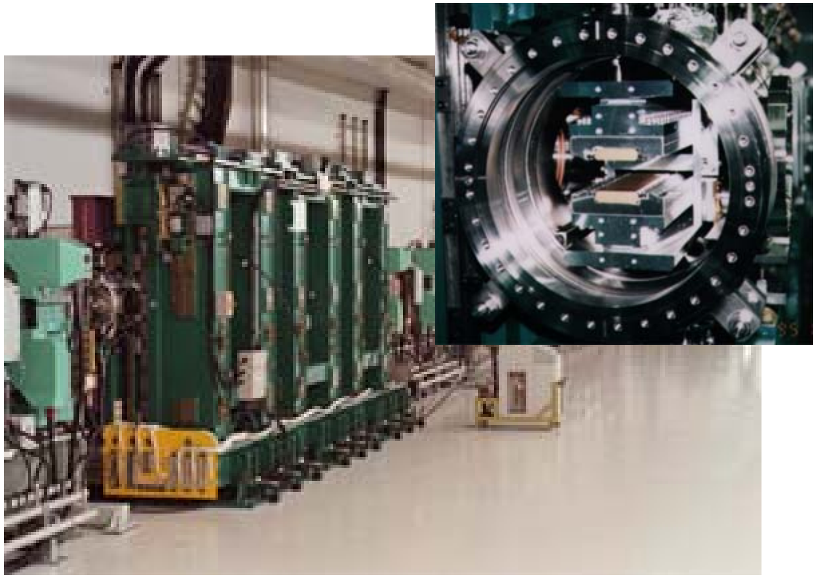


Undulator

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

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



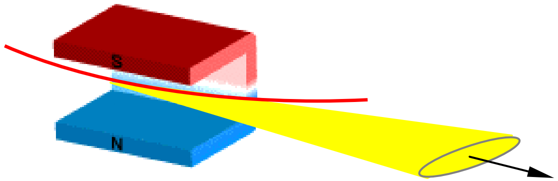


SPring-8 in-vacuum undulator

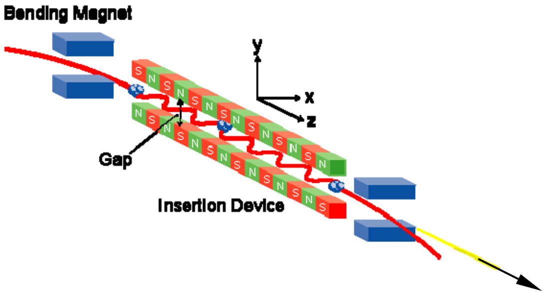
Light sources (3)

SR power → mostly eliminated before/by monochromator

Bending magnet



Undulator



Power distribution

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

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

K: deflection parameter
(*K*= 0.5~2.5)

Total power

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

E= 8 GeV, *I*= 0.1 A, *B*= 0.68 T, *R*= 39.3 m
→ P_{tot}= 0.15 kW/mrad

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

B_0= 0.87 T, *L*= 4.5 m
→ P_{tot}= 14 kW

Monochromator

Key issues from experimental request:

White or monochromatic ? → monochromatic

Energy region ← Bragg's law

Energy resolution ← Source divergence, Darwin width,..

Flux (throughput) ← related to energy resolution

Double-crystal monochromator for fixed-exit

Single-bounce monochromator is for limited case

Heat load ← depending on light source

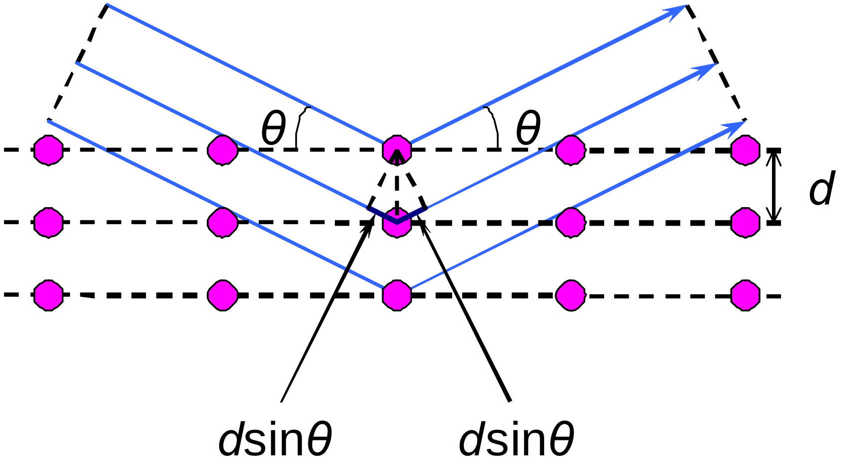
Bragg reflection

Bragg's law in real space

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

2) Phase matching between net planes.

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

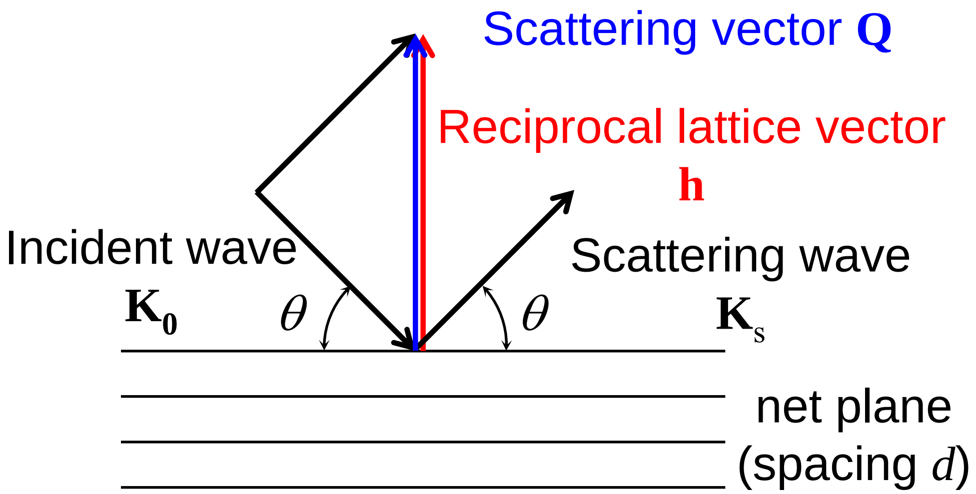


Laue condition (Kinematical) in reciprocal space

$$\boxed{\mathbf{Q} = \mathbf{K}_{\mathrm{s}} - \mathbf{K}_0 = \mathbf{h}}$$

Reciprocal lattice vector $\mathbf{h}$

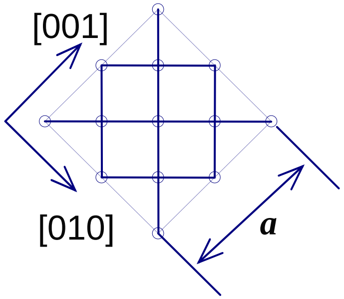
- Normal to net plane
- Length = $1/d$



Miller indices and *d*-spacing for silicon

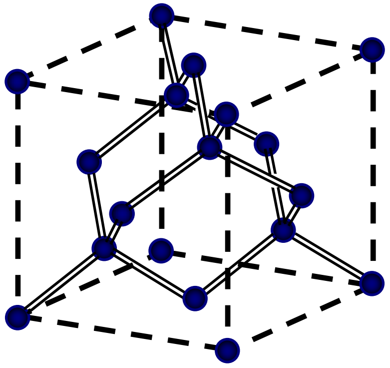
$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Top view

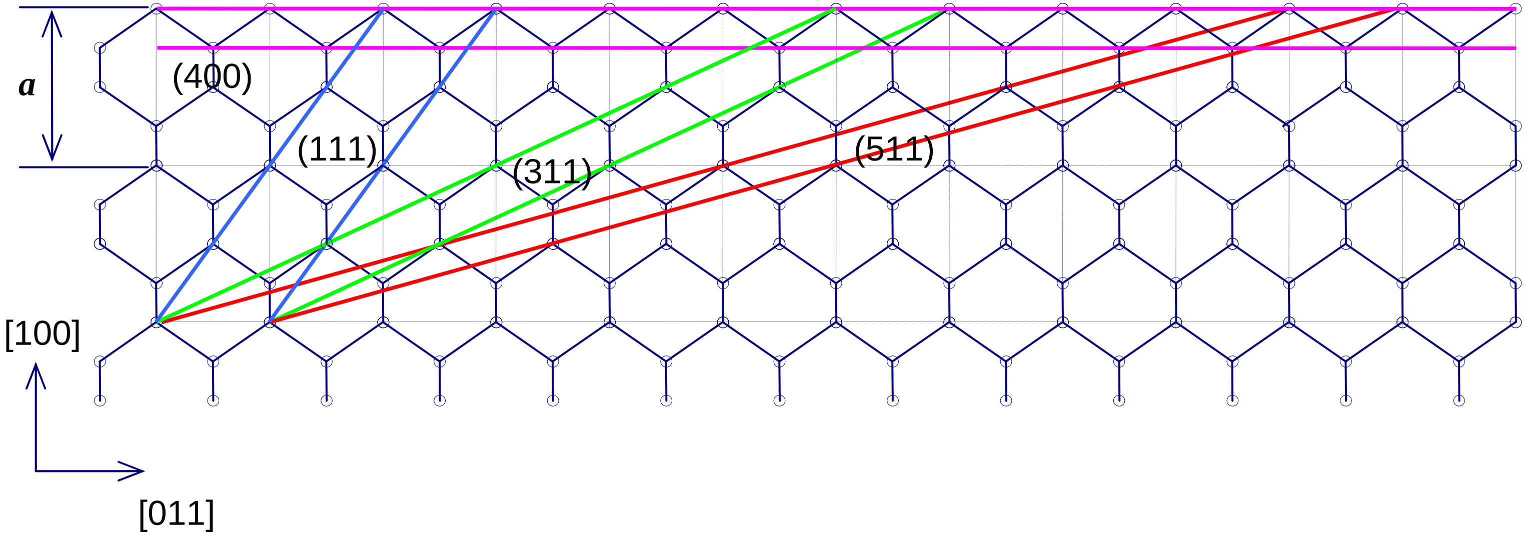


$$a = 5.431\,\text{Å}$$

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



Side view



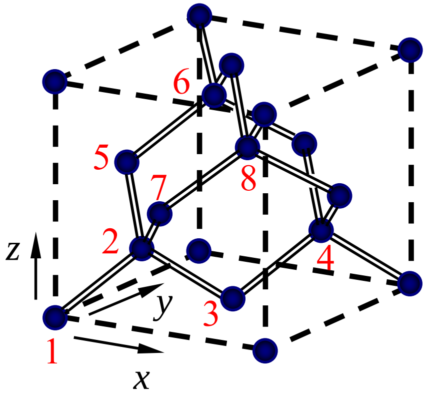
Crystal structure factor for diamond structure

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

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

Atomic scattering factor

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



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,

$$\begin{cases} h+k+l=4m & F=8f & \leftarrow \text{8 atoms in phase} \\ h+k+l=4m\pm1 & F=4(1\pm i)f & \leftarrow \text{Half contribute with phase shift } \pm\pi/2 \\ h+k+l=4m\pm2 & F=0 & \leftarrow \text{Half cancel with } \pi \end{cases}$$

Crystal structure factor for diamond structure

(400), (220),...

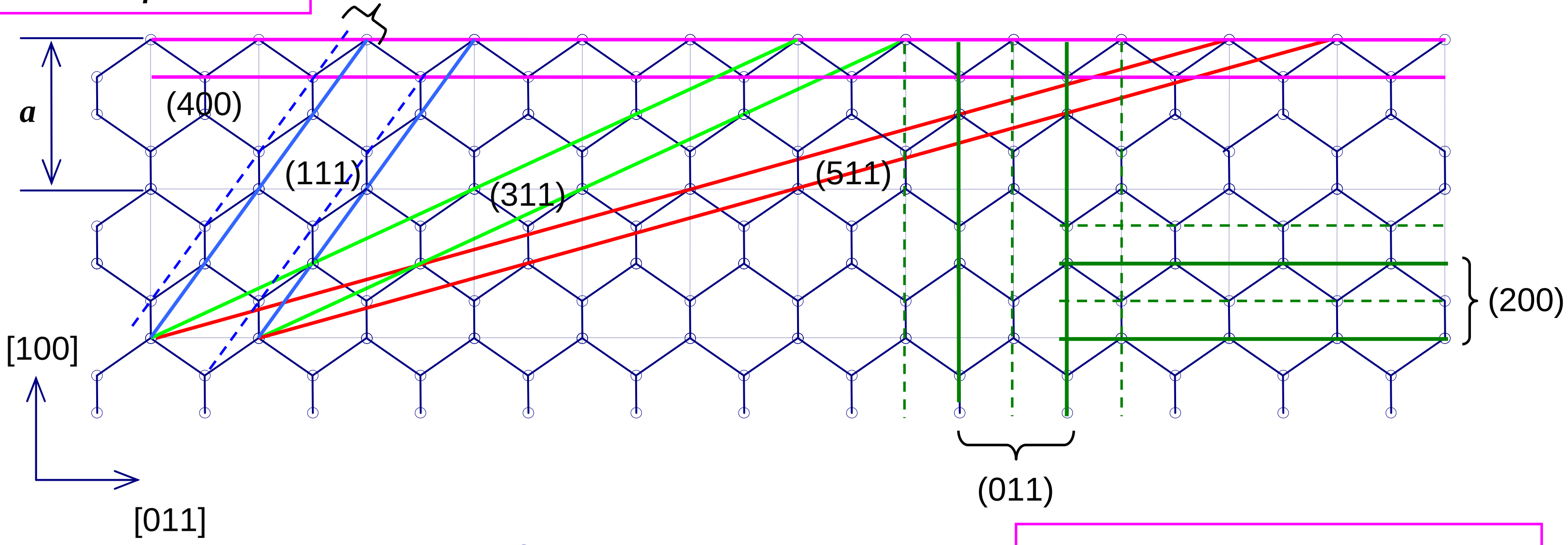
All in phase

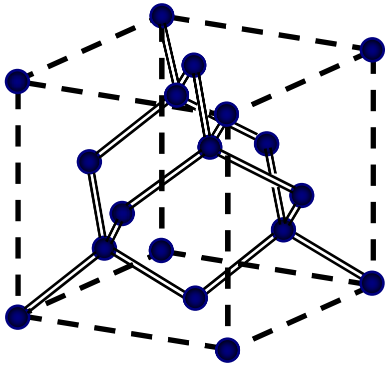
➔ $F = 8f$

(111), (311),...

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

➔ $F = 4(1 \pm i)f$





(011), (200),...

Half cancel with π

➔ Forbidden reflection

$F = 0$

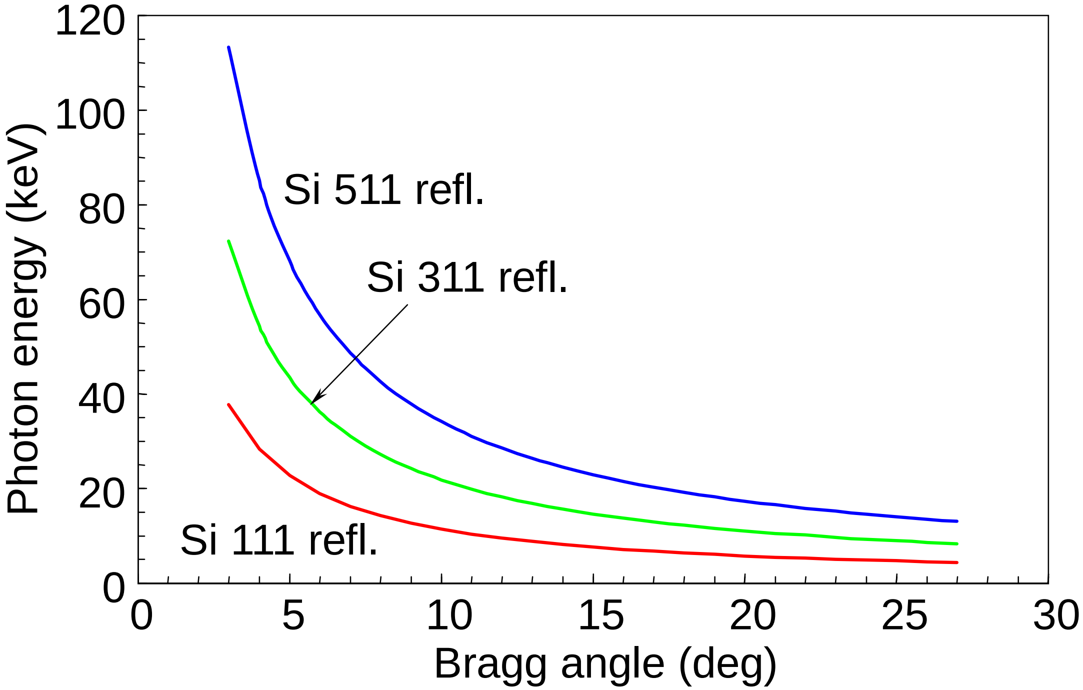
X-ray monochromator using perfect crystal

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

Photon energy range:

- Crystal & lattice plane

- Bragg angle range



e.g. for SPring-8 standard DCM

Bragg angle: 3~27°

Reflectivity (dynamical theory)

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

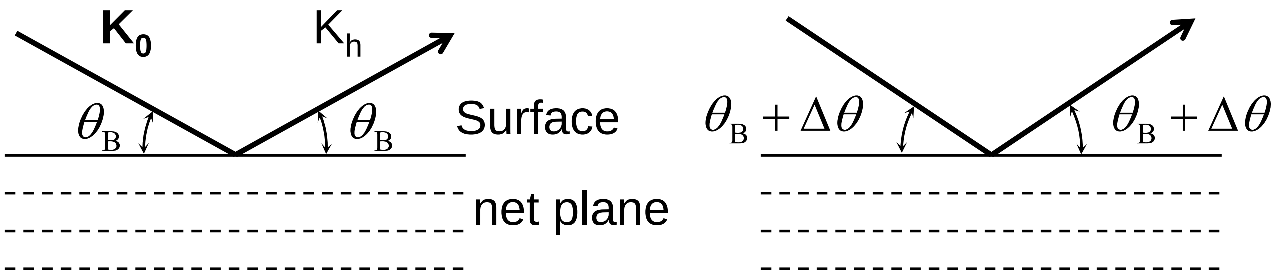
$$W = \left(\underbrace{\Delta\theta \sin 2\theta_{\mathrm{B}}}_{\text{Angular deviation}} + \underbrace{2\sin^2\theta_{\mathrm{B}} \frac{\Delta E}{E}}_{\text{Energy deviation}} + \underbrace{\chi_0}_{\text{Refraction}} \right) \frac{1}{|\chi_h|}$$

χ_{h}: Fourier component of polarizability
→proportional to the structure factor

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

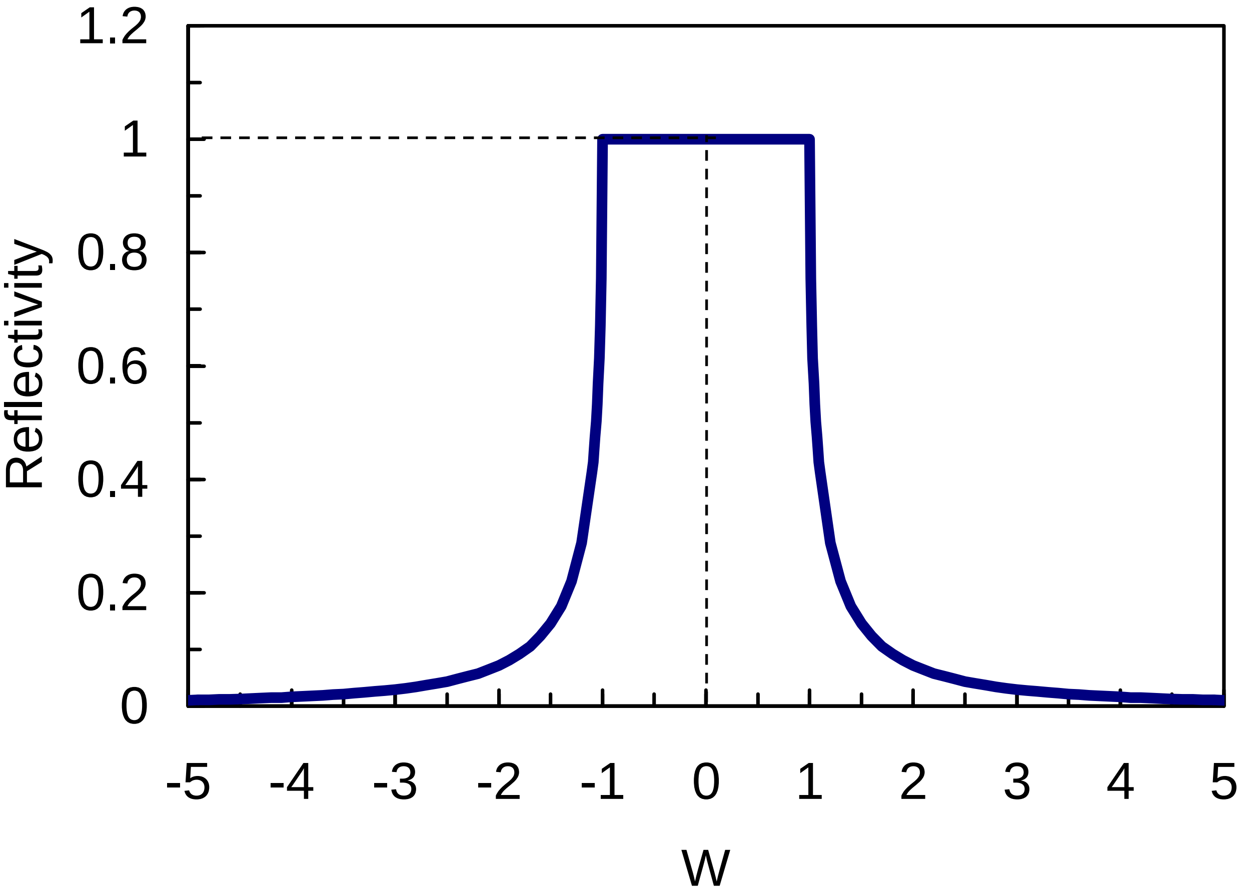
v_{c}: unit cell volume

Geometry for symmetrical Bragg case



Darwin curve

For Bragg case, no absorption, and thick crystal:



Reflectivity with absorption

Fourier component of polarizability for diamond structure

$$\chi_h = \chi'_h + \chi''_h$$

$$\left\{\begin{array}{l}
\boxed{h+k+l=4m} \\
\chi'_h = -\dfrac{r_e\lambda^2}{\pi v_c}8\left(f^0+f'\right)e^{-M} \\
\chi''_h = -\dfrac{r_e\lambda^2}{\pi v_c}8f''e^{-M} \\
\boxed{h+k+l=4m\pm1} \\
\chi'_h = -\dfrac{r_e\lambda^2}{\pi v_c}4(1+i)\left(f^0+f'\right)e^{-M} \\
\chi''_h = -\dfrac{r_e\lambda^2}{\pi v_c}4(1+i)f''e^{-M} \\
\boxed{h=k=l=0} \\
\chi'_0 = -\dfrac{r_e\lambda^2}{\pi v_c}8\left(Z+f'\right) \\
\chi''_0 = -\dfrac{r_e\lambda^2}{\pi v_c}8f''
\end{array}\right.$$

Reflectivity

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

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

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

$$W = \left(\Delta\theta\sin 2\theta_{\mathrm{B}} + 2\sin^2\theta_{\mathrm{B}}\frac{\Delta E}{E} + \chi'_0\right)\frac{1}{\left|\chi'_h\right|}$$

$$g = \frac{\chi''_0}{\left|\chi'_h\right|},\quad \kappa = \frac{\left|\chi''_h\right|}{\left|\chi'_h\right|}$$

Reflectivity curve for silicon

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

Si 111 refl., 10 keV

$$\chi_0' = -9.78\times10^{-6}$$

$$\chi_0'' = -1.48\times10^{-7}$$

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

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

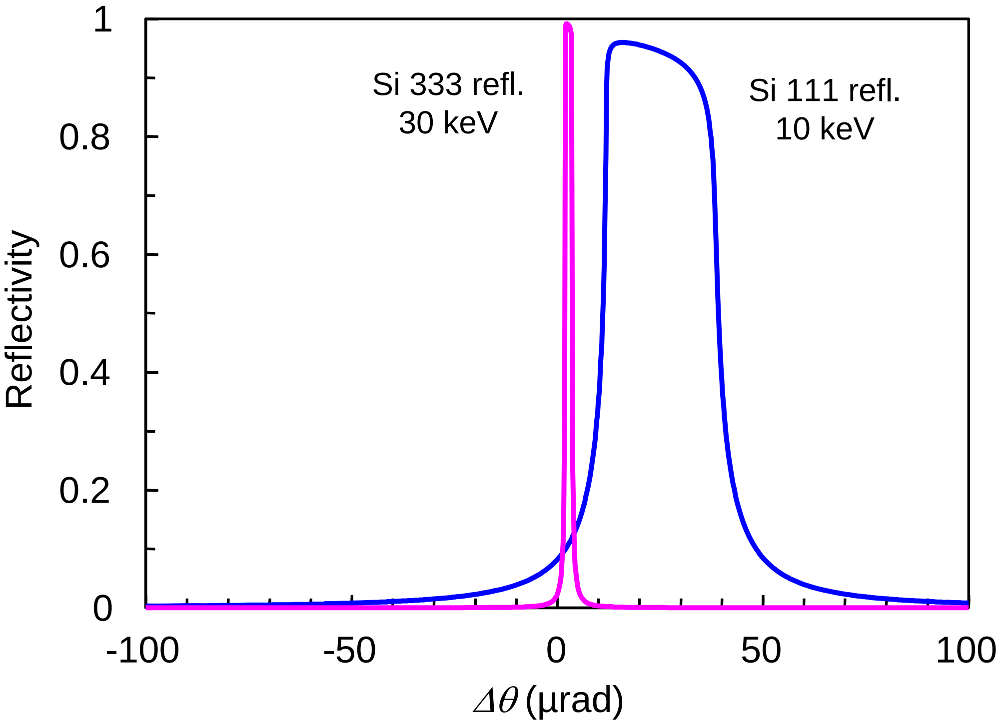
Si 333 refl., 30 keV

$$\chi_0' = -1.07\times10^{-6}$$

$$\chi_0'' = -1.75\times10^{-9}$$

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

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



- 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)

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

← Δ W= 2

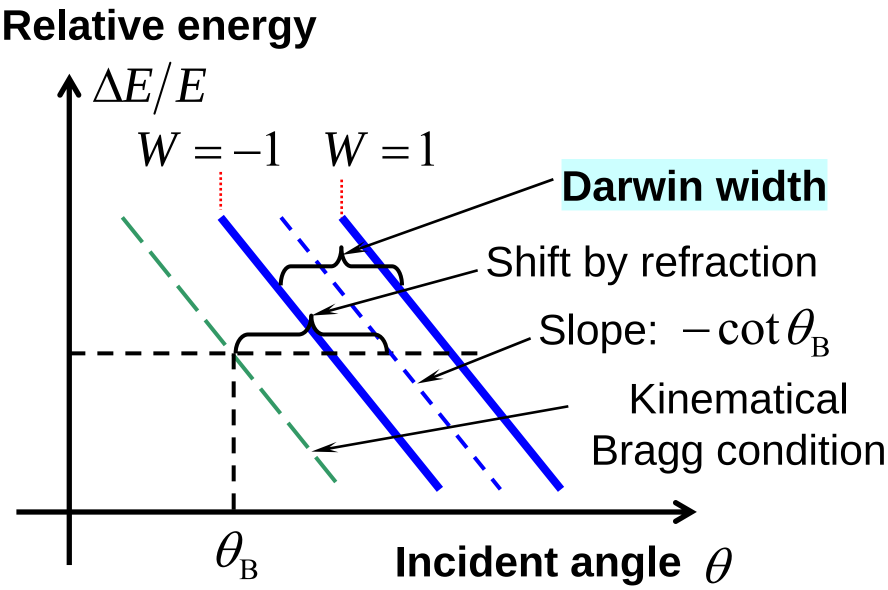
Energy resolution

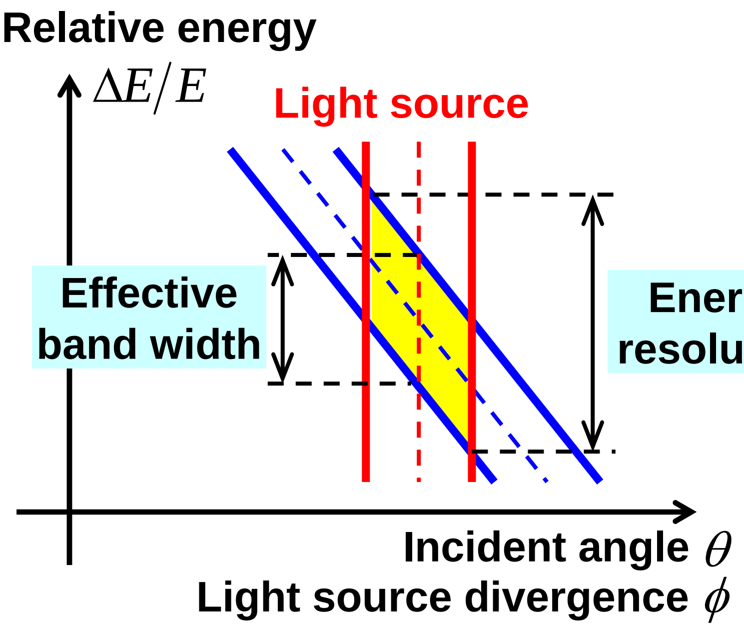
$$\frac{\Delta E}{E} = \cot\theta_{\text{B}}\sqrt{\Omega^2 + \Delta\theta_{\text{Darwin}}{}^2}$$

← Gaussian approximation for both light source and reflection curve

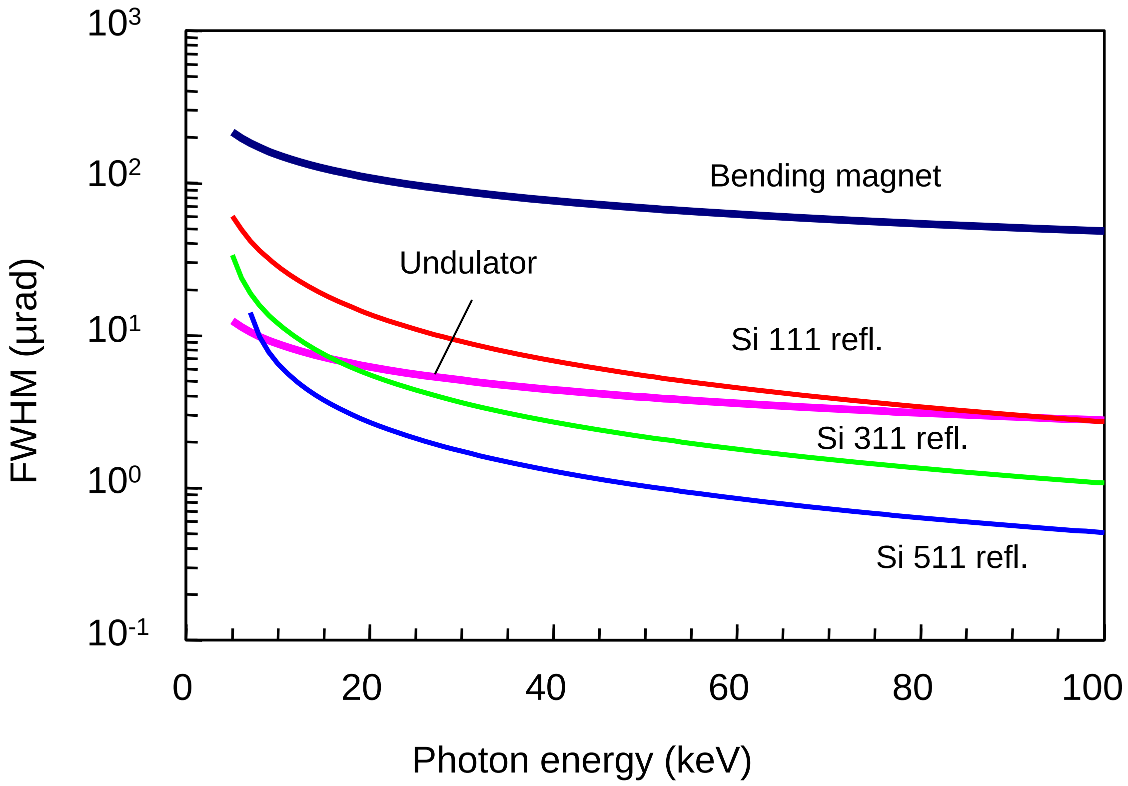
Effective band width

$$\frac{\Delta E}{E} \approx \frac{\left|\chi'_h\right|}{\sin^2\theta_{\text{B}}}$$





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)

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

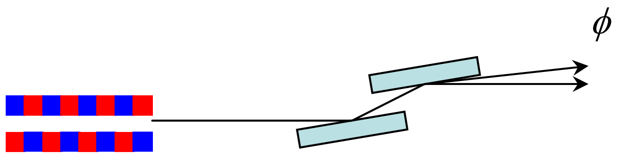
Divergence of undulator radiation ~ diffraction width

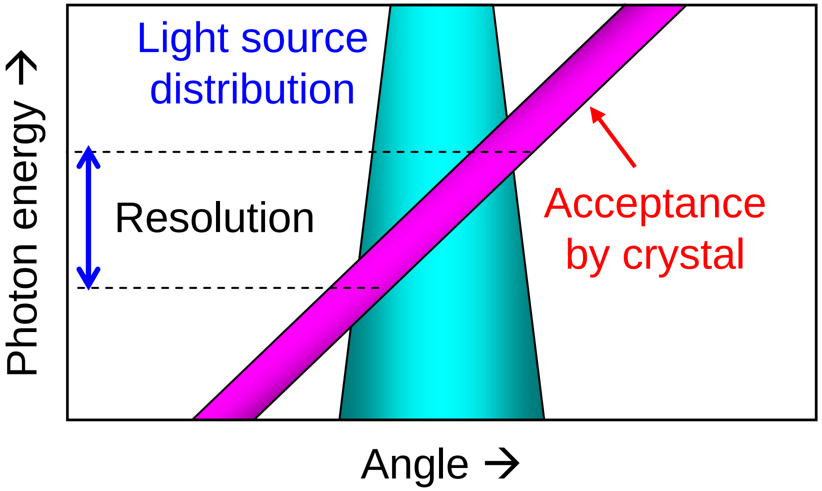
Energy resolution

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

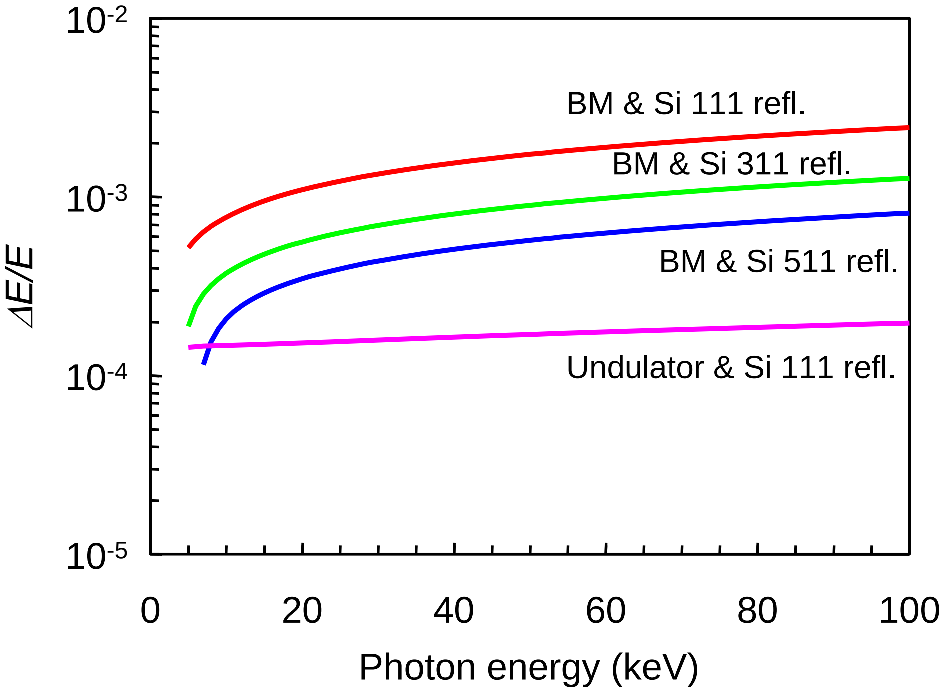
Ω: source divergence,

ω: diffraction width



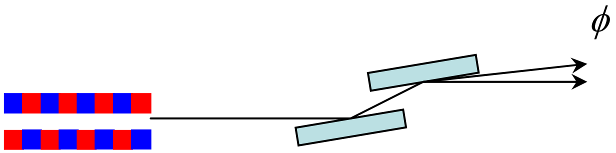


Angle-energy diagram (DuMond diagram)



For usual beamline : $\Delta E/E=10^{-5}\sim10^{-3}$

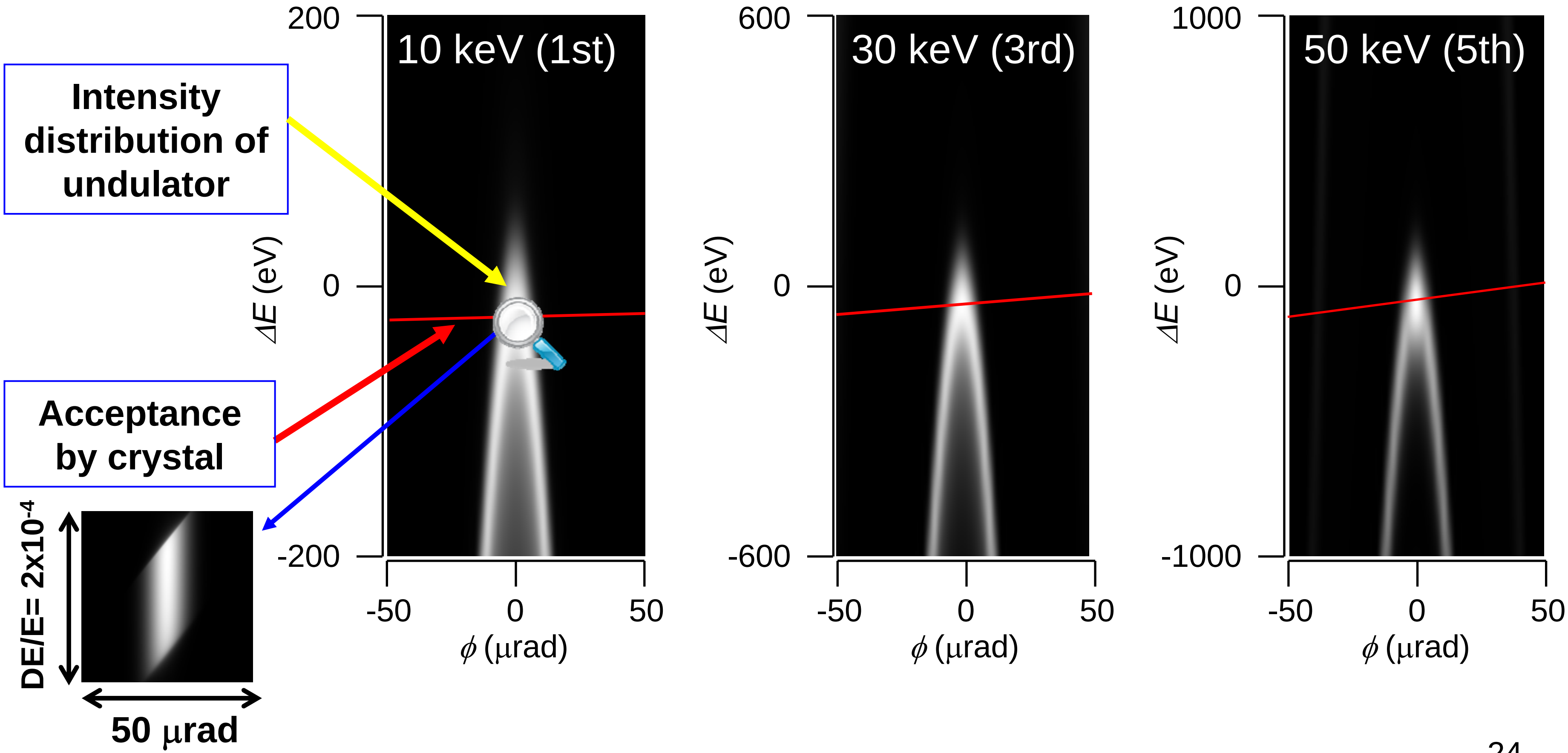
DuMond diagram: undulator & DCM



SPring-8 standard undulator

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

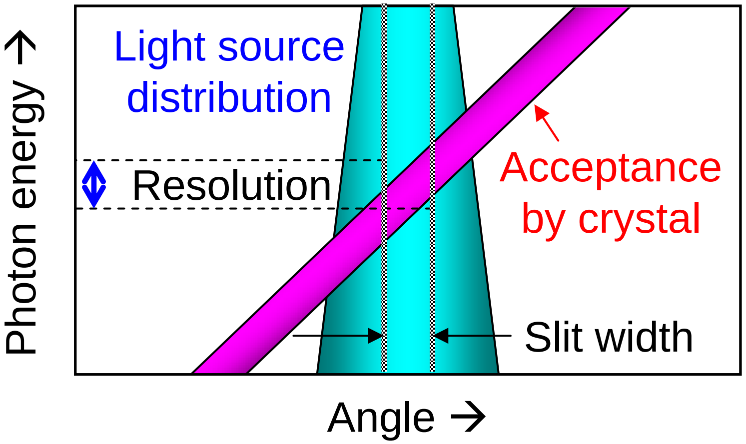
+ DCM (Si 111 refl.)


Intensity distribution of undulator

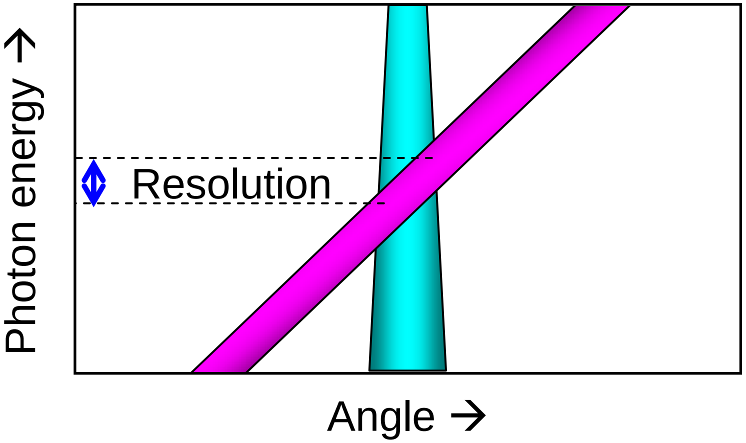
Acceptance by crystal

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

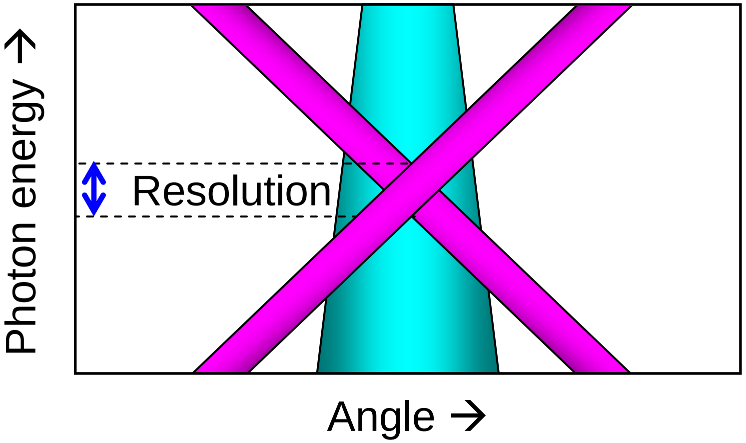
Improvement of energy resolution



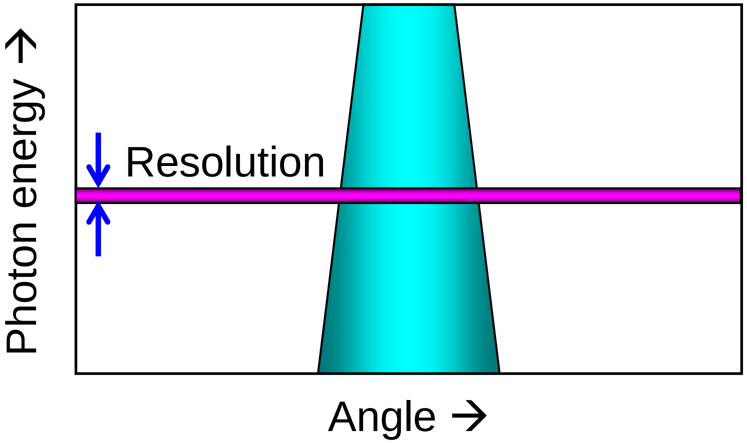
(A) Collimation using slit



(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

Photon flux after monochromator

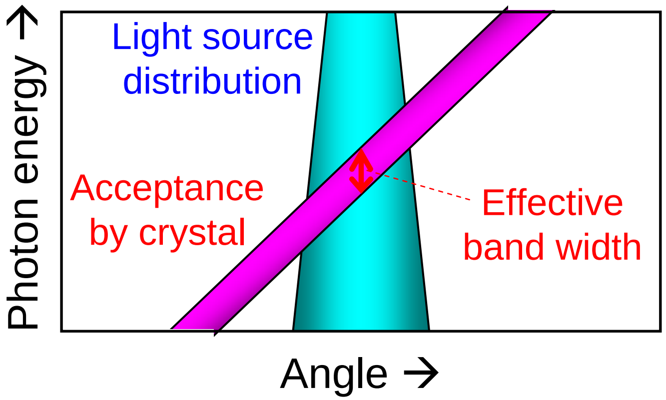
Photon flux (throughput) after monochromator can be estimated using effective band width:

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

$$\frac{\Delta E}{E} \approx \frac{|\chi'_h|}{\sin^2 \theta_{\mathrm{B}}}$$

$$\chi'_h \propto \lambda^2 \{ f_0(d_{hkl}) + f'(\lambda) \}$$

Neglecting anomalous scattering factor *f’*

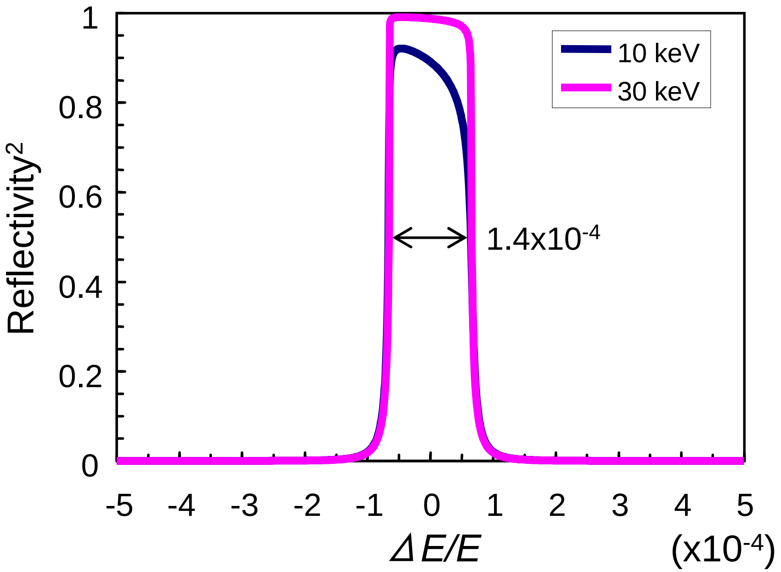
$$\chi'_h \propto \lambda^2 f_0(d_{hkl})$$

$$\frac{\Delta E}{E} = -\frac{\Delta\lambda}{\lambda} \approx \frac{|\chi'_h|}{\sin^2 \theta_{\mathrm{B}}}$$

$$= 4 d_{hkl}{}^2 \frac{|\chi'_h|}{\lambda^2}$$

$$\frac{\Delta E}{E} = -\frac{\Delta\lambda}{\lambda} \propto d_{hkl}{}^2 f_0(d_{hkl})$$

Independent of photon energy



e.g. for Si 111 refl. DCM case

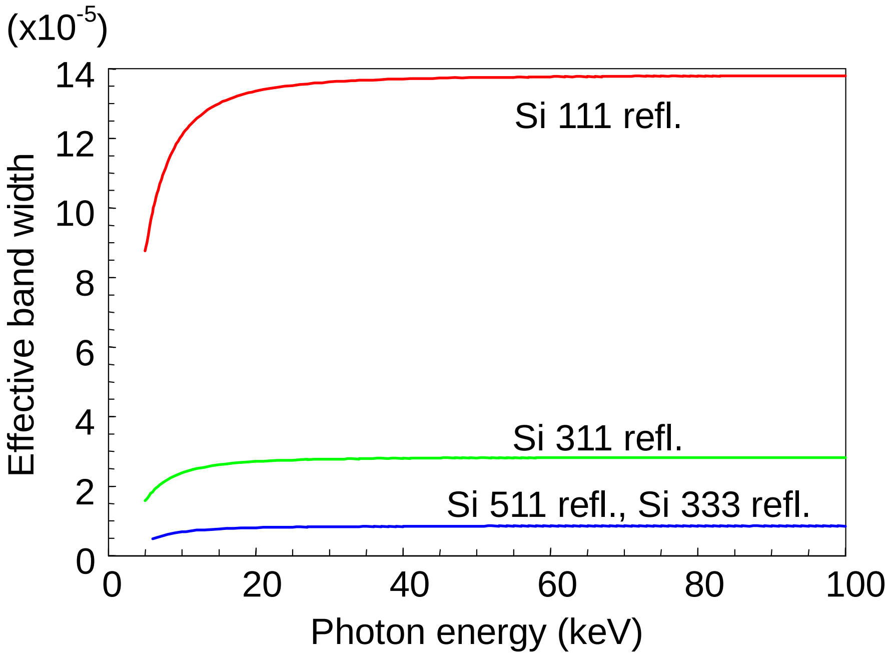
Note relative energy width is constant.

Effective band width (Integrated intensity)

For double-crystal monochromator

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

= ~2



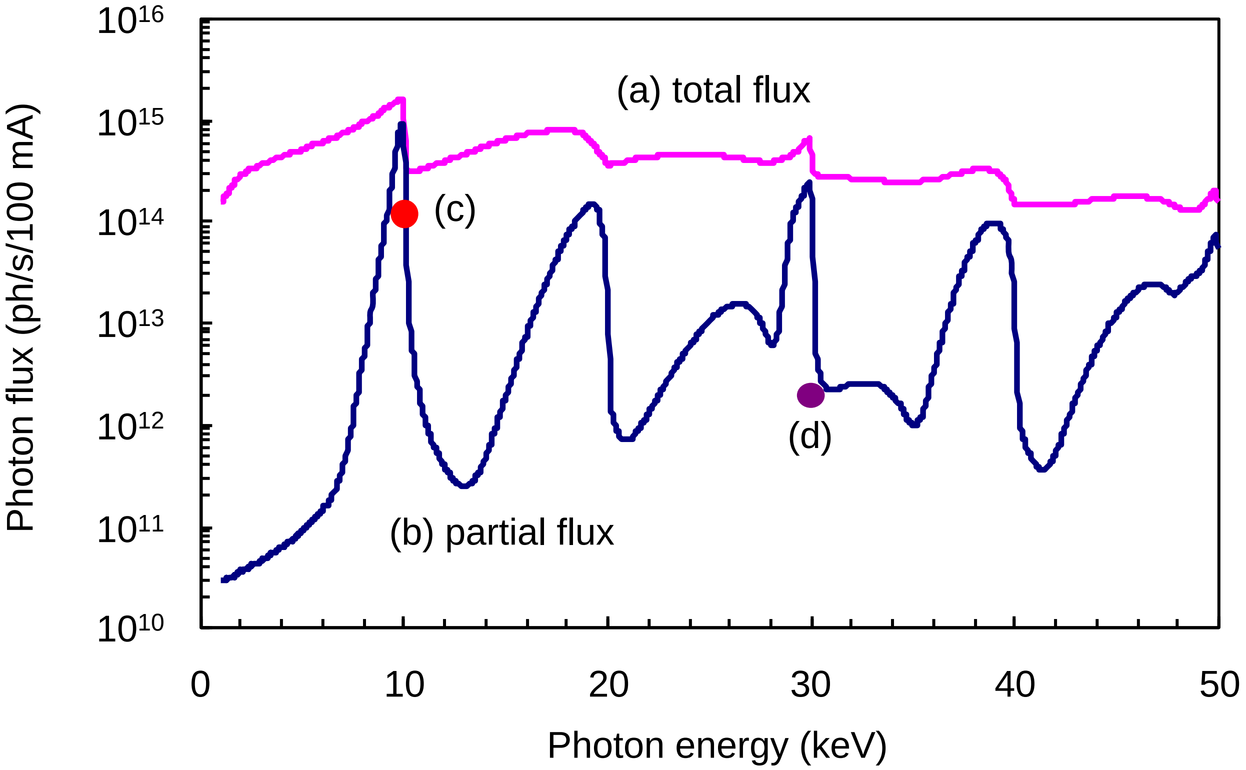
Effective band-width is obtained

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. = $8.0x10^{-6}$

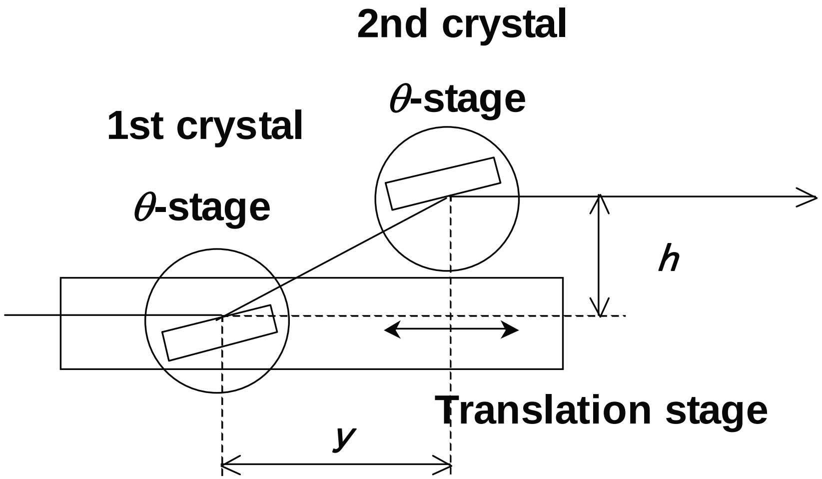
Higher harmonics elimination more → mirror or detuning of DCM

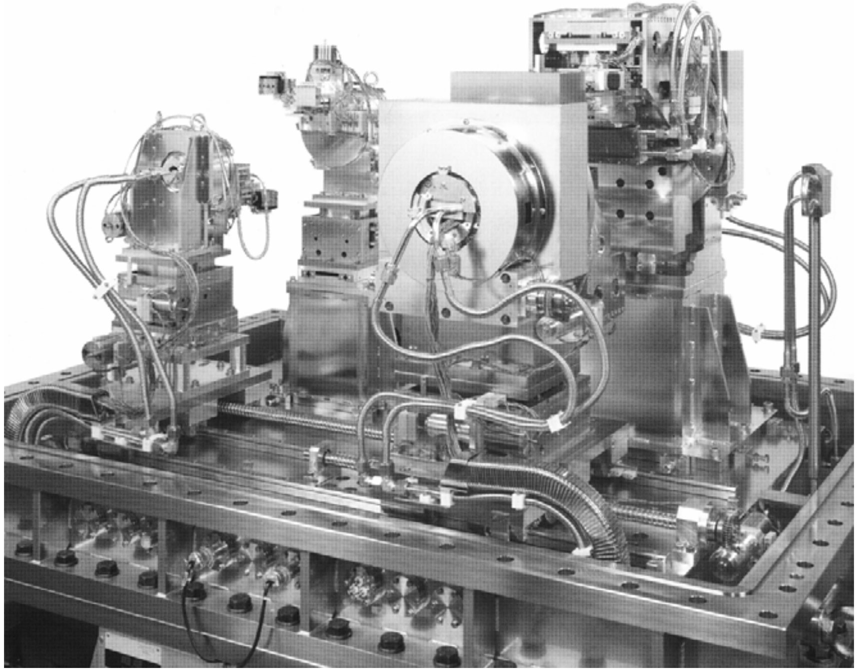
We can obtain photon flux of 10^{13}～10^{14} ph/s/100 mA/mm^2 using standard undulator sources and Si 111 reflections at SPring-8 beamlines.

Double-crystal monochromator

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

θ_1 + translation + θ_2 computer link





SPring-8 BL15XU

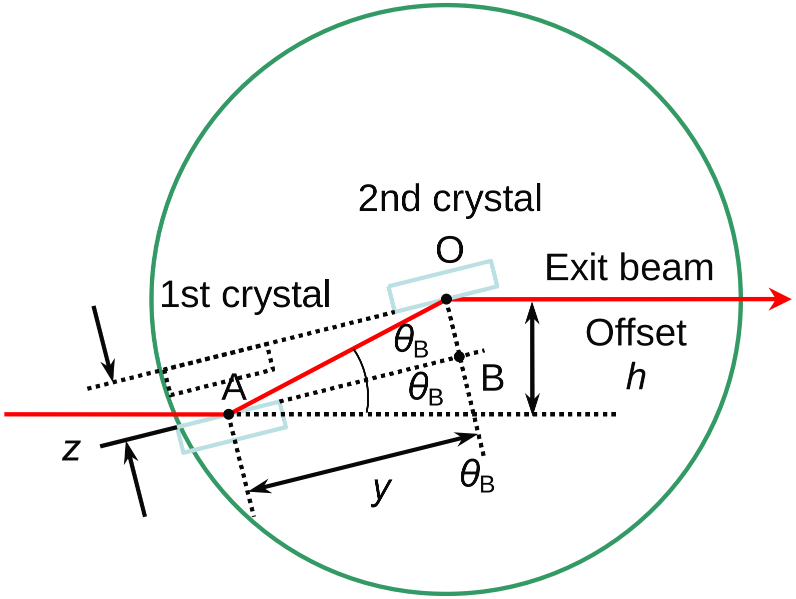
SPring-8 information Vol. 5, No.1 (2000)

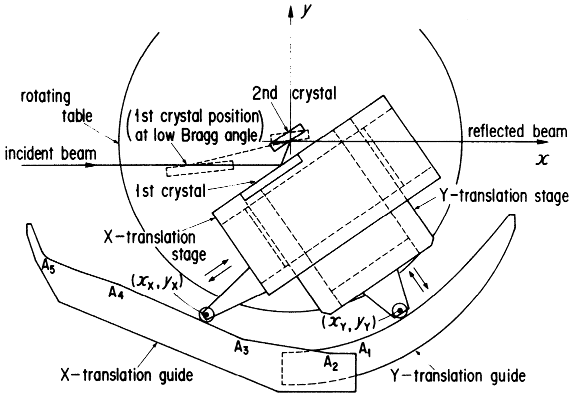
h= 100 mm, θ_B= 5.7~72° (for lower energy range)

Large offset, long-stroke translation

Difficulty of adjustment between 1st and 2nd crystal

θ + two translation (KEK-PF)





PF BL-4C..

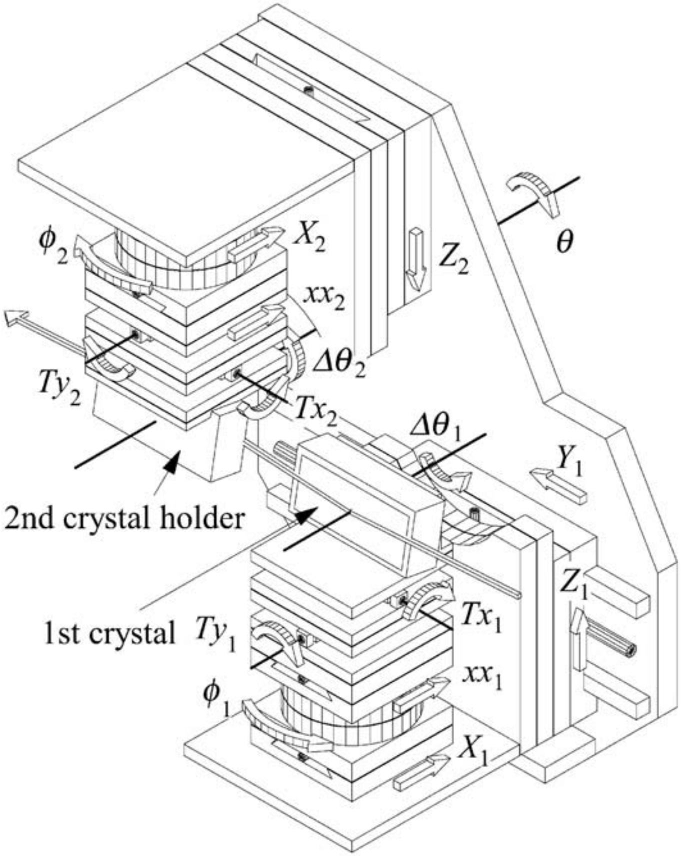
Matsushita et al., NIM A246 (1986)

h= 25 mm, θ_B= 5~70°

Two cams for two translation-stages

Rotation center at 2nd crystal

SPring-8 standard DCM



Offset h= 30 mm

θ_B =3~27º for higher energy range

High-precision adjustment stages

for undulator beamline DCM

Sub-μm & sub-μrad control

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)

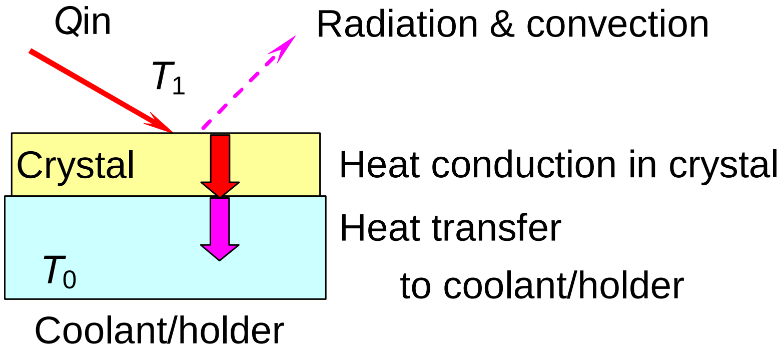
α: thermal expansion coefficient

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 !



Solution for crystal cooling

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) Large contact area between crystal and coolant/holder → larger

(S-3) Irradiation area → Larger, and power density → smaller

Figure of merit

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

Figure of merit of cooling:

Good for silicon (80 k) and diamond (300 K)

For SPring-8 case

Bending magnet beamline

Power and density : ~100 W, ~1 W/mm^2 @40 m

Method:

→ Direct cooling with fin crystal ← S-2

Undulator beamline

(Linear undulator, N= 140, λu= 32 mm)

Power and density : ~500 W , ~500 W/mm^2 @40 m

Methods:

→ Direct cooling of silicon pin-post crystal ← S-2

+ Rotated inclined geometry (→10 W/mm^2) ← S-3

→ or Cryogenic cooling using LN$_2$ circulation ← S-1

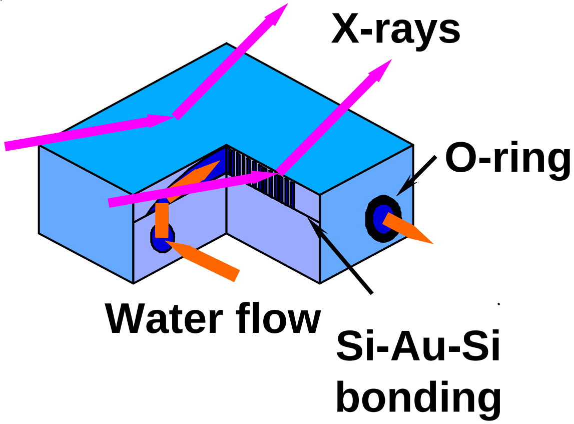
→ or Indirect cooling of IIa diamond crystal ← S-1

Crystal monochromator at SPring-8

<Bending magnet beamline>

Power & power density:
~100 W, ~1 W/mm^2

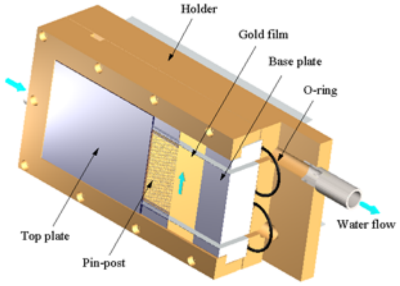
Fin crystal direct-cooling - (S2)

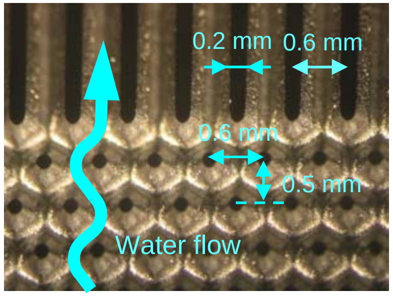


<Undulator beamline>

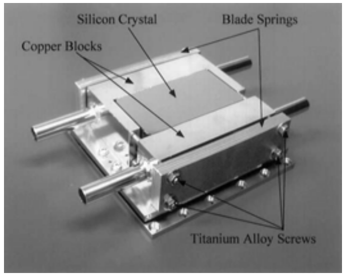
Linear undulator, *N*= 140, λu= 32 mm
Power & power density: 300~500 W ,
300~500 W/mm^2

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

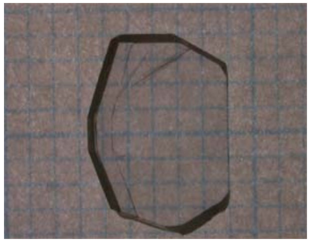


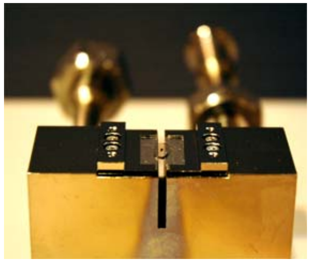


b) Silicon cryogenic cooling - (S1)



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





Example of x-ray beamline

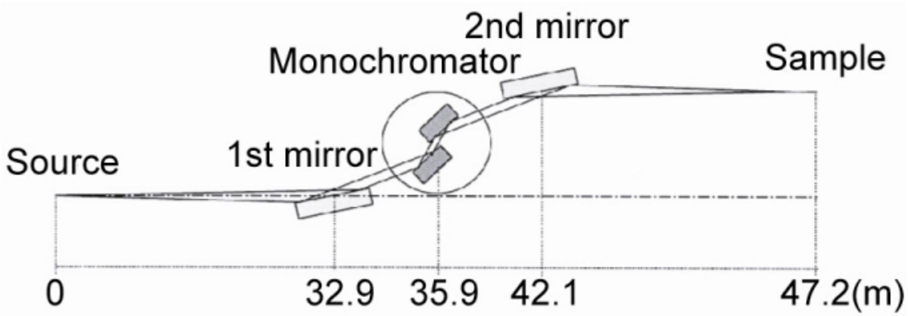
- SPring-8 case -

XAFS & single crystal diffraction

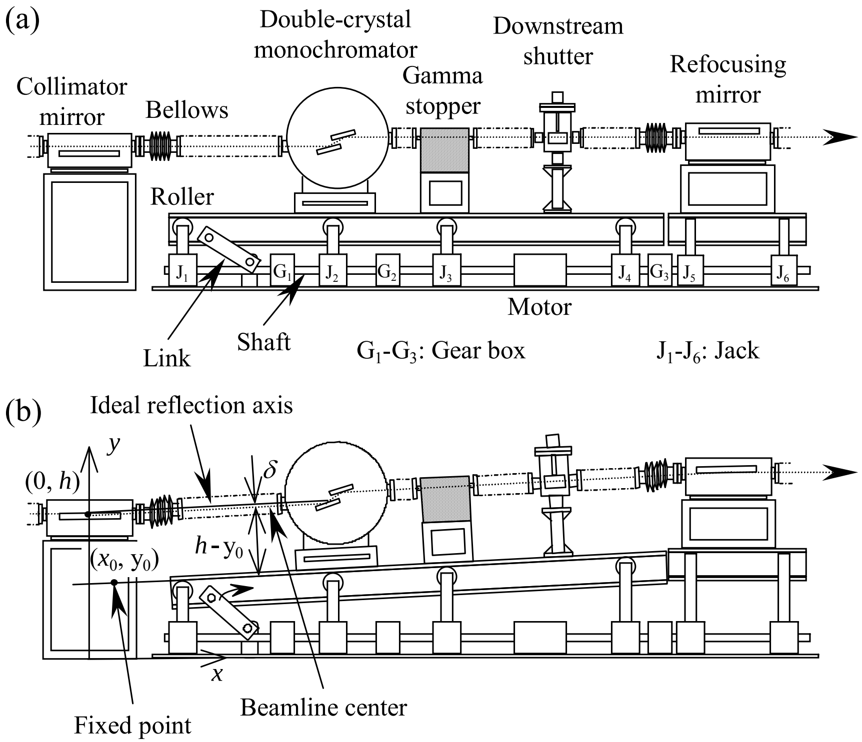
- Bending magnet
- Collimator mirror,

  + DCM,

  + refocusing mirror

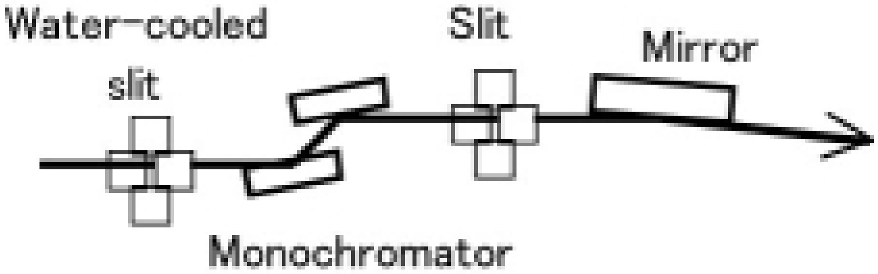


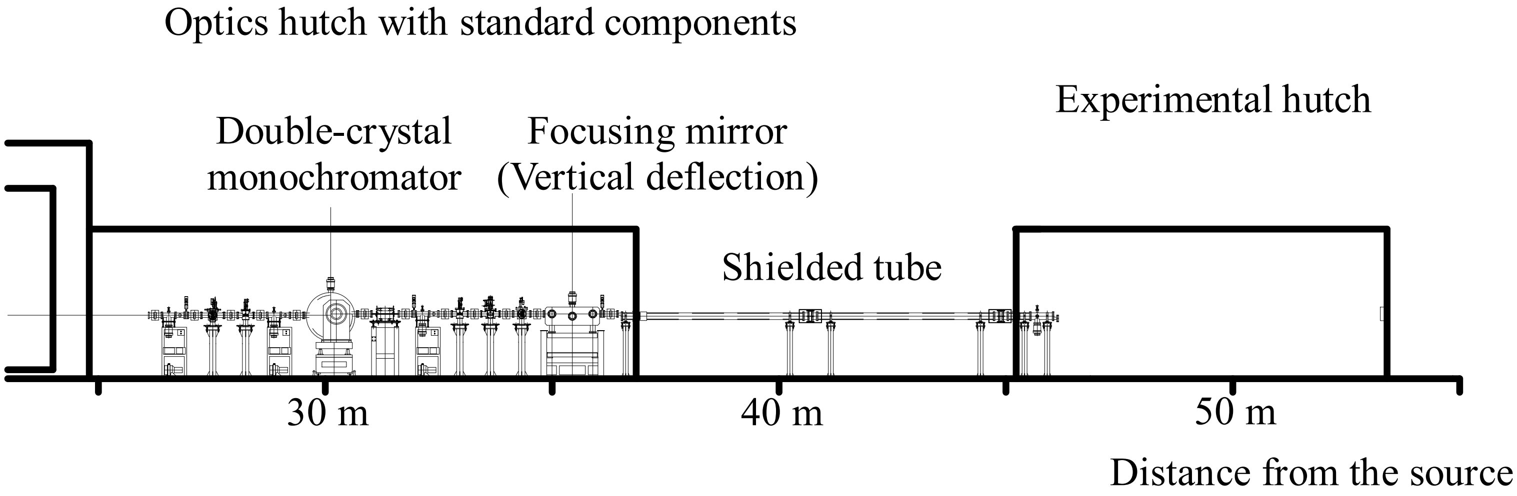
Optical layout for energy range less than 60 keV



Protein crystallography

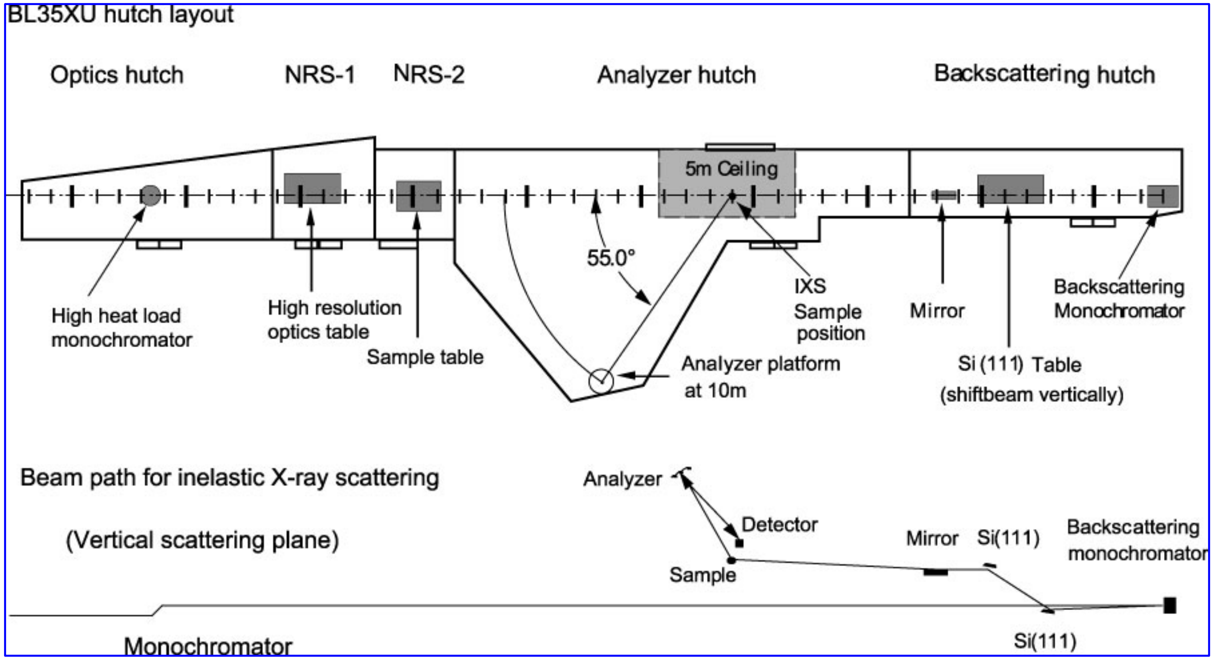
- Bending magnet
- DCM + focusing mirror

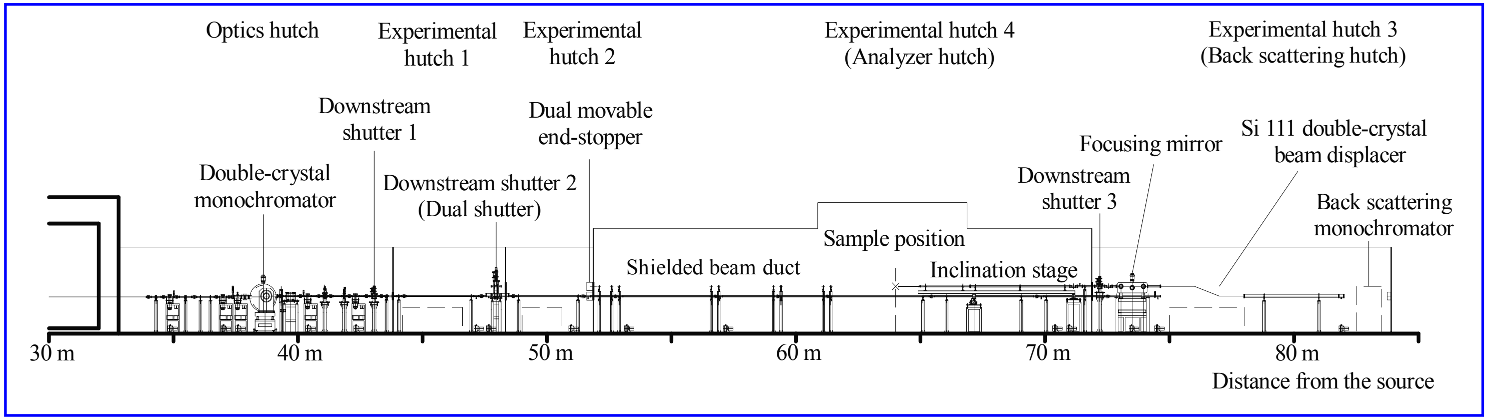




High resolution inelastic scattering

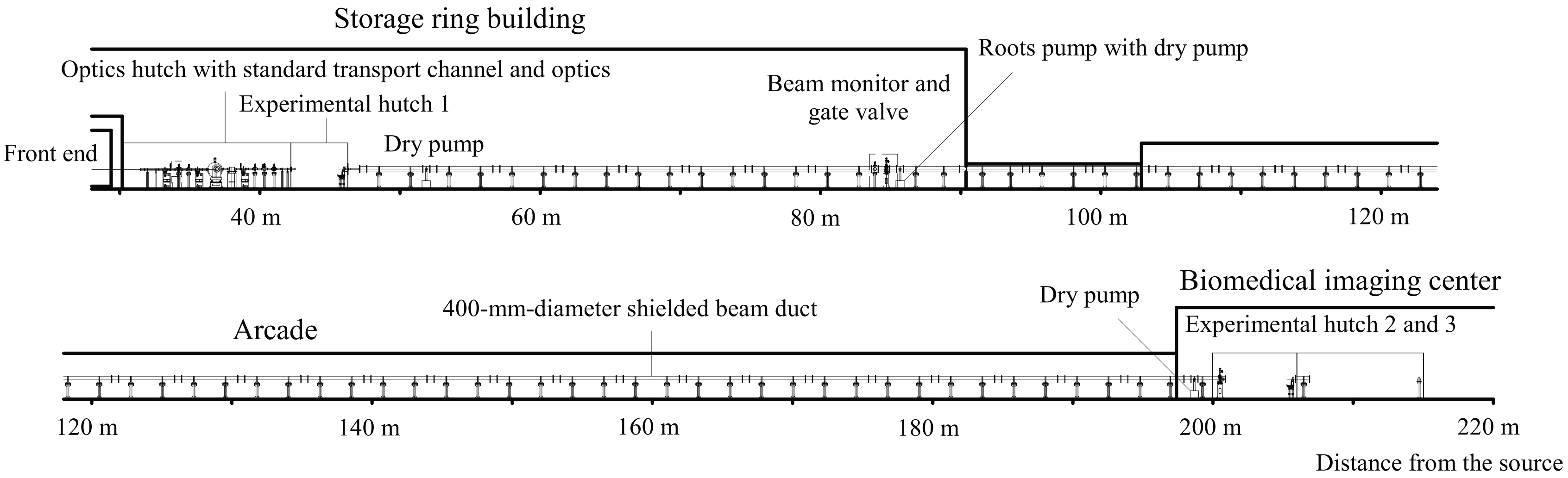
- Undulator
- DCM + back-reflection monochromator & analyzer (w/ ~meV resolution)

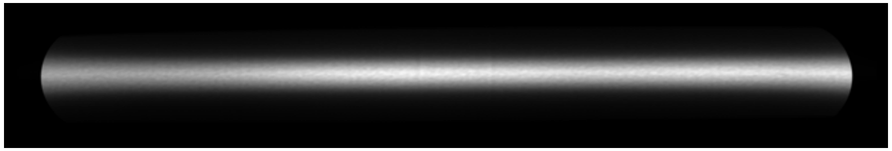




200-m-long beamline

- Bending magnet
- DCM





300-mm-wide beam at end-station

Summary

- Starting point of X-ray beamline design is shown here,

w/ light source and **monochromator**.

- It helps to figure out what we can do at the beamline.

- We will have to go into details of design refinement using;

FEA (ANSYS), ray-tracing (SHADOW,...).

- Ray-tracing → wave simulation for "diffraction limited source and optics"