October 10, 2010

Cheiron School 2010

X-ray Beamline Design

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SPring-8/JASRI

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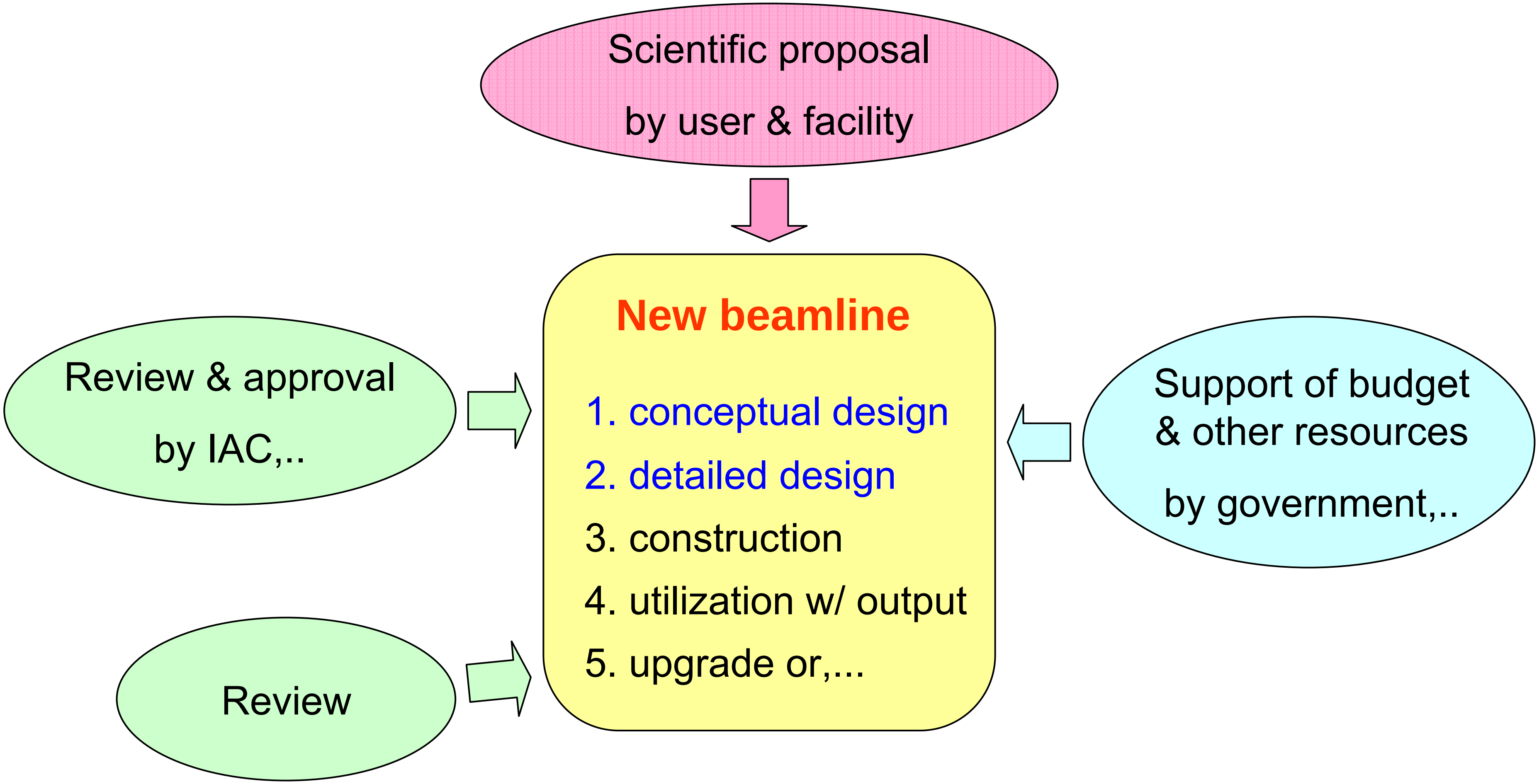
Process of beamline construction

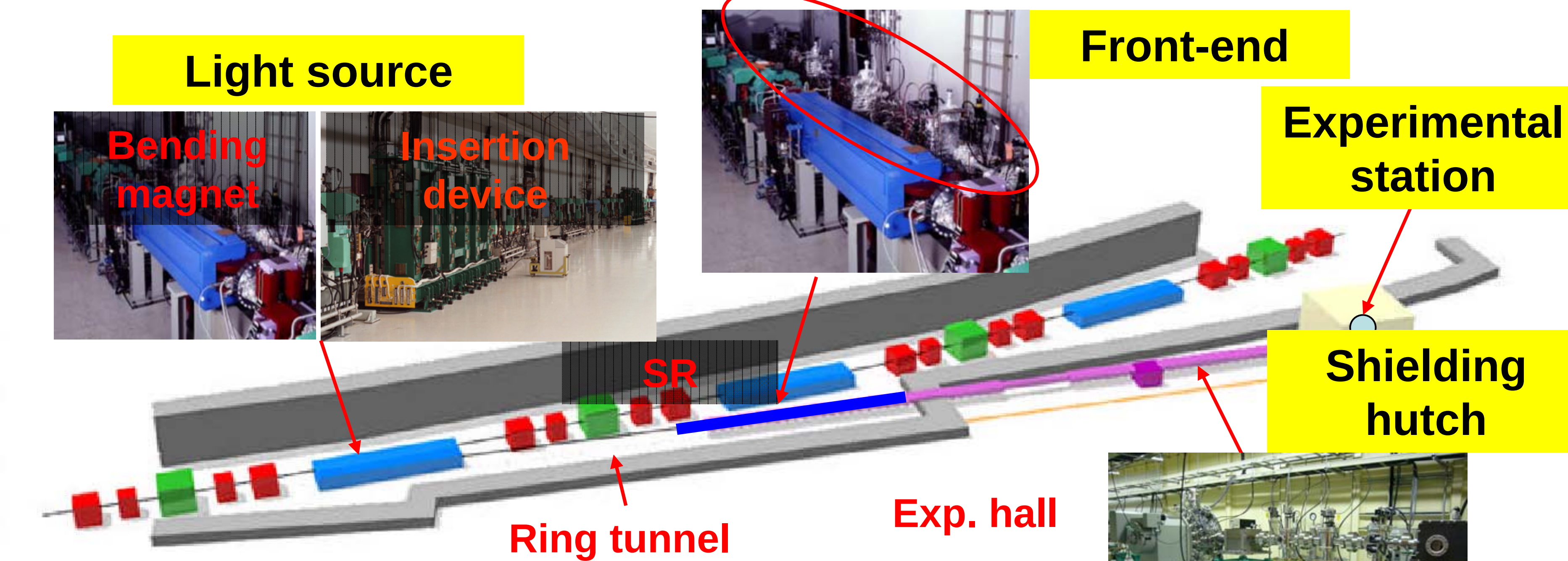


Beamline design is first step and crucial for success of the beamline !

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

Beamline structure

Beamline = "Bridge" between light source & experimental station



Monochromator, mirror

shutter, slit

pump,..

- → **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

Light sources & X-ray optics

Check points to be considered for your application:

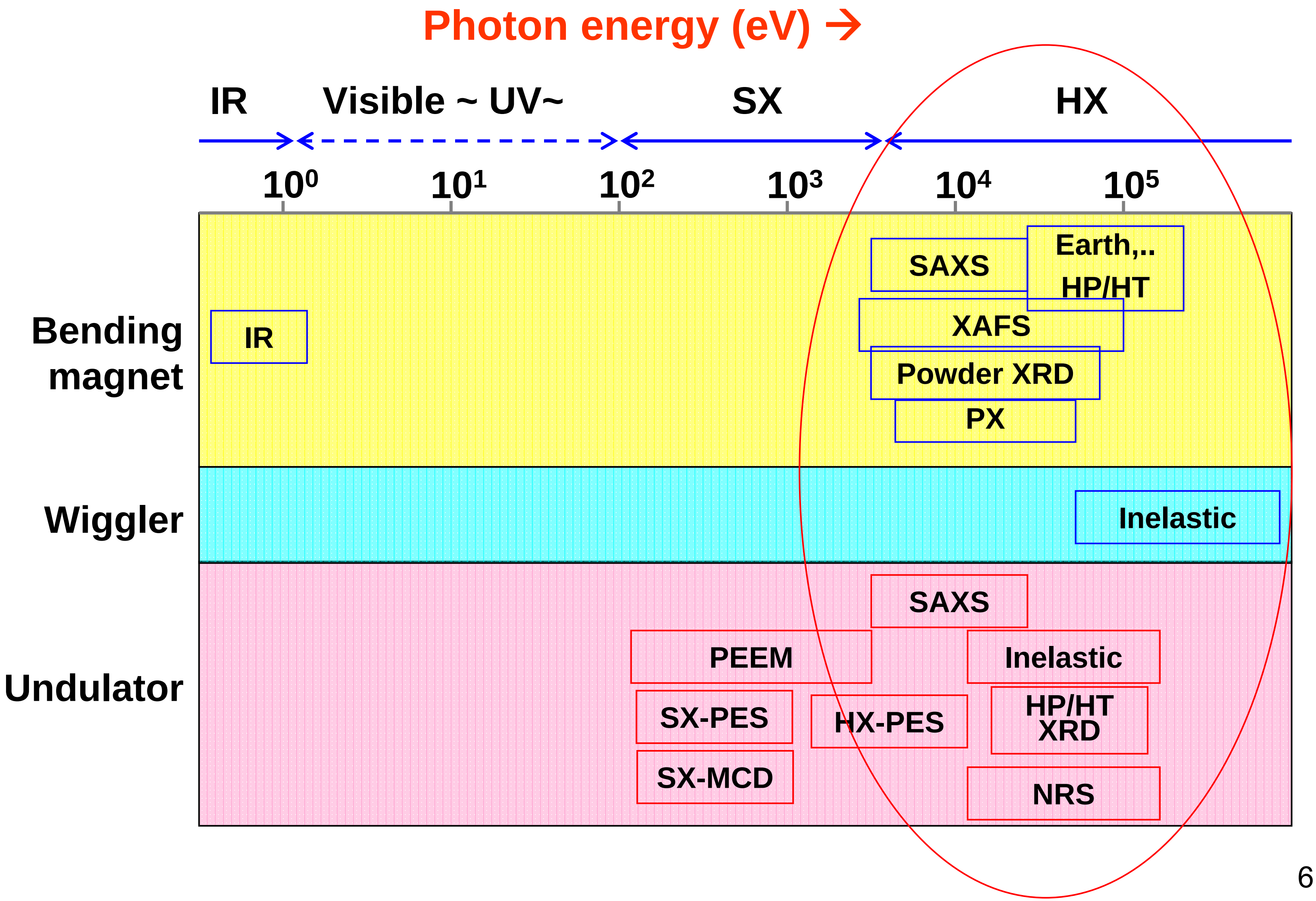
- White or monochromatic
- Energy range
- Energy resolution
- Flux & flux density
- Beam size at sample (micro beam?,...)
- Beam divergence/convergence at sample (Resolution in k-space)
- Higher order elimination w/ mirror
- Polarization conversion
- Spatial coherency

....

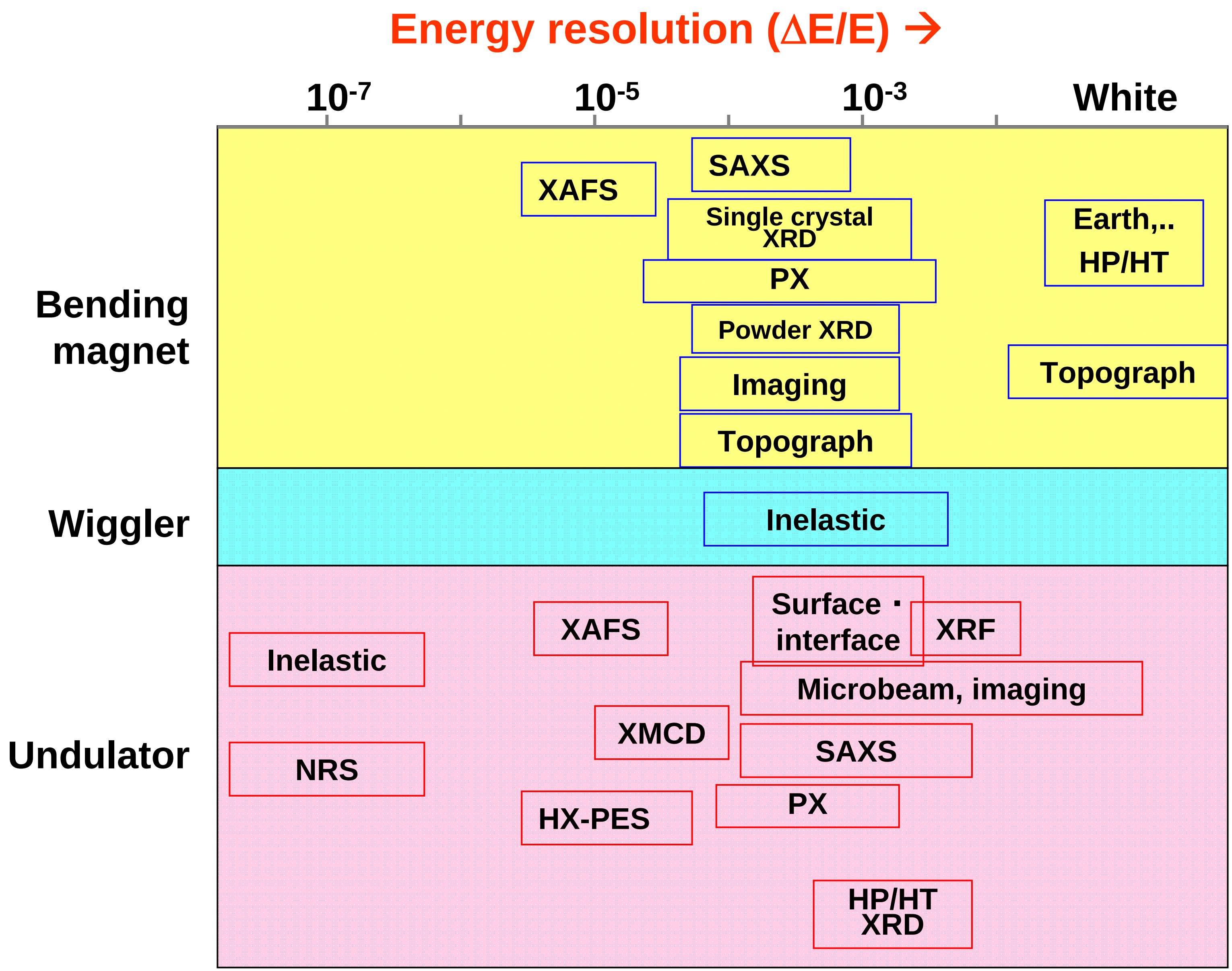
→ Light source, monochromator, mirror,

and other optical devices and components

BL classification (energy region)



BL classification (energy resolution)



Light sources

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):

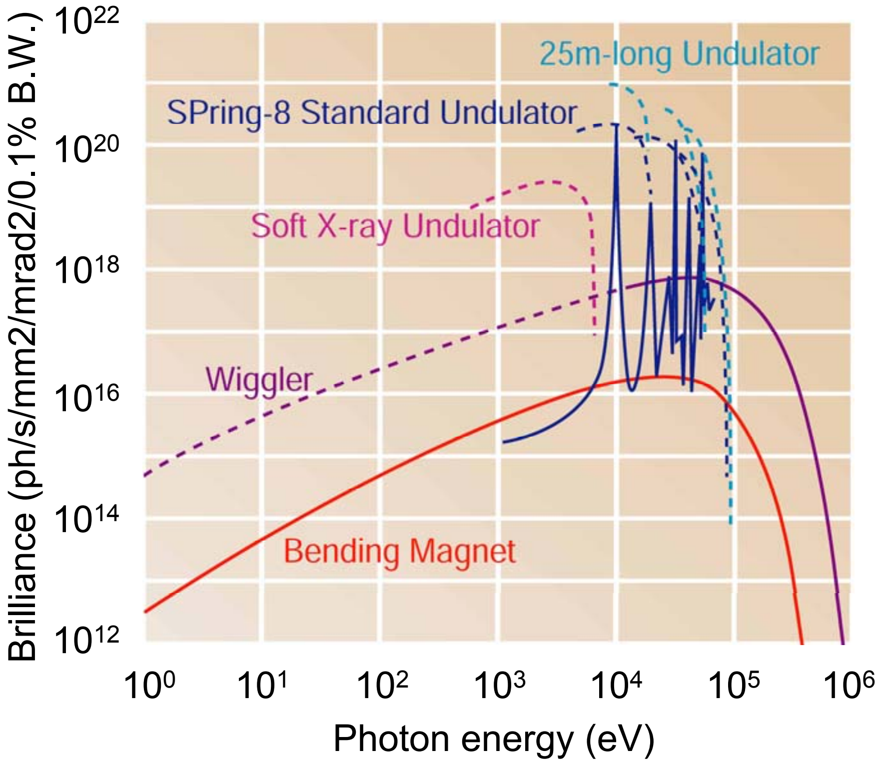
for high-brilliance beam

for micro-/ nano-focusing beam

Wiggler:

for higher energy X-rays > 100 keV.

→ *short-period-length undulator*



Brilliance for SPring-8 case

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

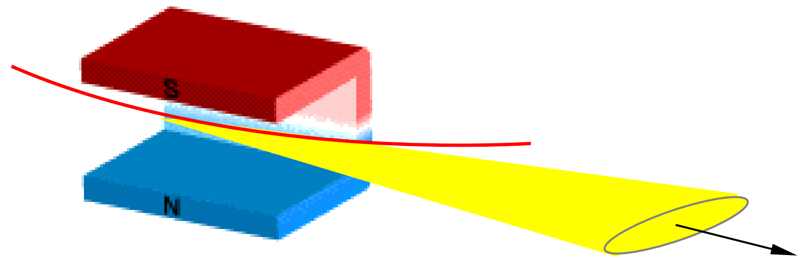
e.g. “SPECTRA” by T. Tanaka & H. Kitamura

Light sources

Angular divergence and band width

- Bending magnet

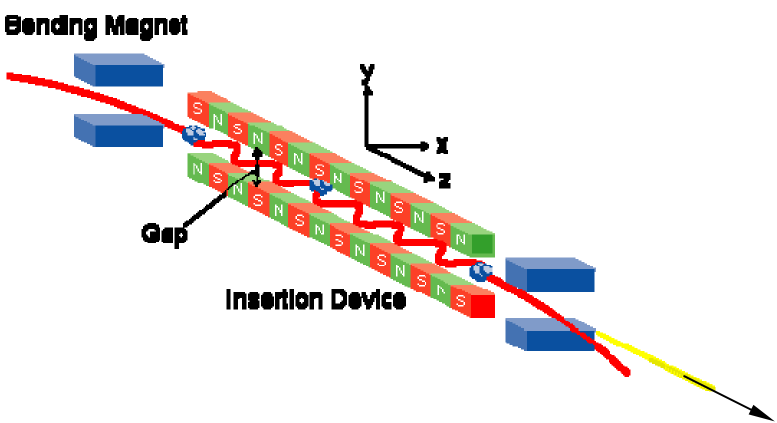
$$\sigma_{r'} \approx 0.597 \frac{1}{\gamma} \sqrt{\frac{\lambda}{\lambda_c}}$$

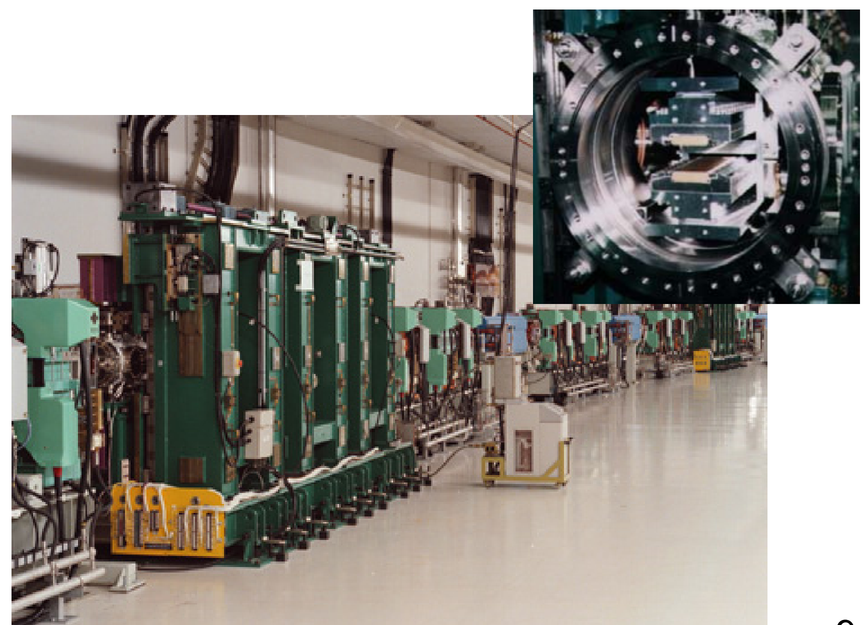


- Undulator

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

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





SPring-8 in-vacuum undulator

Monochromator

Key issues from experimental request:

White or monochromatic ? → monochromatic

Energy region ← Bragg's law

Energy resolution ← Source divergence, Darwin width,..

Throughput ← related to energy resolution

Double-crystal monochromator for fixed-exit

Single-bounce monochromator is for limited case

Heat load ← depending on light source

X-ray monochromator using perfect crystal

→ Principle of monochromator

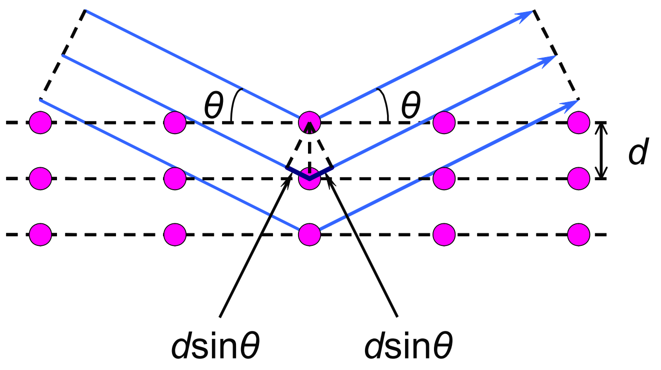
Bragg reflection from perfect single crystal

$2d \sin \theta_B = n \lambda$

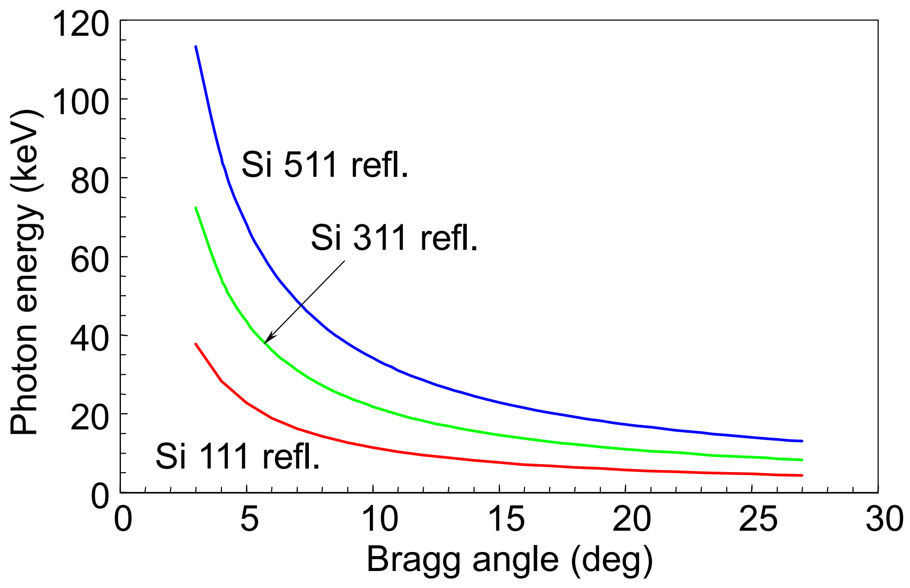
d: Latiice *(d)*-spacing,

θ_B: glancing angle (Bragg angle),

λ: X-ray wavelength



→ Crystal: silicon, diamond,..



e.g. for SPring-8 standard DCM

Bragg angle: 3~27°

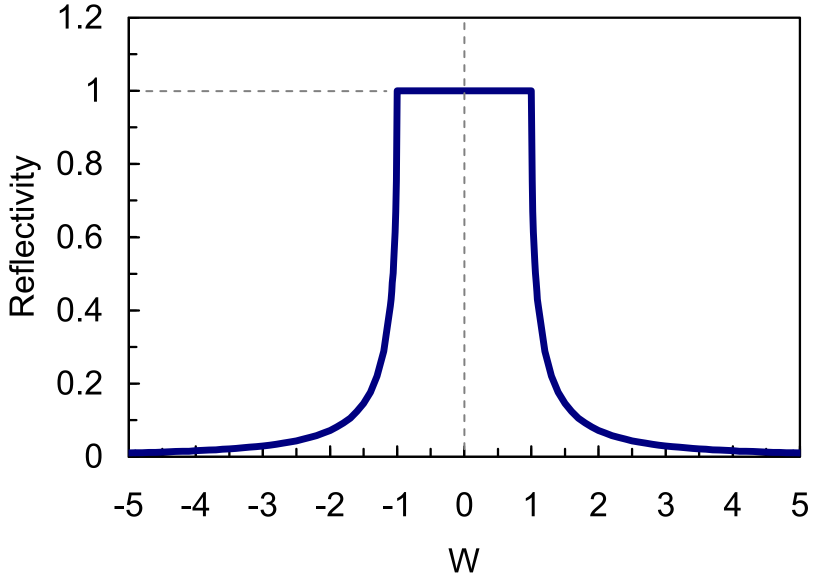
Photon energy range:

- Crystal & lattice plane
- Bragg angle range

Reflectivity (intrinsic rocking curve)

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

$$
\begin{cases}
R = \dfrac{|\gamma_h|}{\gamma_0}\left|\dfrac{E_h}{E_0}\right|^2 = \left(W + \sqrt{W^2 - 1}\right)^2 & (W < -1) \\
R = 1 \quad (-1 \le W \le 1) & \leftarrow \text{Total reflection region} \\
R = \left(W - \sqrt{W^2 - 1}\right)^2 & (W > 1)
\end{cases}
$$



For symmetric Bragg case, sigma polarization:

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

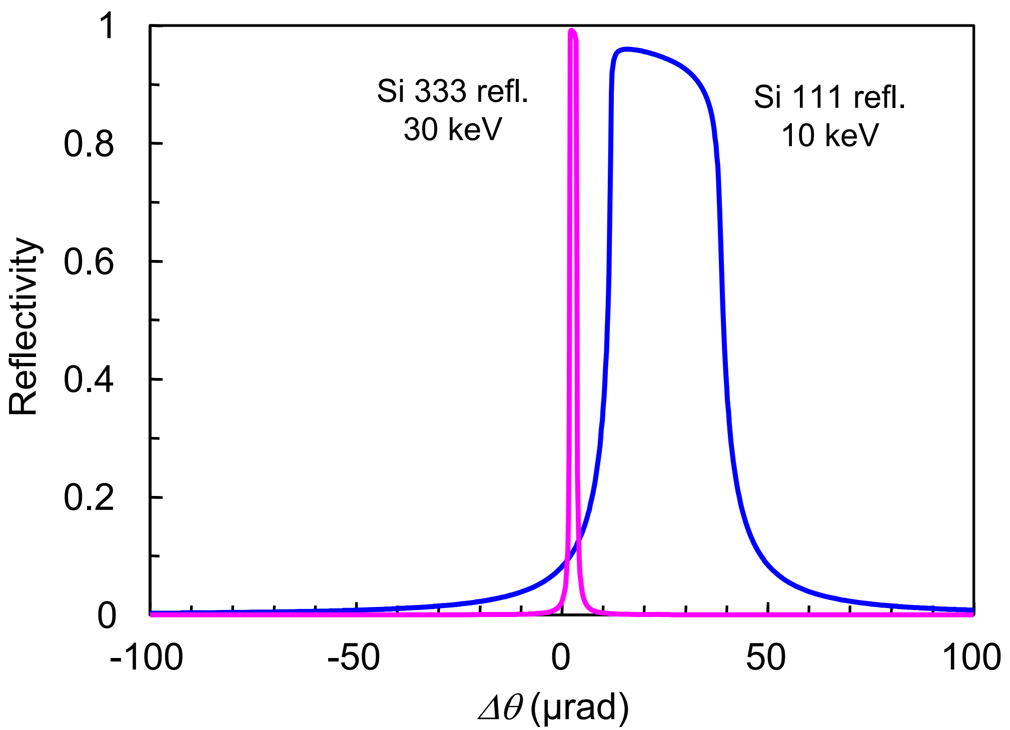
Darwin width → $\Delta W = 2$

$$\omega = \frac{2|\chi_{hr}|}{\sin 2\theta_{BK}} \propto |F_h|$$

Crucial for energy resolution and throughput!

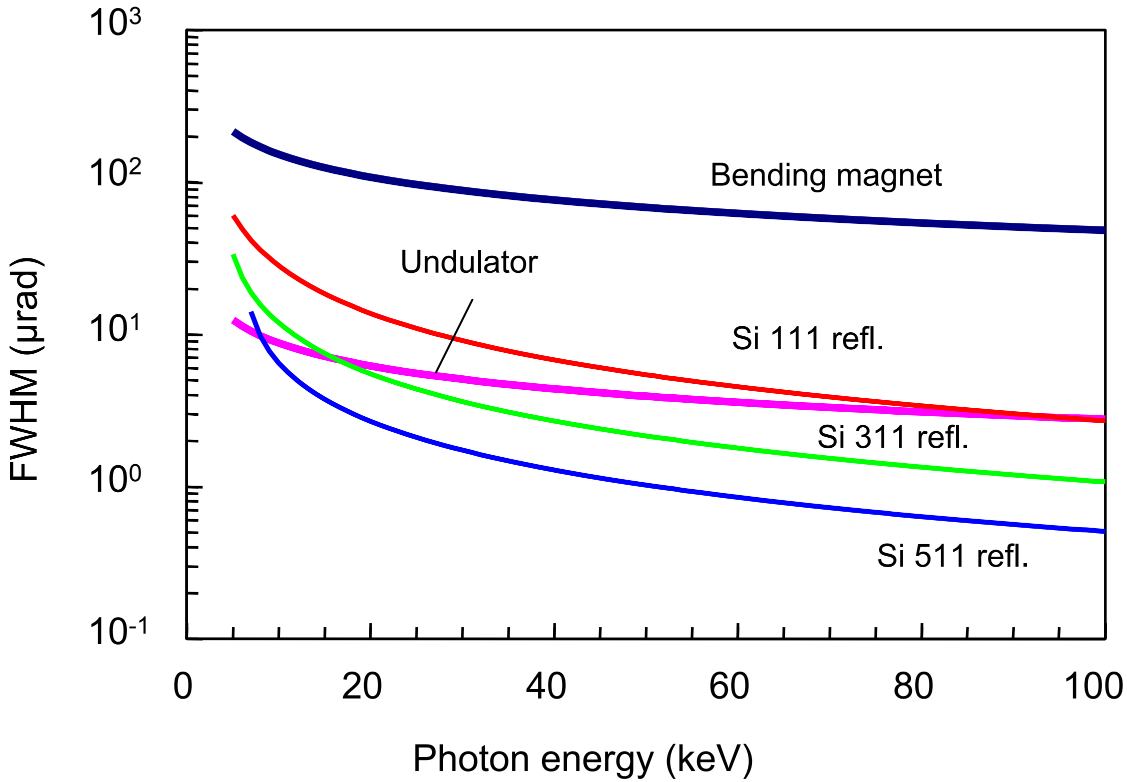
Intrinsic rocking curve for silicon

For Bragg case, with absorption, and thick crystal:



- Darwin width of 0.1～100 μrad
- Peak ~1 with small absorption

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)

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

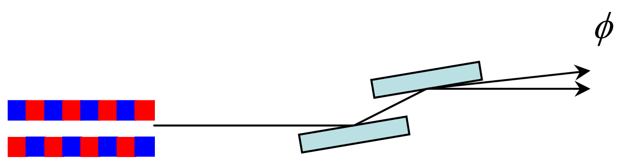
Divergence of undulator radiation ~ diffraction width

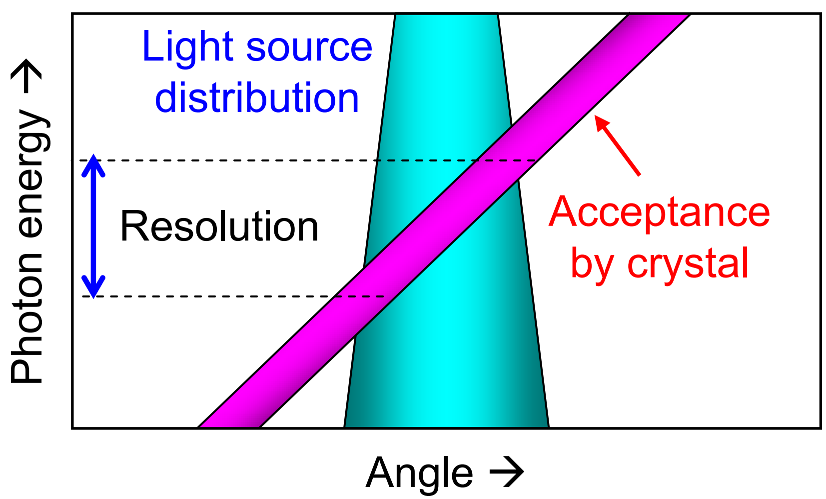
Energy resolution

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

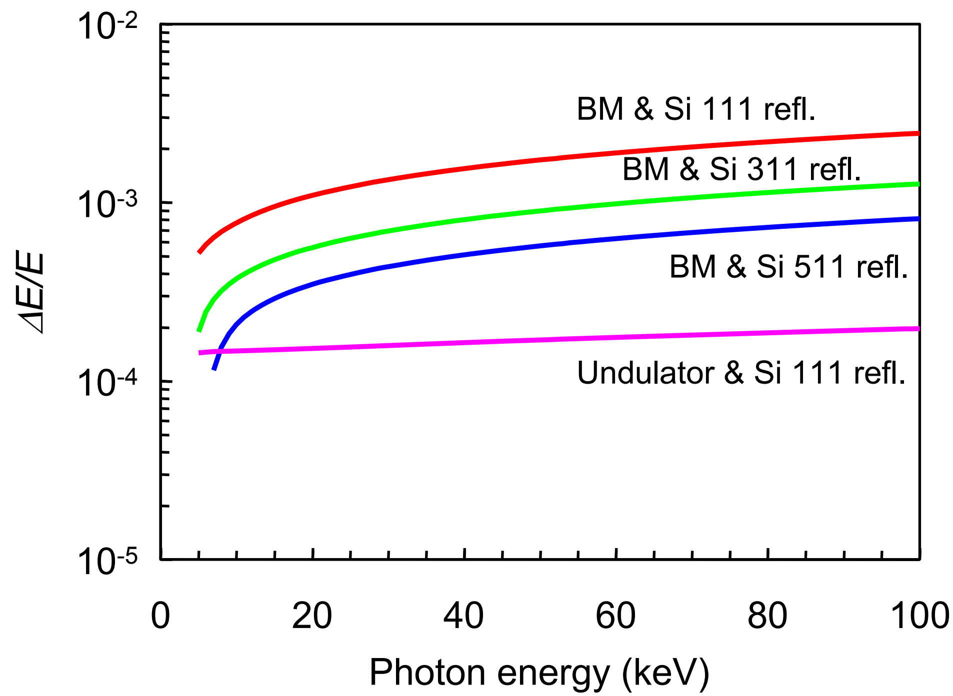
Ω: source divergence,

ω: diffraction width



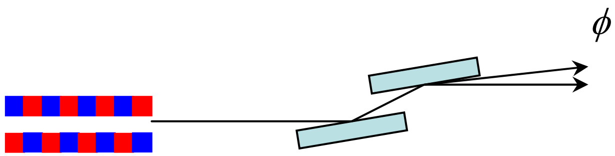


Angle-energy diagram
(DuMond diagram)



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

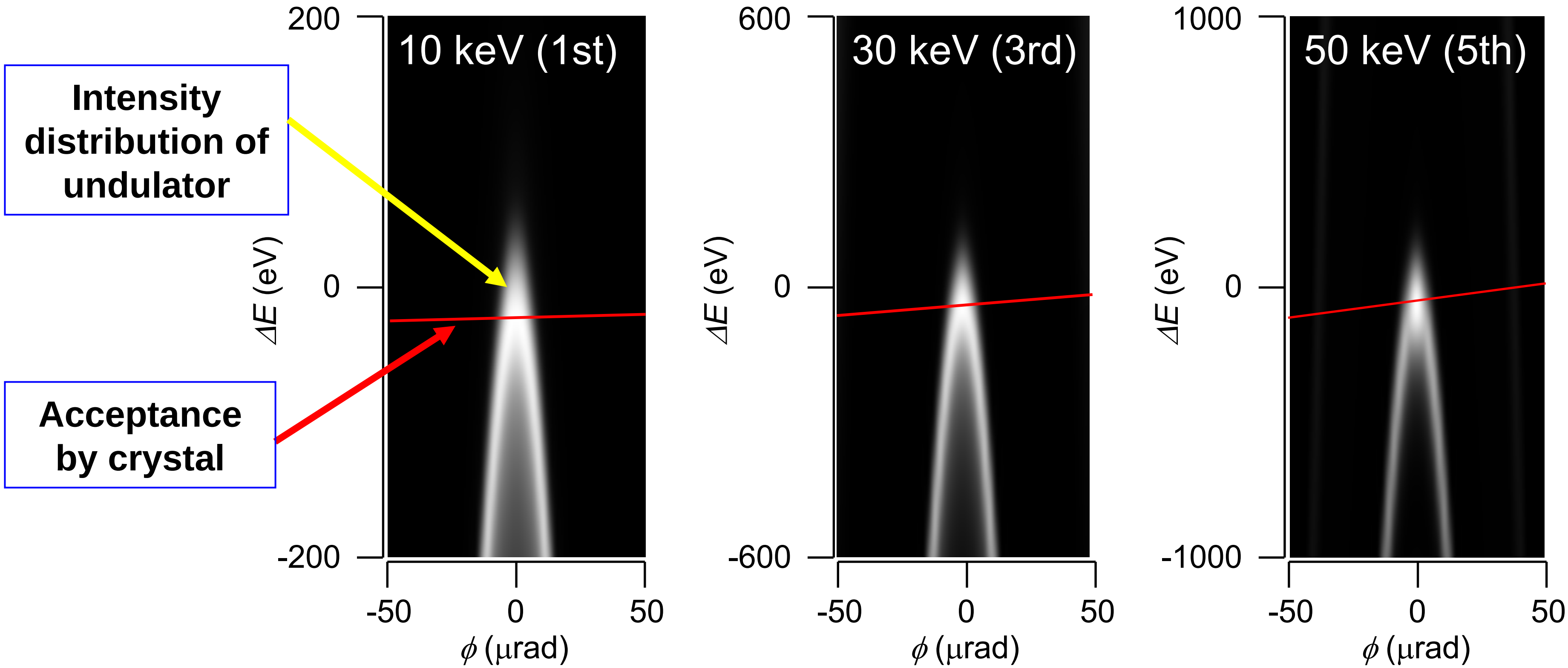
DuMond diagram: undulator ~ DCM



SPring-8 standard undulator

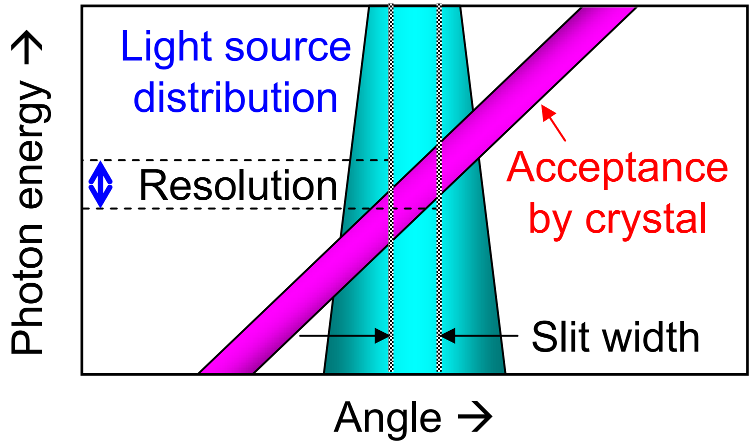
(λu= 32 mm, N= 140, K= 1.34, E_{1st}= 10 keV)

+ DCM (Si 111 refl.)

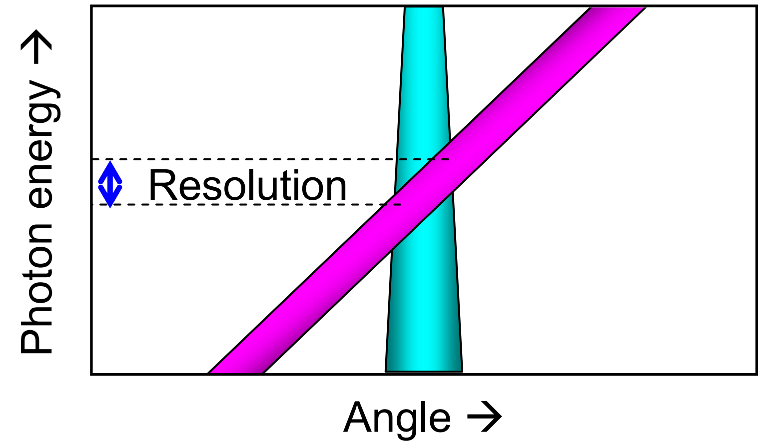


Wider slit increases unused photons (power) on the monochromator !

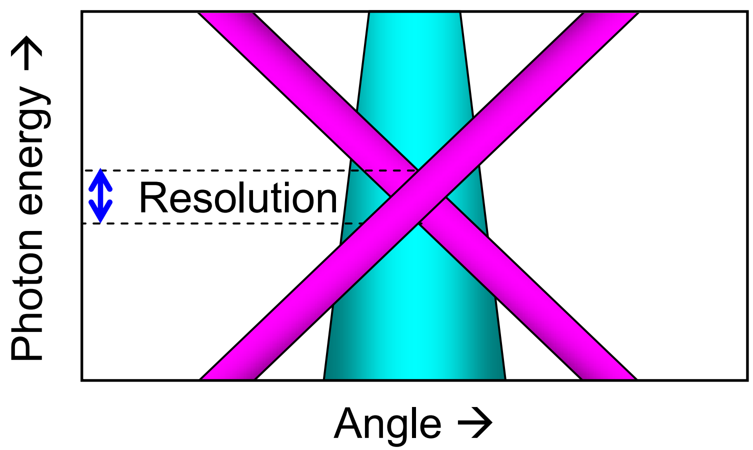
Improvement of energy resolution



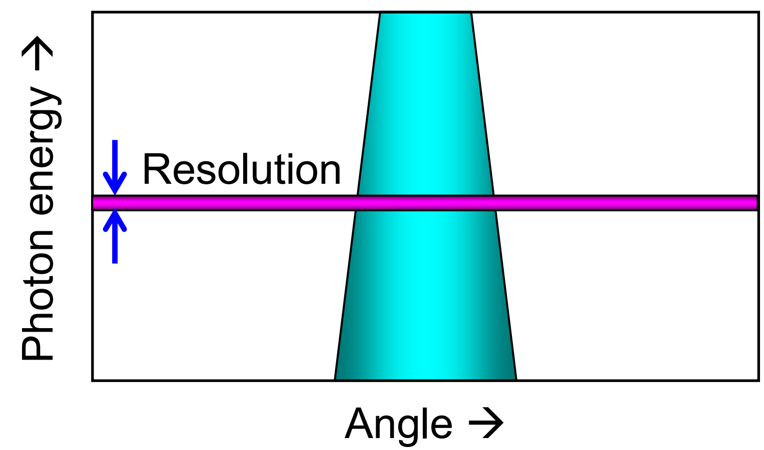
(A) Collimation using slit



(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

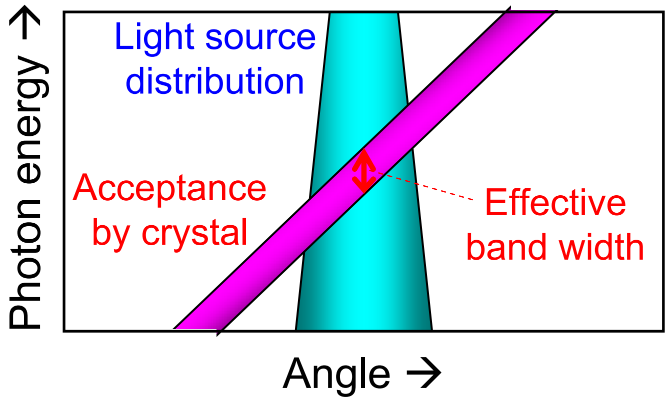
Photon flux (throughput) after monochromator can be estimated using effective band width:

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.

Darwin width → energy width

Starting with Darwin width and neglecting anomalous scattering factor *f'*

$$\chi_{hr} \propto \lambda^2 f_0(d_{hkl})$$

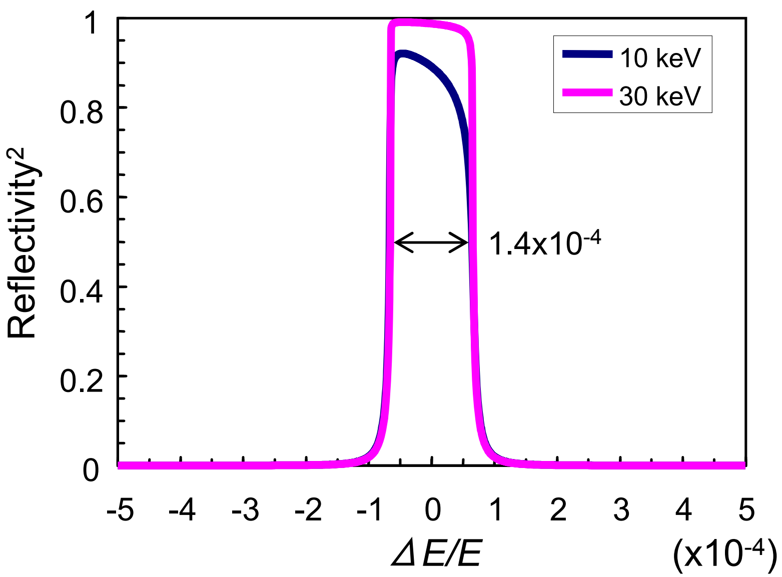
$$\frac{\Delta\lambda}{\lambda} = \omega \cot\theta_B = \frac{2|\chi_{hr}|}{\sin 2\theta_B} \cot\theta_B$$

$$\frac{\Delta\lambda}{\lambda} = \frac{|\chi_{hr}|}{\sin^2\theta_B} = 4 d_{hkl}{}^2 \frac{|\chi_{hr}|}{\lambda^2}$$

Energy width:

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

Independent of photon energy



e.g. for Si 111 refl. DCM case

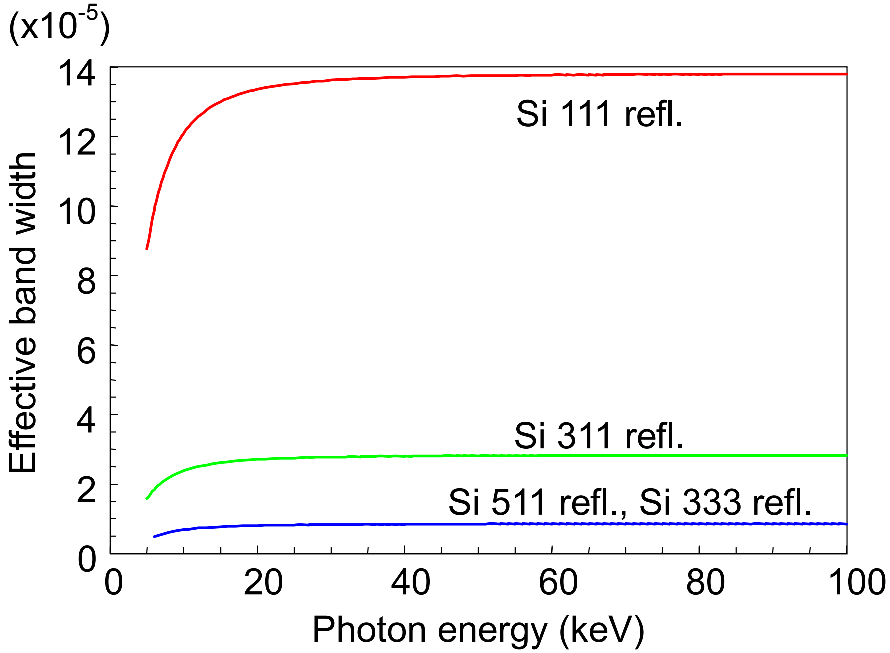
Note relative energy width is constant.

Effective band width (Integrated intensity)

For double-crystal monochromator

$$\left(\frac{\Delta E}{E}\right)_{\text{Eff}} = \frac{|\chi_{hr}|}{2\sin^2\theta_{\text{BK}}} \underline{\int R(W)^2 dW}$$

= ~2



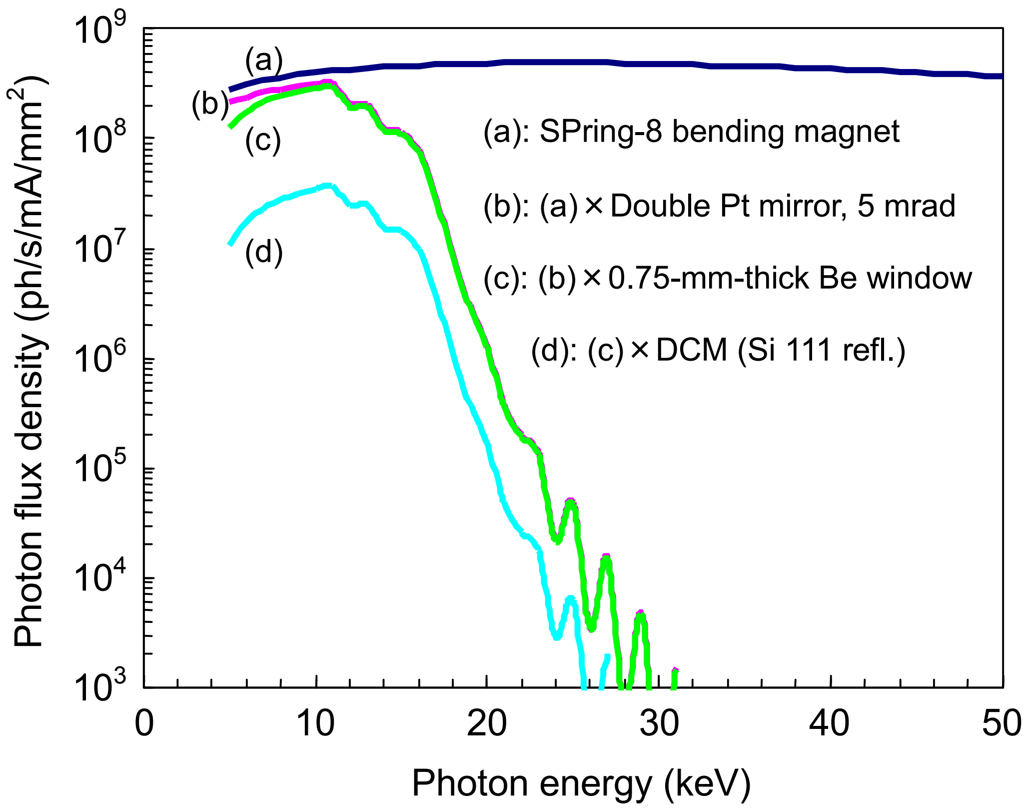
Effective band-width is obtained

by integration of rocking curve.

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

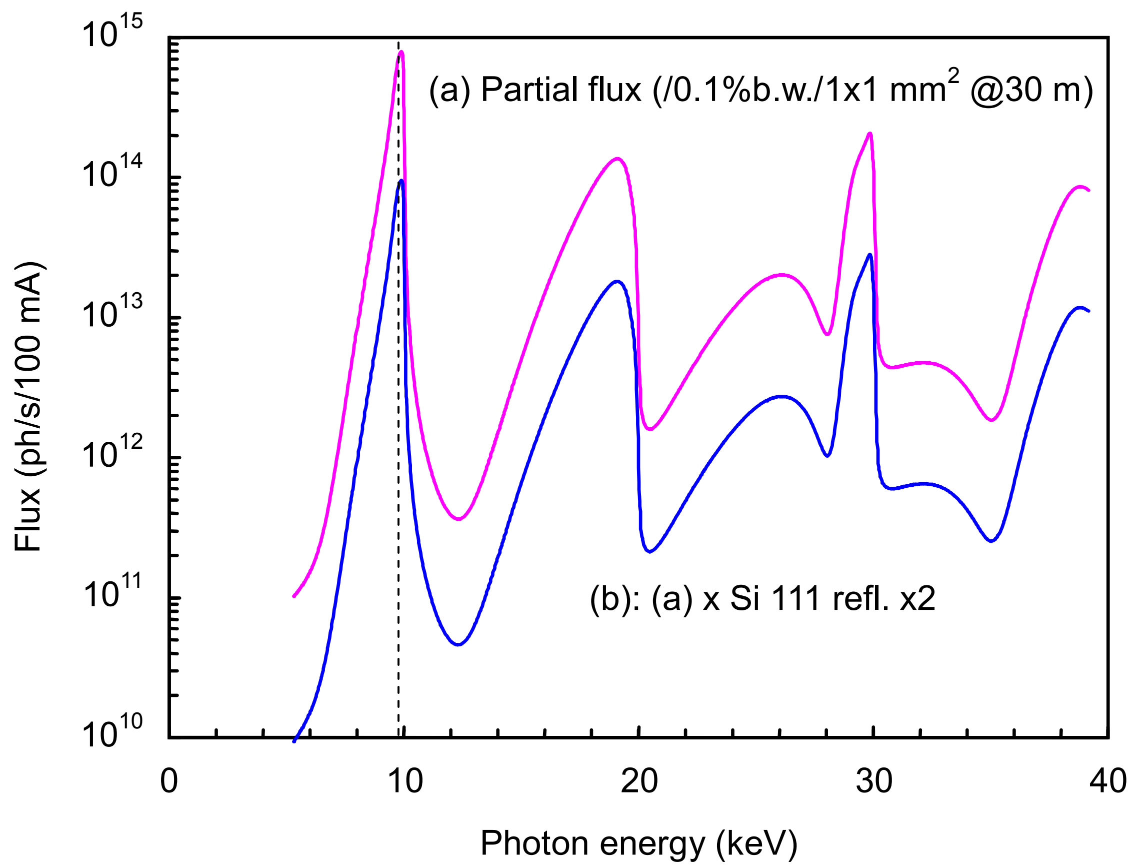
When you need resolution → Higher order (Si 311, Si 511 refl,..)

Photon flux at bending magnet beamline



Example of photon flux estimation at bending magnet beamline BL02B1. (Photon flux density at 50 m from the source)

Photon flux at undulator beamline



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

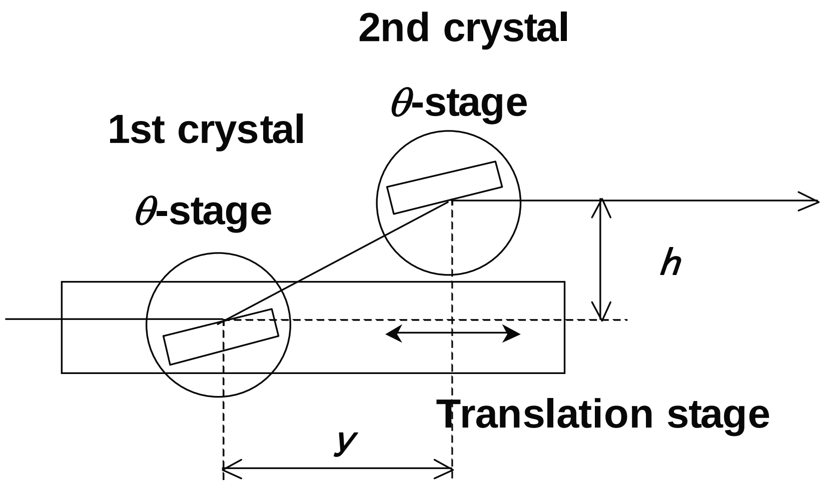
Double-crystal monochromator

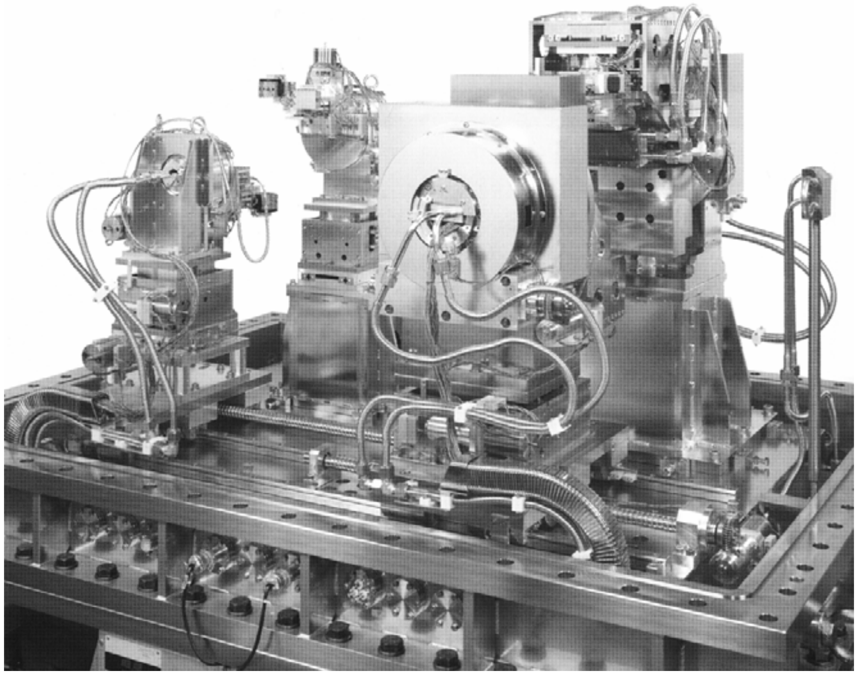
Fixed-exit operation for usability at experimental station.

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

Precision, stability, rigidity,...

θ_1 + translation + θ_2 computer link





SPring-8 BL15XU

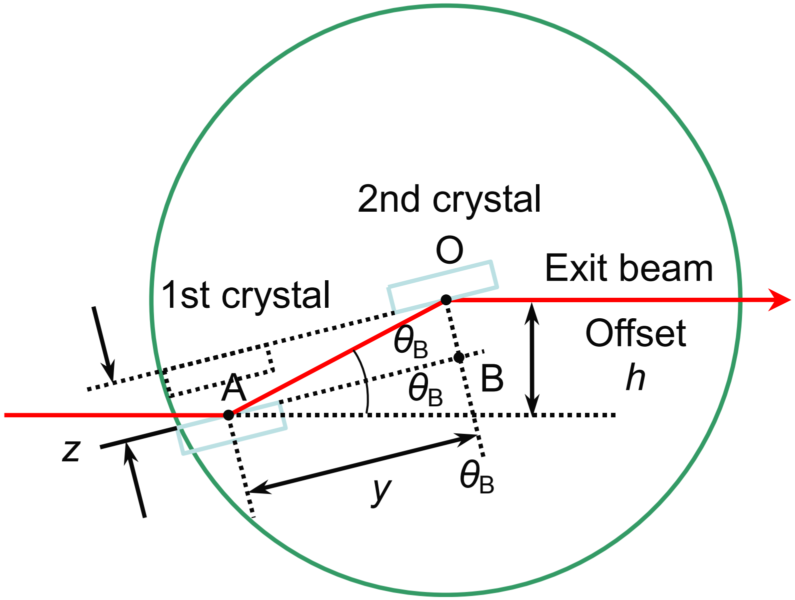
SPring-8 information Vol. 5, No.1 (2000)

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

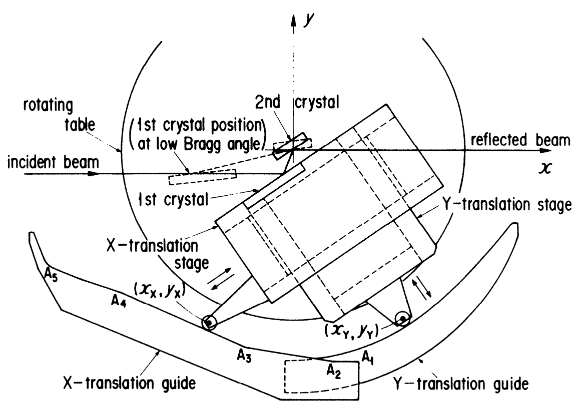
Large offset, long-stroke translation

Difficulty of adjustment between 1st and 2nd crystal

θ + two translation (KEK-PF)



h= 25 mm, θ_B= 5~70°



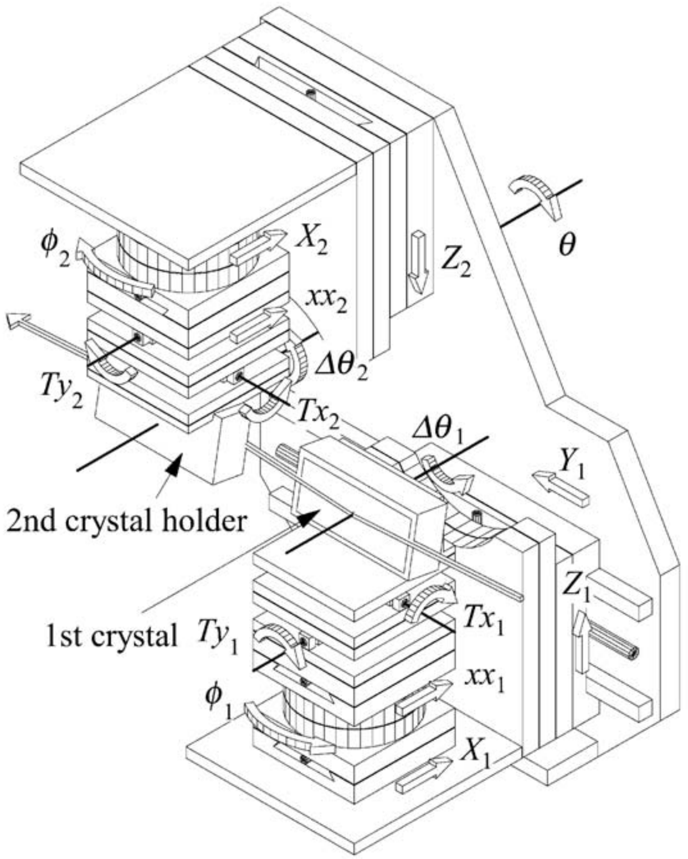
Two cams for two translation-stages

Rotation center at 2nd crystal

PF BL-4C..

Matsushita et al., NIM A246 (1986)

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)

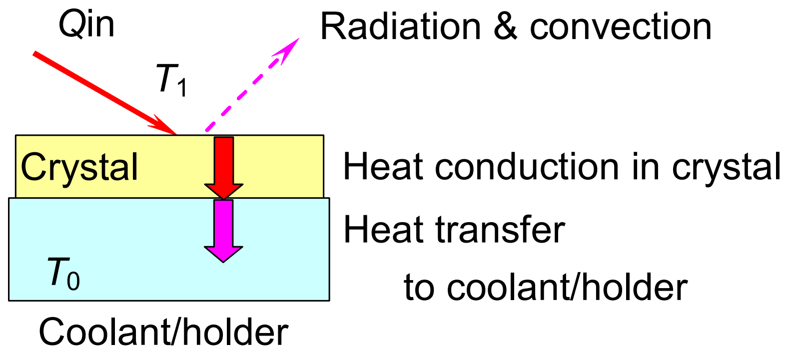
α: thermal expansion coefficient

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)	$2.5\text{x}10^{-6}$	$-5\text{x}10^{-7}$	$1\text{x}10^{-6}$
κ / α $\text{x}10^{6}$	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

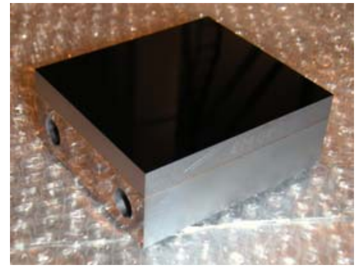
→ or Indirect cooling of IIa diamond crystal ← S-1

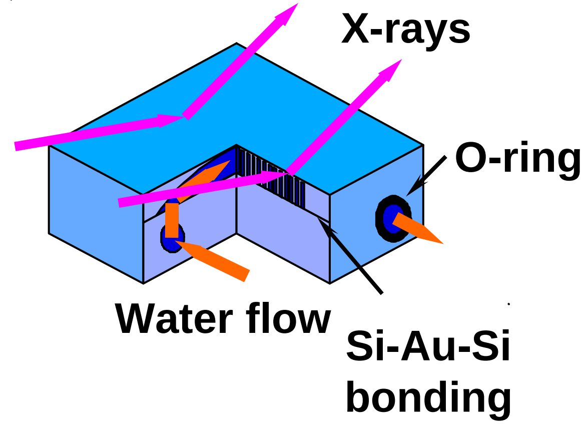
Crystal monochromator at SPring-8

<Bending magnet beamline>

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

Fin crystal direct-cooling - (S2)



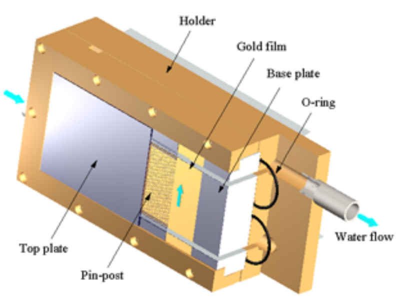


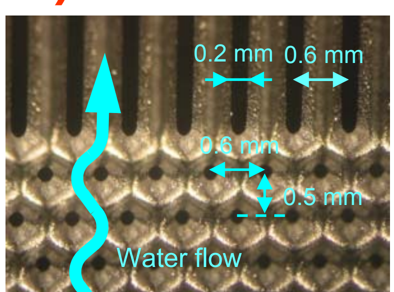
<Undulator beamline>

Linear undulator, N= 140, λu= 32 mm

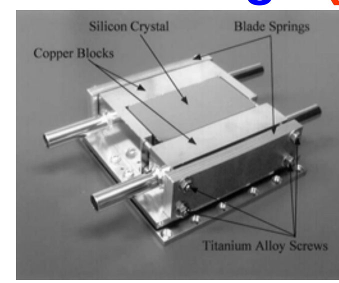
Power & power density: 300~500 W , 300~500 W/mm^2

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





b) Silicon cryogenic cooling - (S1)



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

Mirror

- Higher harmonics rejection

- Bent mirror for focusing/collimation

- Figured mirror for micro~nanobeam

Mirror quality

Mirror quality must be considered.

→ Micro-roughness

- Reduction of reflectivity
- Lower-energy shift of critical energy
- Diffuse scattering

Optical (Zygo) range (<1 mm): ~ 0.3 nm rms or less

AFM range (<1 μm): ~ 1 nm rms or less

→ Insufficient coating

- Reduction of reflectivity
- Lower-energy shift of critical energy

Should be ~100%

→ Slope error

- Beam shape deformation
- Wave-front distortion
- Flux density loss

LTP range (<1 m): ~1 μrad or less

Mirror reflectivity

Mirror reflectivity for sigma-polarization:

$$R = \left| \frac{k_{iz} - k_{tz}}{k_{iz} + k_{tz}} \exp(-2k_{iz}k_{tz}\sigma^2) \right|^2$$

$$k_{iz} = \frac{2\pi}{\lambda}\cos\theta,\ k_{tz} = \frac{2\pi}{\lambda}\sqrt{n^2 - \cos^2\theta}$$

k_{iz}, k_{tz}: Normal components of incidence and transmitted wave vectors

n: complex index of refraction

θ: glancing angle

σ: high-spatial-frequency roughness (AFM region)

Surface roughness must be considered
around critical energy (angle).

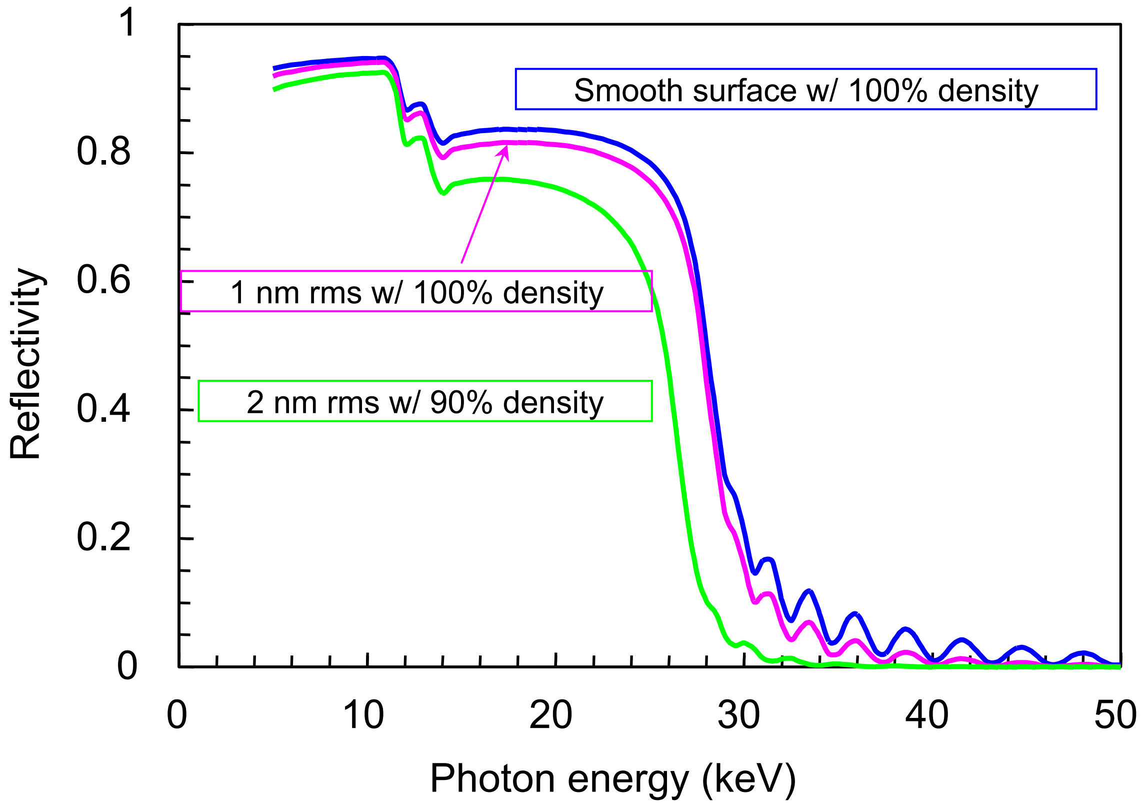
Effect of roughness

e.g. reflectivity of Pt mirror

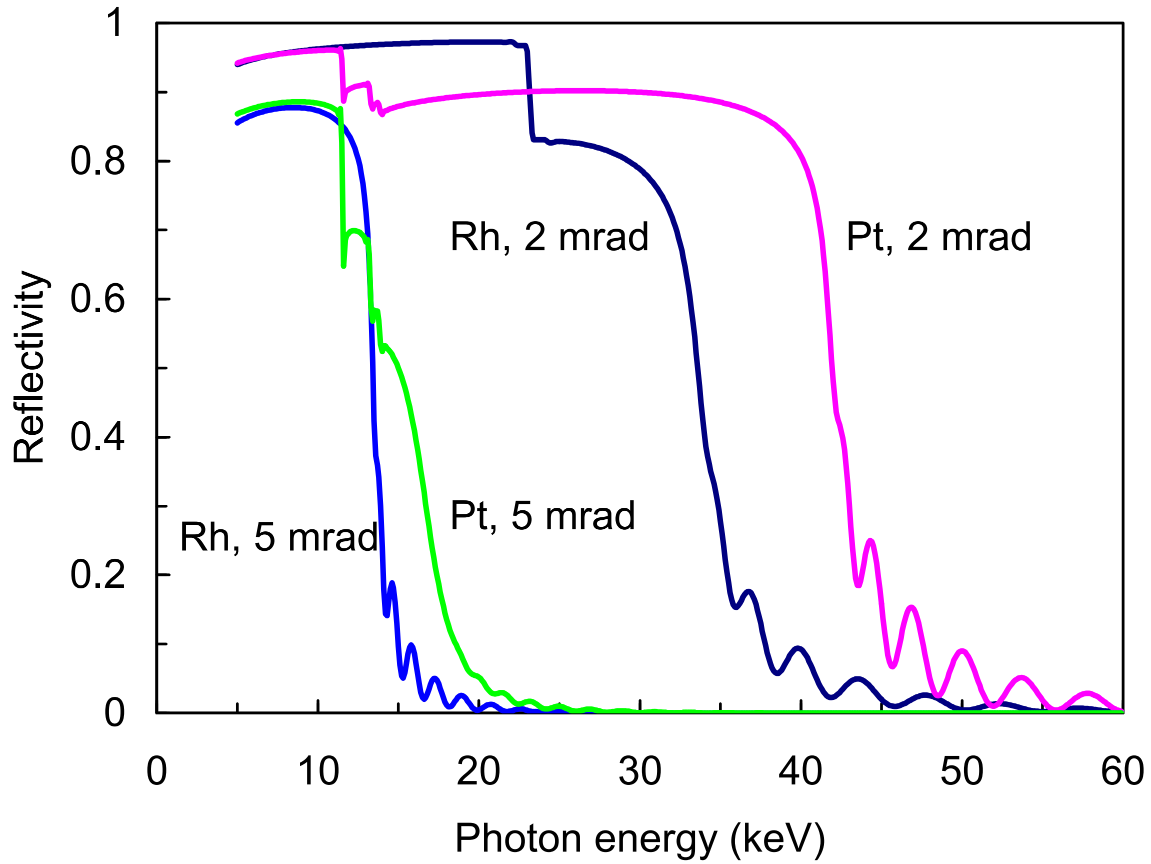
s-polarization

Glancing angle: 3 mrad

Film thickness: 50 nm



Example of mirror reflectivity



Thickness 50 nm, roughness 1 nm

Material, glancing angle, length

- **Material**
  Si, SiC for white radiation
  SiO_2, Glass,.. for monochromatic beam
- **Coating**
  Pt, Rh, Ni,...
  Depending on energy, reflectivity, absorption edges,..
- **Glancing angle**
  2~10 mrad (For SPring-8 X-ray beamline)
  Depending on energy, reflectivity, absorption edges,..
- **Mirror length**
  400 mm~1 m (For SPring-8 X-ray beamline)
  Depending on the beam size and glancing angle
  e.g. 100 μrad × 50 m/5 mrad= 1 m

Focusing with mirror

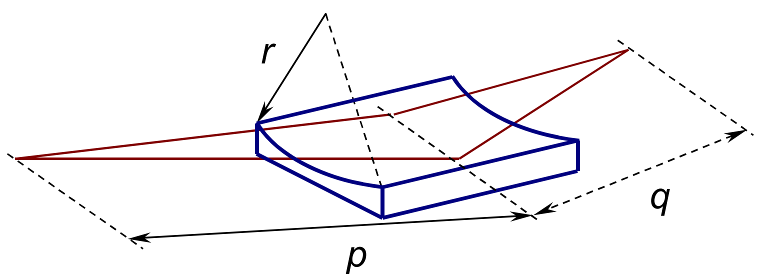
For beam focusing or collimation, we need;

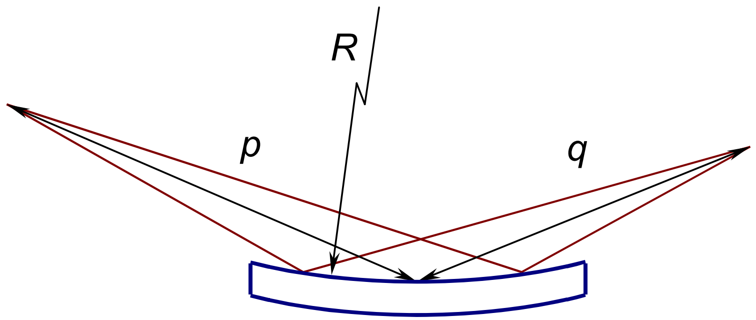
elliptical mirror, ellipsoidal mirror, parabolic mirror, paraboloidal mirror,...

➔We can approximate by bending:

flat → meridional cylinder,

sagittal cylinder → toroidal,...





Sagittal focusing

w/ sagittal cylinder

$$r = \frac{2pq}{p+q}\sin\theta$$

Meridional focusing

w/ meridional cylinder

$$R = \frac{2pq}{(p+q)\sin\theta}$$

e.g.) θ= 5 mrad, p= 40 m, q= 10 m

r= 80 mm, R= 3.2 km

※ When $q \to \infty$

We obtain parallel beam:

$$r = 2p\sin\theta$$

$$R = 2p/\sin\theta$$

SPring-8 standard mirror support

For SPring-8 X-ray beamline

- **For undulator beamline**
  400-mm-long, vertical deflection, plane
  700-mm-long, horizontal deflection, plane

- **For bending magnet beamline**
  1-m-long, vertical deflection,
  plane/cylindrical

Options

- Bender
- Indirect water-cooling (side cooling)

High heat-load 1st mirror for undulator beamline is installed with cryogenic cooling or water-cooling at some BL in SPring-8.

For 400-mm-long mirror,
Vertical deflection, w/ bender

For 1-m-long mirror,
vertical deflection,
w/ bender, Indirect water-cooling

Focusing with mirror

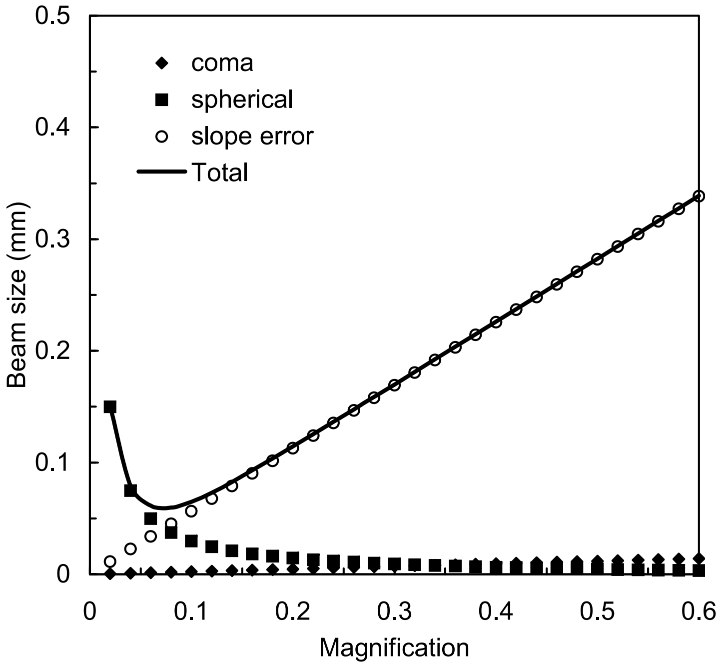
Beam size using meridional cylinder mirror:

$$F_{coma} = 2.35\Sigma M$$

$$F_{spherical} = \frac{3L^2\theta(1-M^2)}{16pM}$$

$$F_{Fabrication} = 2\times 2.35\Delta_{fabrication}Mp$$

$$F_{total} = \left[\left(F_{coma}+F_{spherical}\right)^2 + F^2{}_{fabrication}\right]^{1/2}$$



e.g.

Σ = 10 μm

L = 400 mm

$\Delta_{fabrication}$ = 3 μrad

θ = 4 mrad

p = 40 m

Σ: source size

M: magnification = q/p

L: mirror length

$\Delta_{fabrication}$: slope error

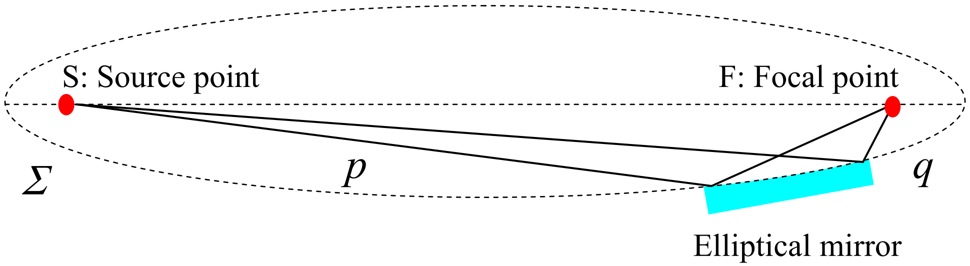
θ: glancing angle

For micro~nonofocusing, we need precisely-polished and large NA elliptical K-B mirror near exp. station.

J. Susini, Opt. Eng. **34**, 361 (1995)

Diffraction-limited focusing

Focusing w/ figured mirror



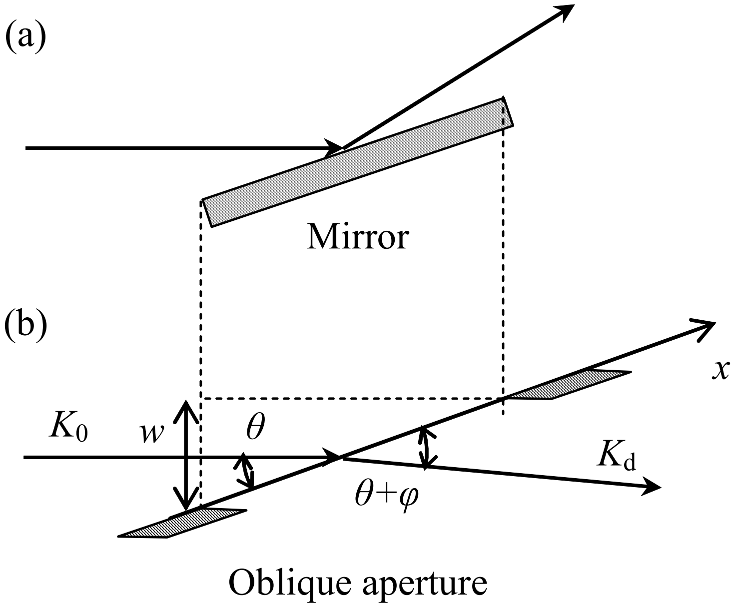
Estimation by oblique aperture model

→ **Angular spread due to Fraunhofer diffraction**

$$FWHM_{\phi} = 2.7831 \frac{\lambda}{\pi w} \approx 0.8858 \frac{\lambda}{L \sin\theta}$$

→ **Spatial spread at *q***

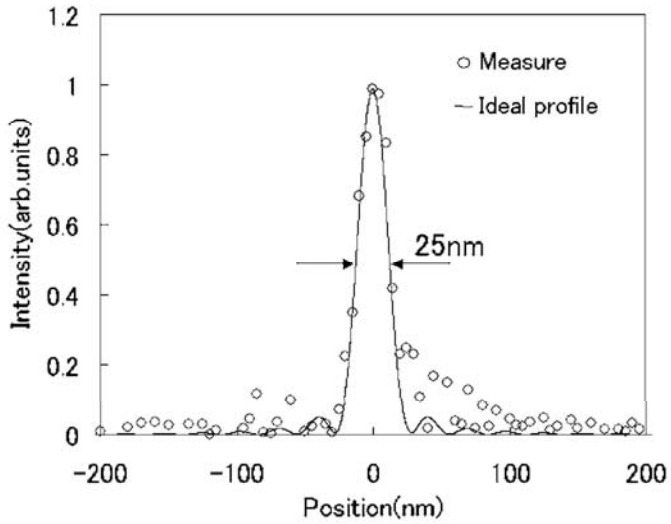
$$FWHM_{X} = 0.8858 \frac{\lambda q}{L \sin\theta}$$



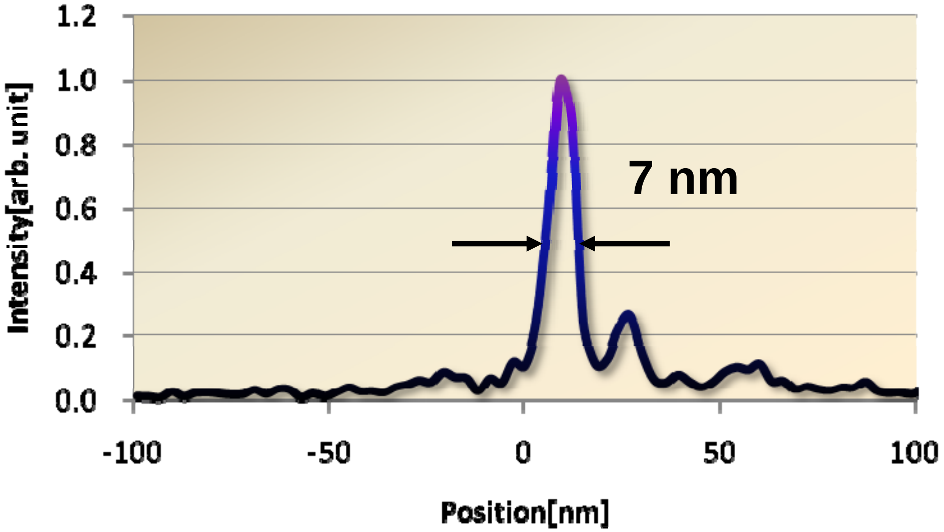
$$FWHM_{X} > \frac{q}{p}\Sigma$$

← diffraction-limited focusing

Diffraction-limited focusing



H. Mimura et al.,
Appl. Phys. Lett. 90, 051903 (2007)



H. Mimura et al.,
Nature physics **6**, 122-125 (2010)).

θ_{ave}= 3 mrad

λ= 0.083 nm (E= 15 keV)

L= 45 mm

q= 50 mm

➔ FWHM ~ 27 nm

θ_{ave}= 7 mrad

λ= 0.062 nm (E= 20 keV)

L= 80 mm

q= 75 mm

➔ FWHM ~ 7.3 nm

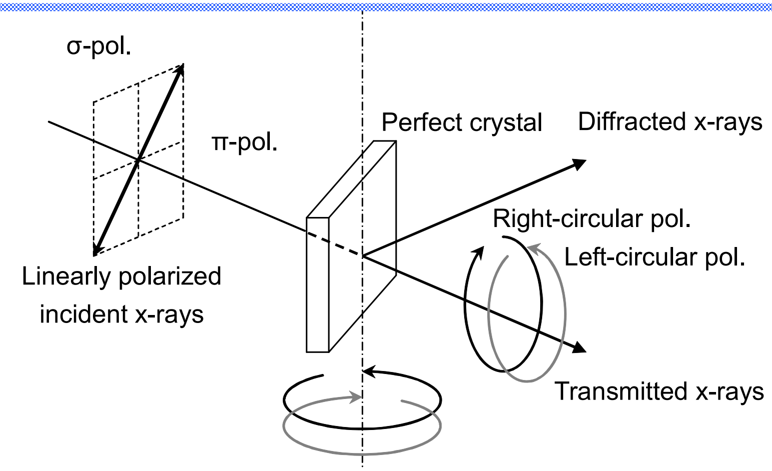
Polarization conversion

Phase retarder is used to convert the polarization for XMCD and other applications.

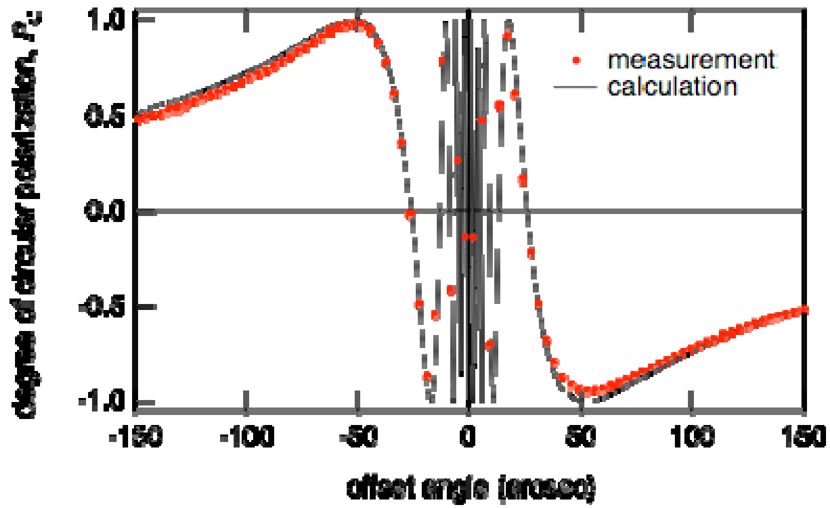
Horizontal polarization → right-/left-circular polarization
Horizontal polarization → vertical polarization
...

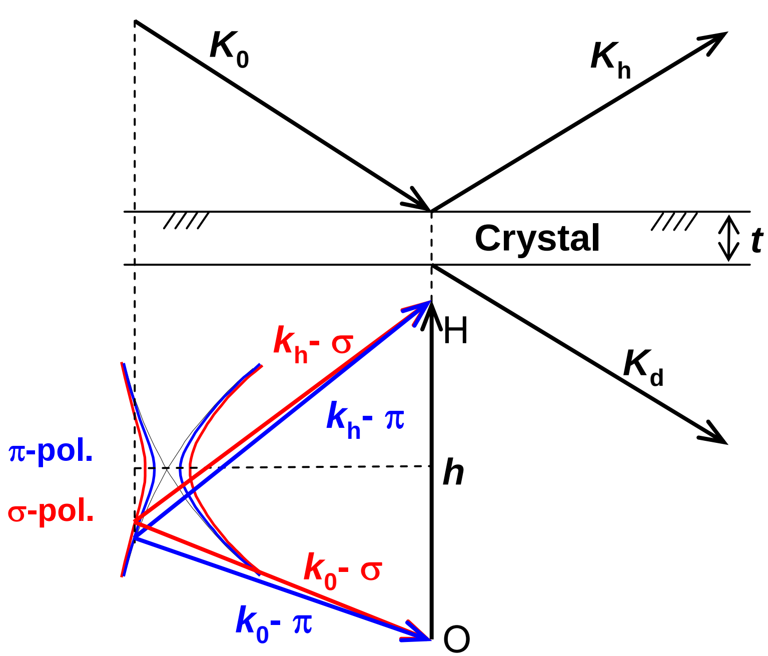
Crystal: IIa diamond,..

Polarization conversion

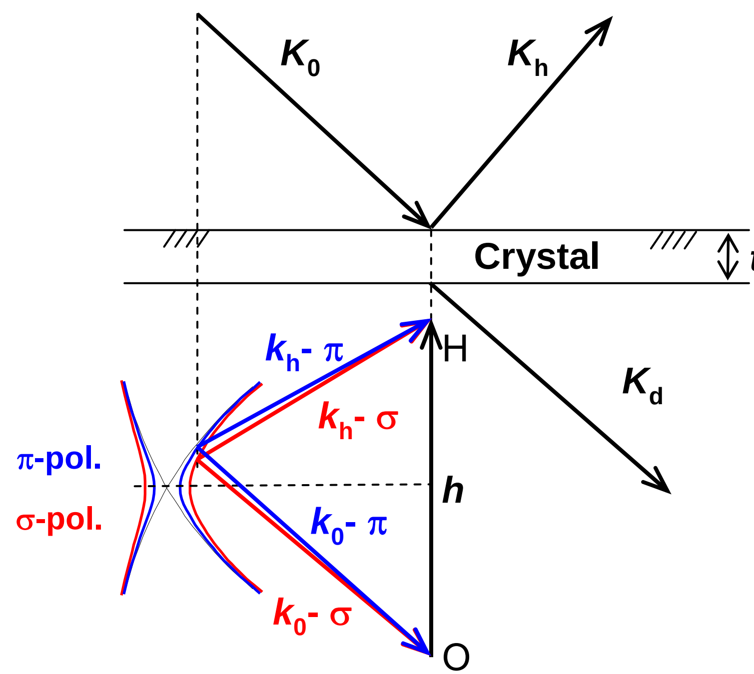


Offset angle of crystal: $\theta_B \pm \Delta\theta$



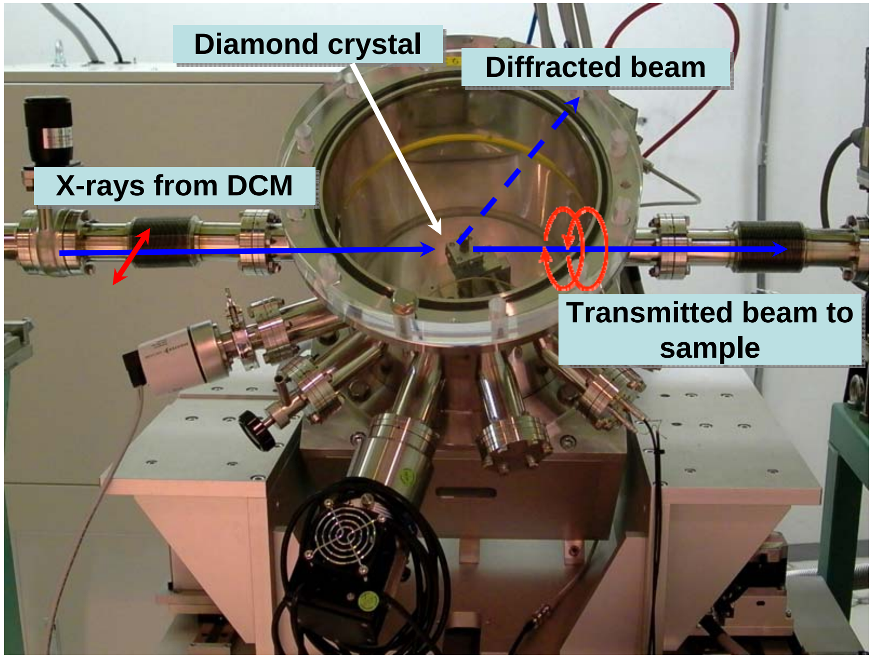


Offset angle (-)

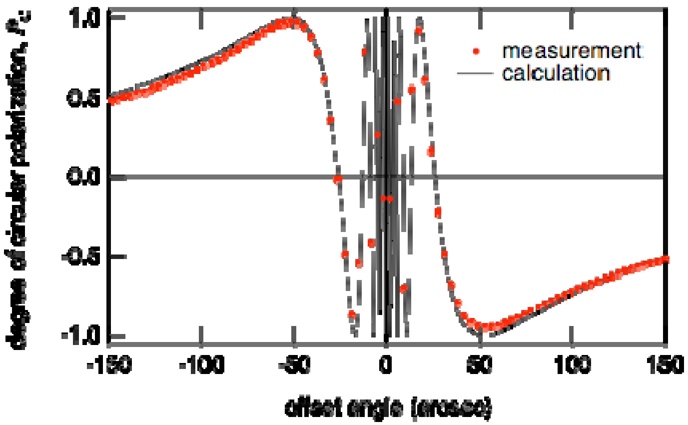


Offset angle (+)

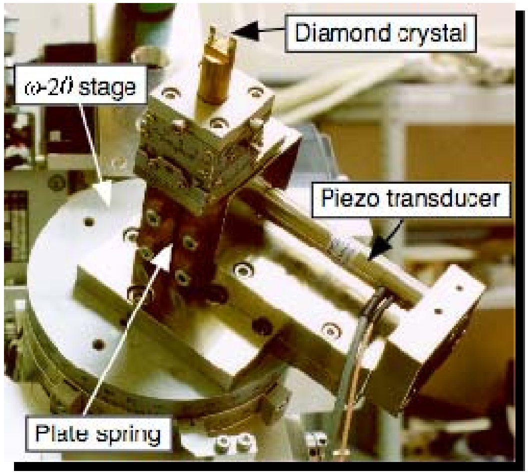
Diamond phase plate system BL39XU



Stages and vacuum chamber of phase retarder



0.45-mm-thick (111) diamond plate



Switcher of phase

Selection of phase plate

Thickness (mm)	Index	Reflection	Energy (keV)	Transmittance (%)
0.34	(111)	111 Bragg	5~5.8	3~7
		220 Laue	5.8~7.5	7~41
0.45	(111)	220 Laue	6~9	5~53
0.73	(111)	220 Laue	8~12	22~65
2.7	(001)	220 Laue	11~16	13~47

Spatial coherence

We need:

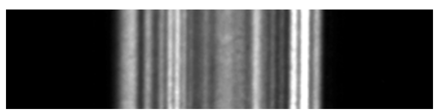
- small source size (σ_s) & long beamline (L)

$$l_{coh} \propto \frac{\lambda L}{\sigma_s}$$

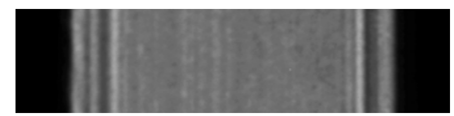
(*depend on machine performance and facility design !*)

- w/ speckle-free optics.

Mirror

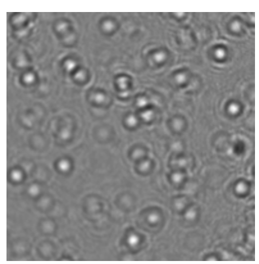


→ultra smooth surface



100 mm

Be window



→void-free & polished

300 μm

e.g. x-ray images using coherent x-rays

Front-end

(1) Vacuum chamber

(with ion pumps,..)

Pressure (10^{-7}～10^{-5} Pa)

(2) Main beam shutter

(MBS)

・Water-cooled absorber

・Beam shutter

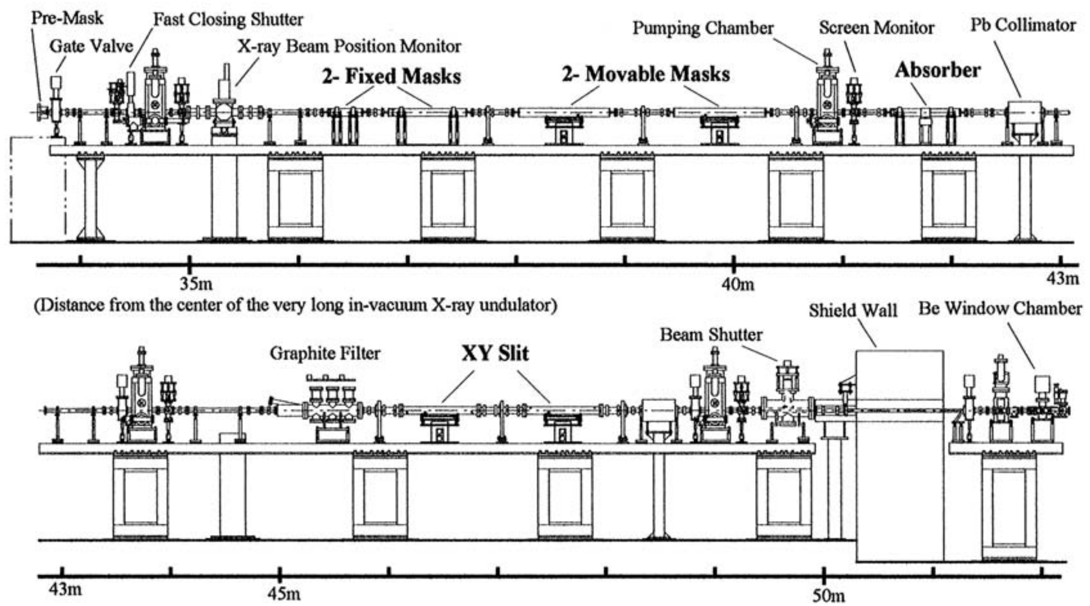
(3) Mask, XY-slit

Spatial power control

(4) Water-cooled Be windows

Protection of UHV

(5) Beam position monitor



e.g. SPring-8 BL19LXU front-end

It reduces source power of 33 kW down to 500 W

for downstream optics

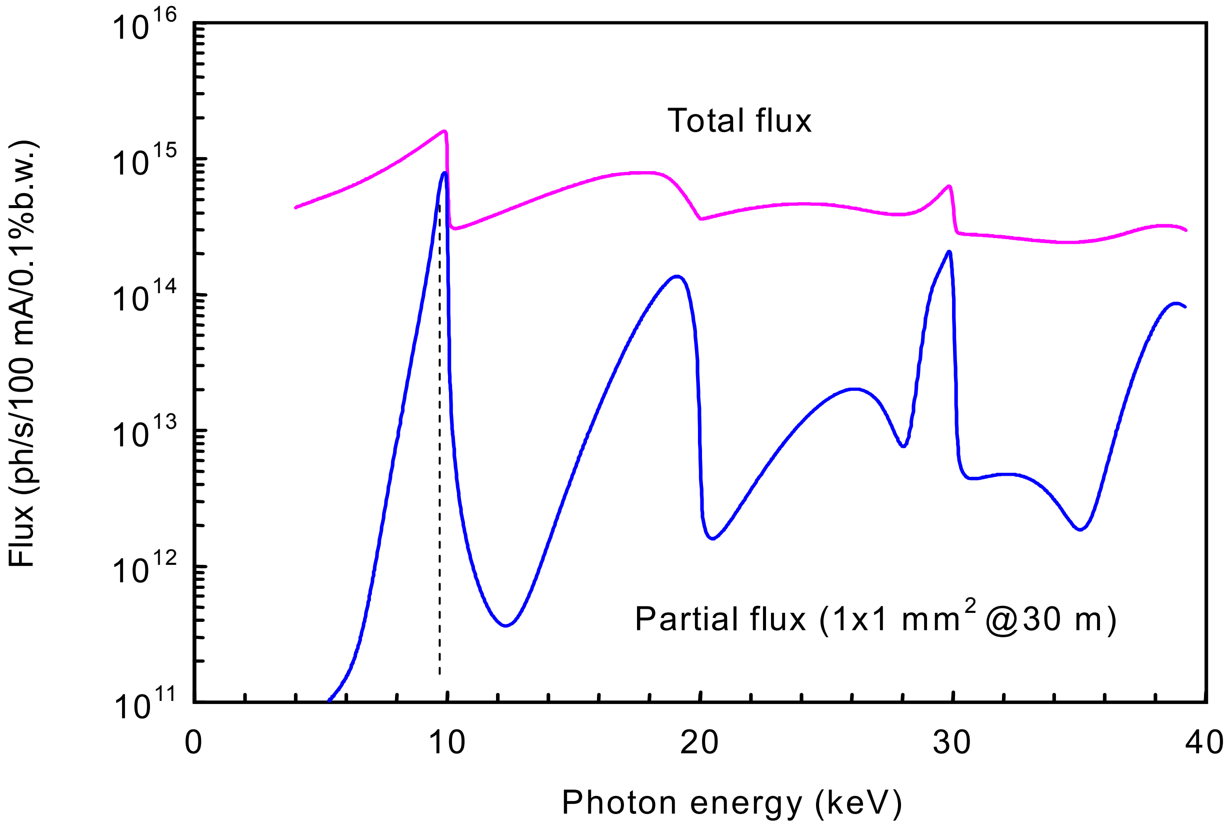
New IXS beamline 43LXU

→ 50 kW to 1.5 kW

Grazing incidence technique w/ GlidCop

→ 10 kW/m

Reduction of power at front-end



e.g. Radiation From standard x-ray undulator λu=32 mm, *N*= 140, fundamental peak of 10 keV

Front-end eliminates the out-of-axis power spatially and reduce the power on the first optical element

Transport channel

e.g. BL14B2

❑ Transport channel components

Exhaustion unit (ion-pump, TMP,..)

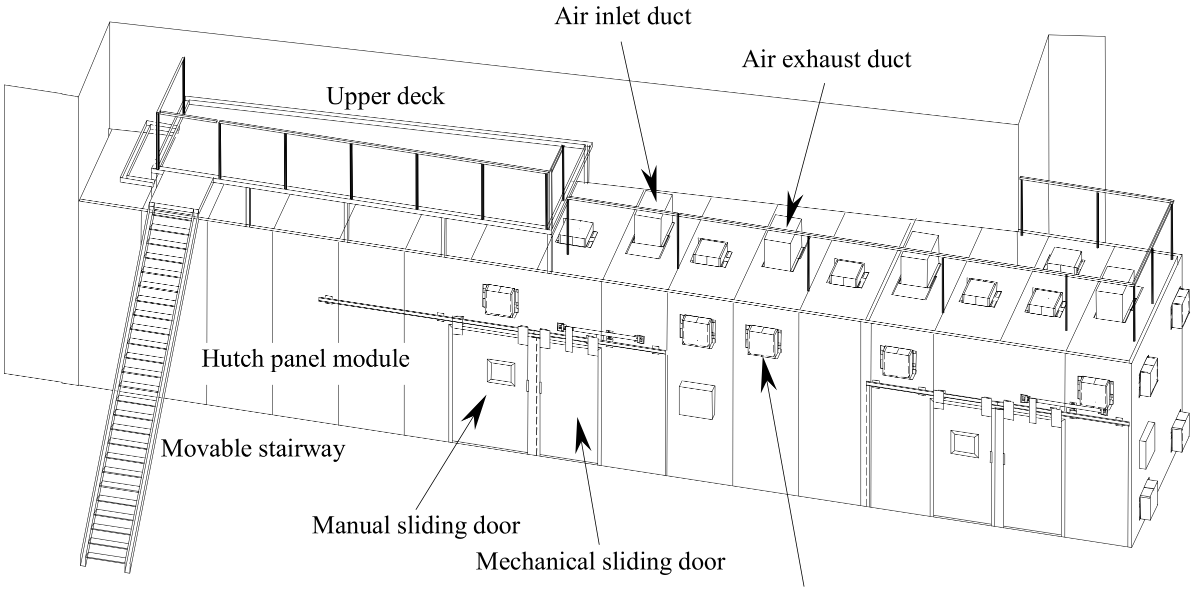
Down stream shutter (W or Pb)

Gamma stopper (Pb)

Beryllium window

Screen monitor

Shielding hutch @SPring-8



❑Optics hutch

contains optics and transport channel components introducing white radiation

❑Experimental hutch

contains experimental station equipments introducing monochromatic beam

・Panel	Steel/ Lead/ steel sandwich structure
・Lead thickness	Depends on the radiation condition (3～50 mm)
・Module	Panel, Door, Cable duct, Air inlet/exhaust duct,...
・Utility	Compressed air, Chilled water, electric power

Other issues on beamline design

- Boundary condition

  Storage ring and tunnel, neighboring beamline,..

- Radiation safety for shielding hutch, shutter,..

  Radiation shielding calculation (EGS4, STAC8,..)

- Control and interlock

  Common scheme in the facility.

  Connection with machine and safety control

- Others

  Utilities: electricity, water, compressed air, air conditioning.

  Environmental: vibration of floor, temperature of air,..

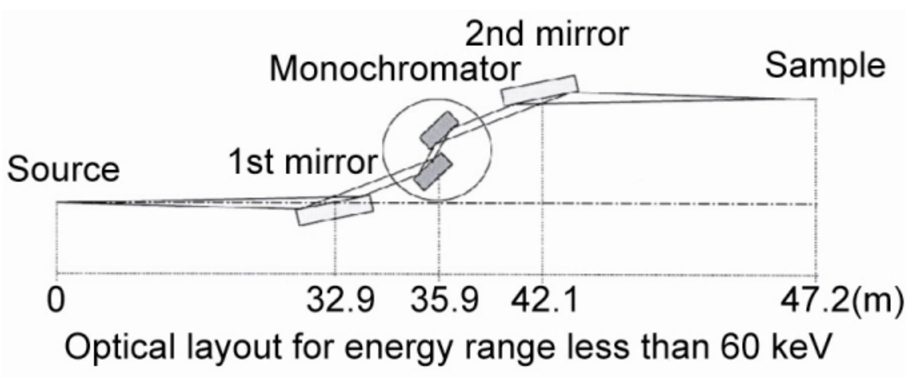
Cooperation with specialists in the facility is crucial !

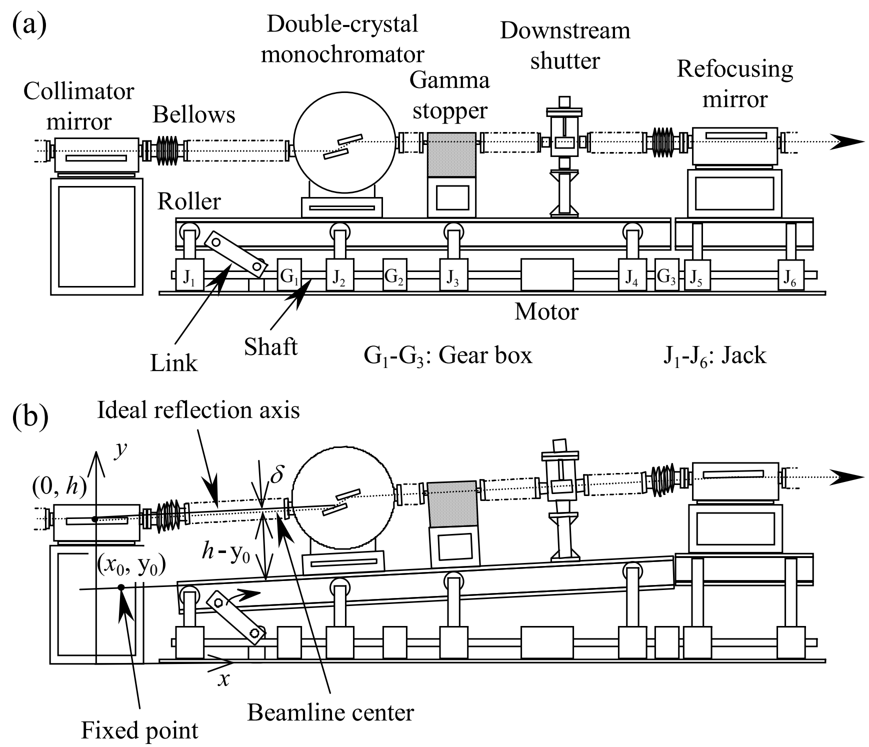
Example of x-ray beamline

- SPring-8 case -

XAFS & single crystal diffraction

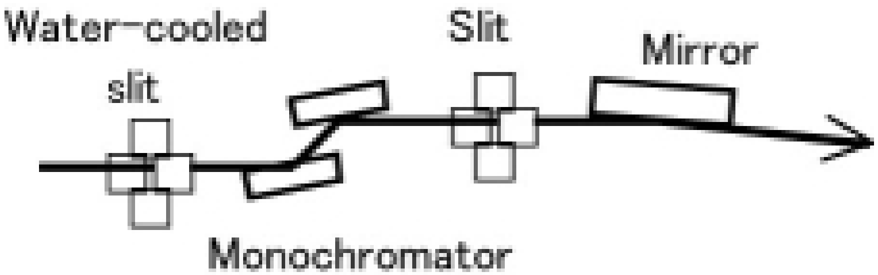
- Bending magnet
- Collimator mirror,
  + DCM,
  + refocusing mirror

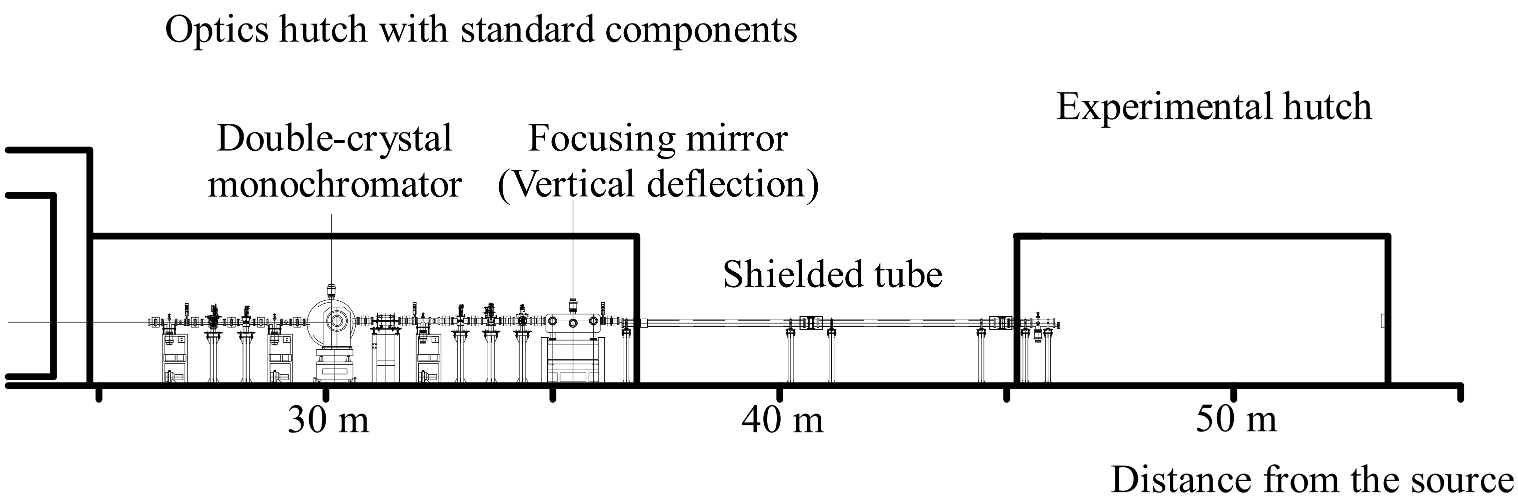




Protein crystallography

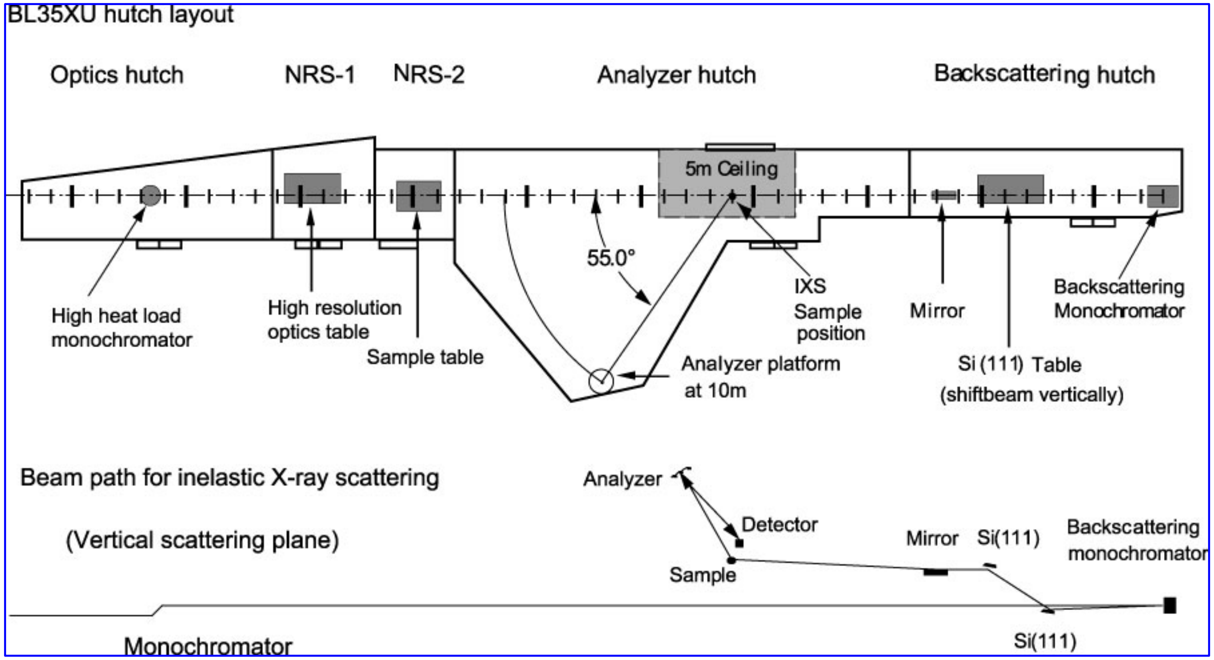
- Bending magnet
- DCM + focusing mirror

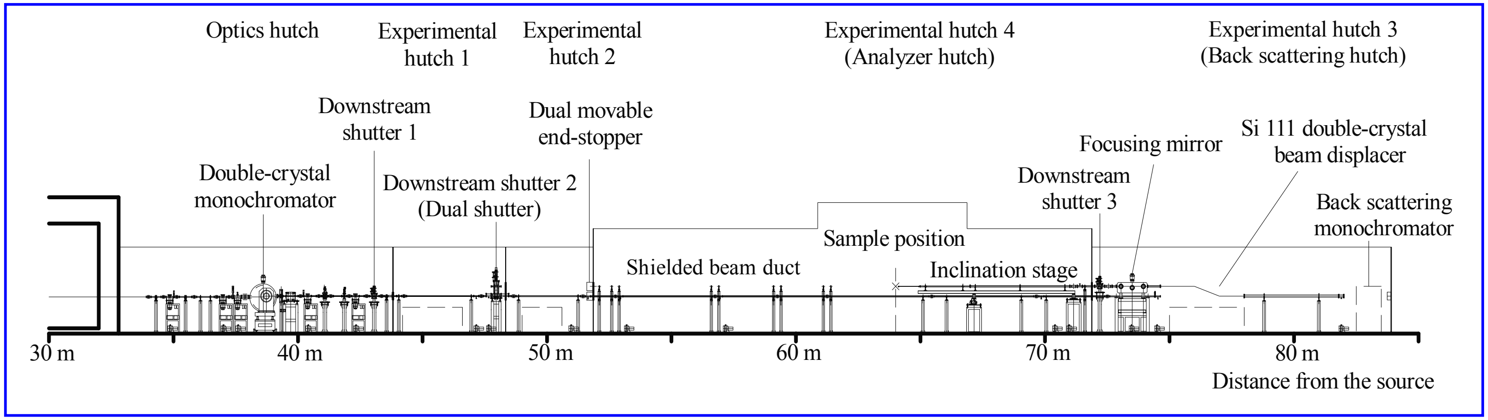




High resolution inelastic scattering

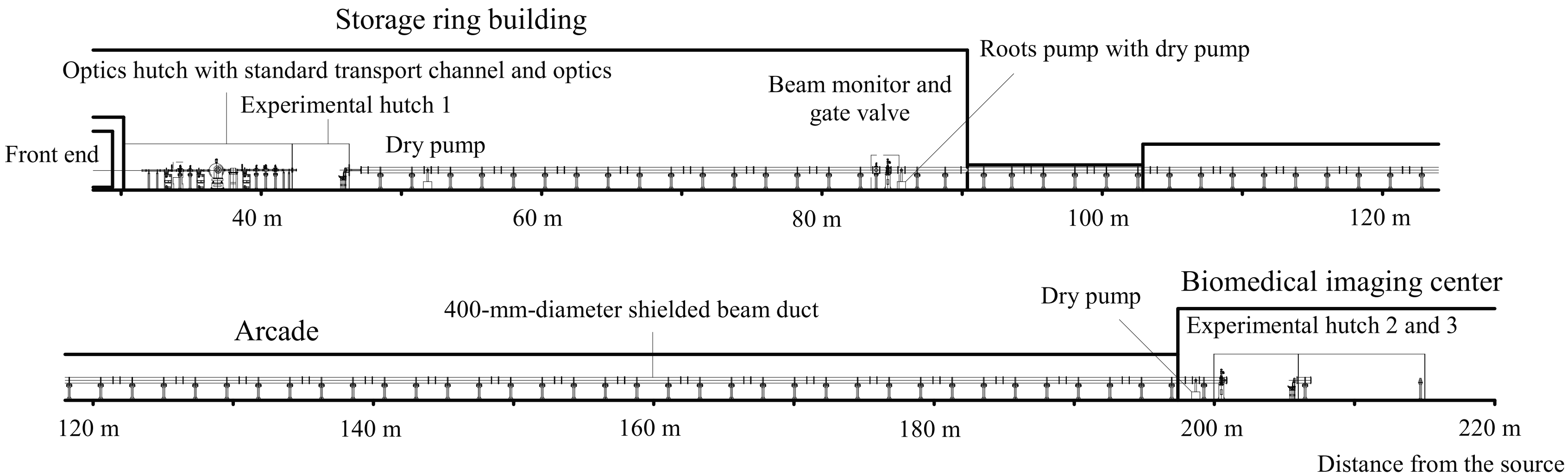
- Undulator
- DCM + back-reflection monochromator & analyzer (w/ ~meV resolution)

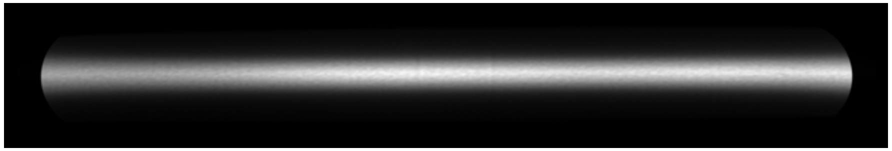




200-m-long beamline

- Bending magnet
- DCM

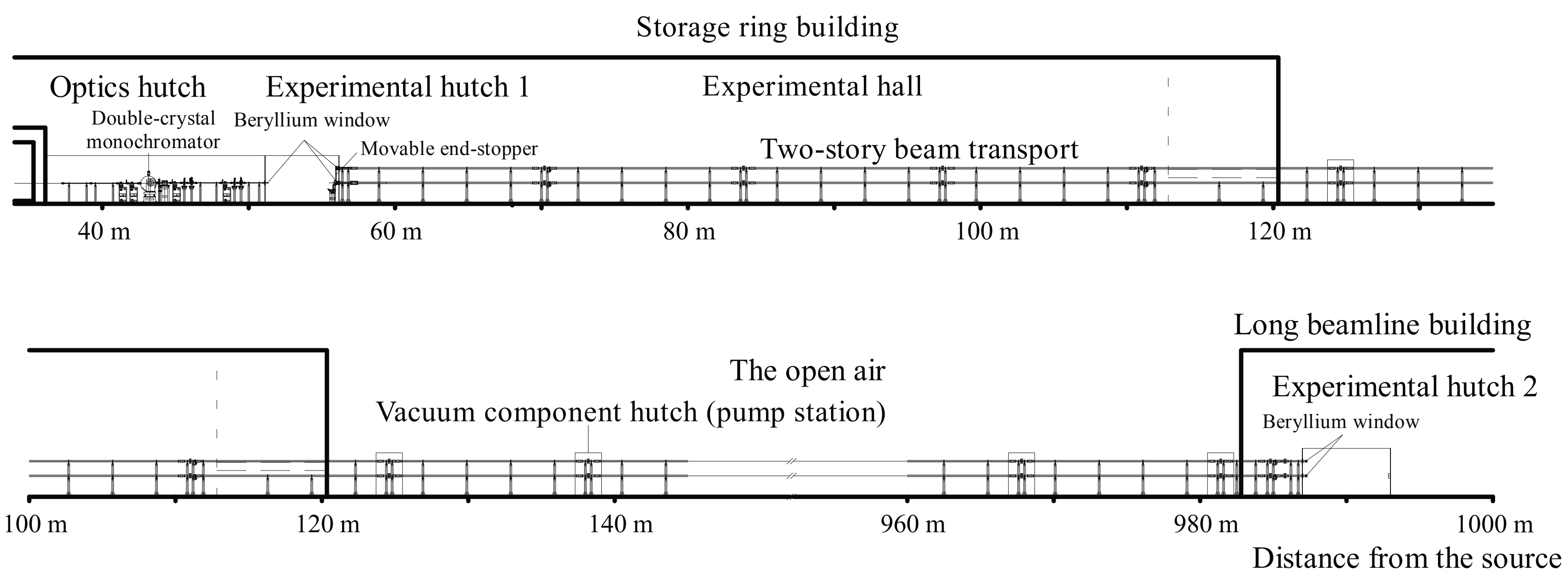




300-mm-wide beam at end-station

1-km-long beamline

- Undulator
- DCM + tandem mirror



Wide and spatially-coherent X-rays at 1-km end station

Summary

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

  w/ light source, monochromator, mirror, and other components.

- 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,...), shielding calculation,...

- Standardization of well-designed components helps beamline construction and maintenance, saves the cost, man-power, and other resources.

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

Thanks to:

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Thank you for your attention.