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School on Synchrotron and Free-Electron-Laser Sources and their Multidisciplinary Applications

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X-ray monochromators and beamline design

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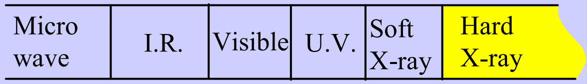
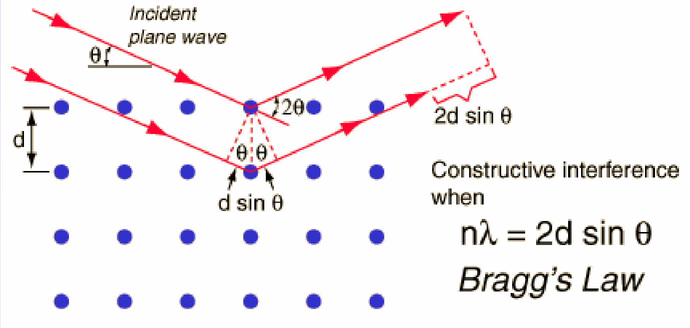
Monochromators



Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

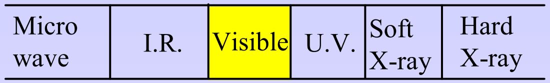
Crystal



Constructive interference when

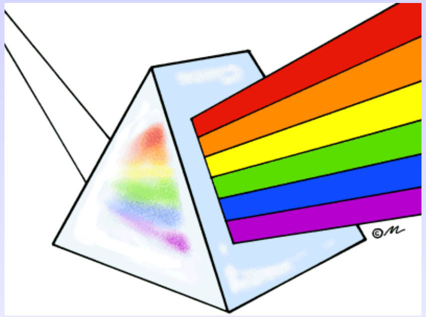
$n\lambda = 2d \sin\theta$

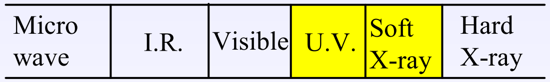
Bragg's Law



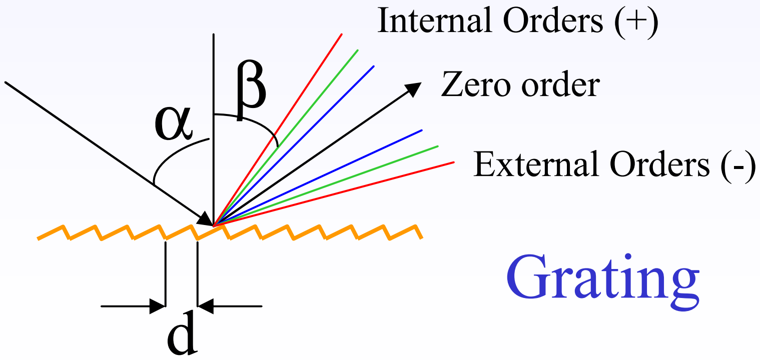
Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Prism





Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

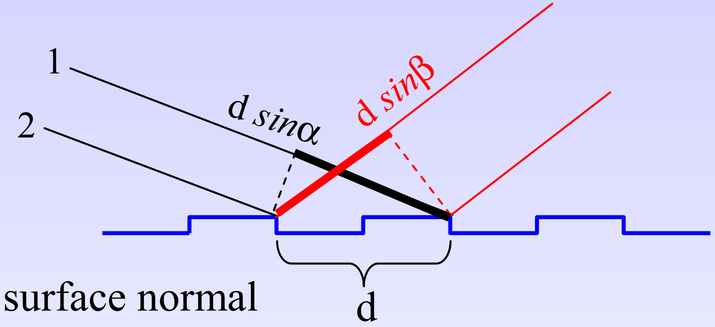


Grating

Gratings

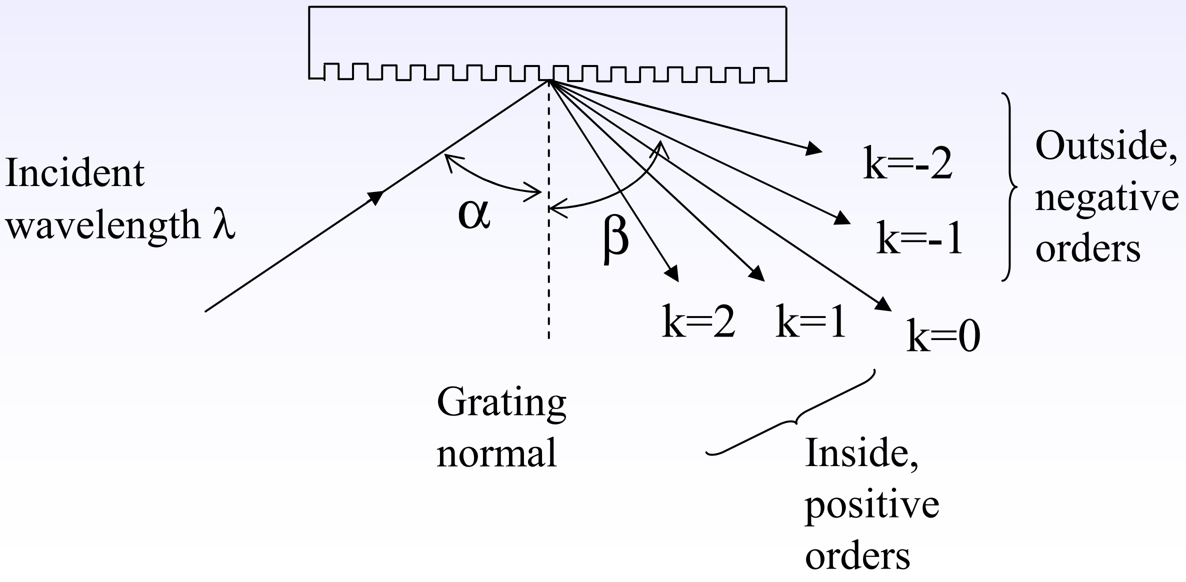
The diffraction grating is an artificial periodic structure with a well defined period d. The diffraction conditions are given by the well-known grating equation:

$$\boxed{\sin\alpha + \sin\beta = Nk\lambda}$$

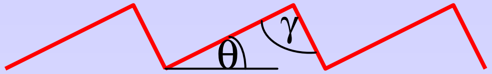


α and β are of opposite sign if on opposite sides of the surface normal

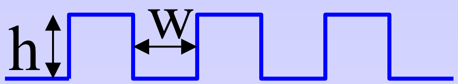
$N=1/d$ is the groove density, k is the order of diffraction (±1,±2,...)



Gratings profiles (1)

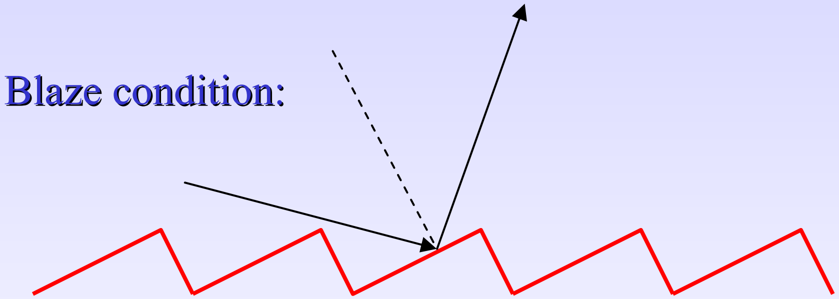


Blaze profile



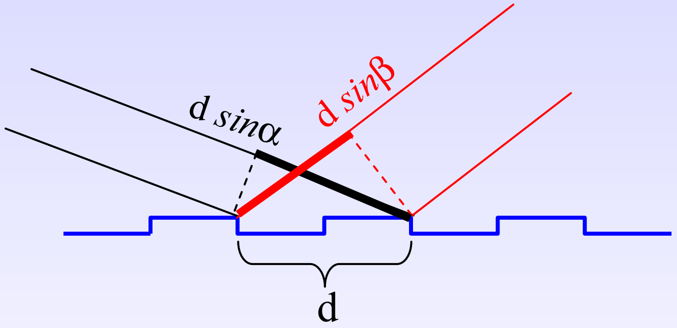
Laminar profile

Blaze condition:



Blaze angle=(α+β)/2

The angle θ is chosen such that for a given wavelength the diffraction direction coincides with the direction of specular reflection from the individual facets

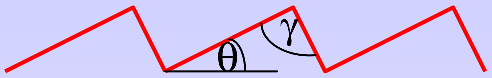


$$\overset{1\lambda}{k\lambda} = d(\sin\alpha + \sin\beta)$$
$$2\frac{\lambda}{2}$$

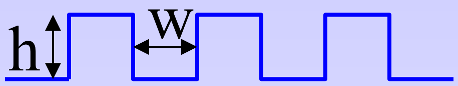
Blaze gratings: higher efficiency

Laminar gratings: higher spectral purity

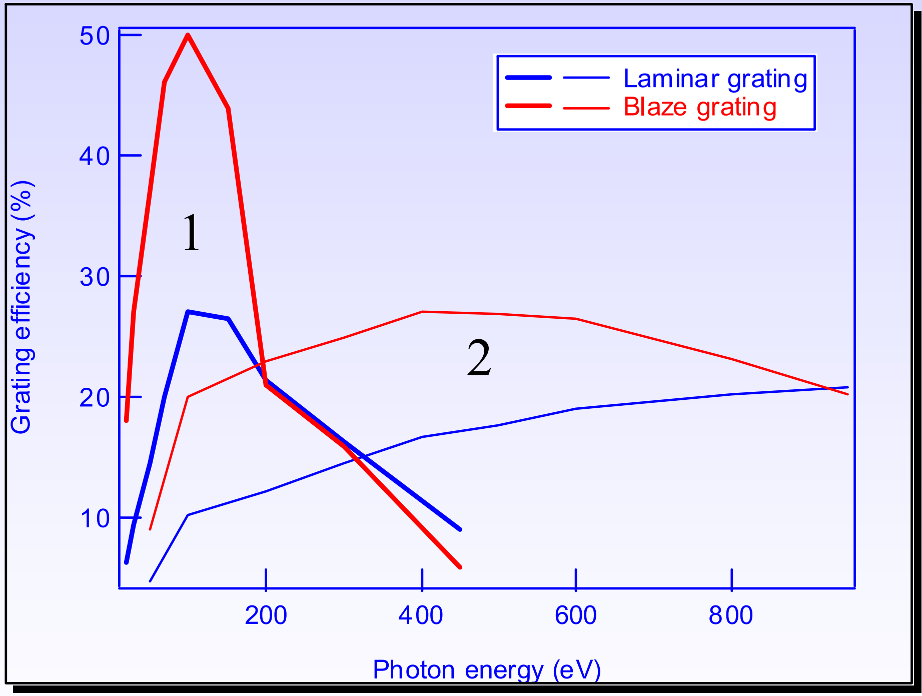
Gratings profiles (2)

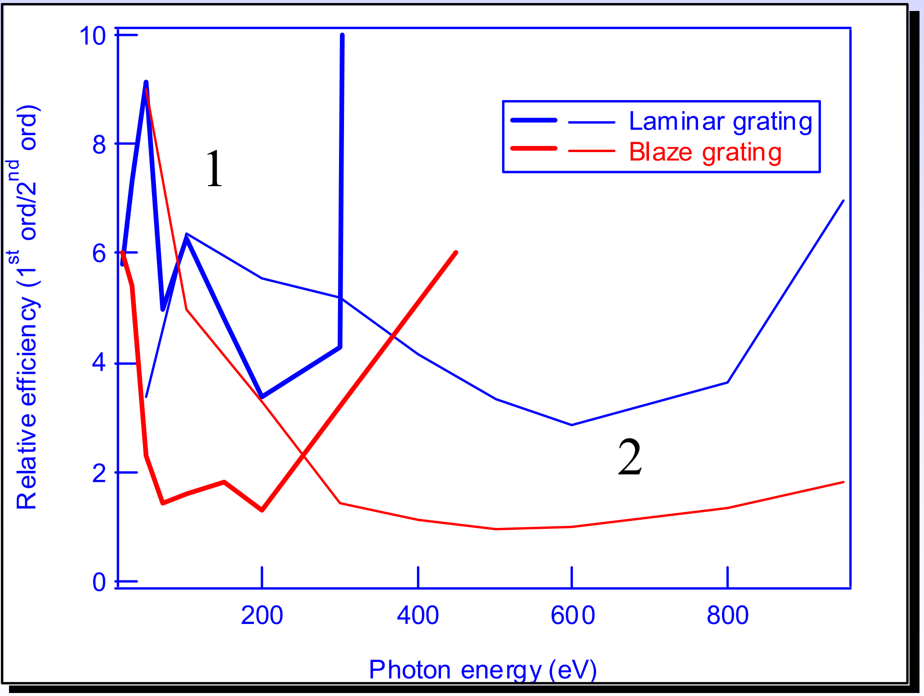


Blaze profile



Laminar profile

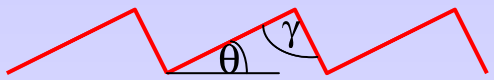




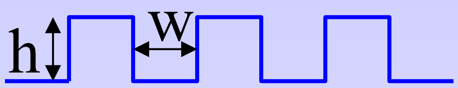
$$d(\sin\alpha + \sin\beta) = k\lambda$$

Grating 1: N=200 g/mm (d=5 µm)
Grating 2: N=400 g/mm (d=2.5 µm)

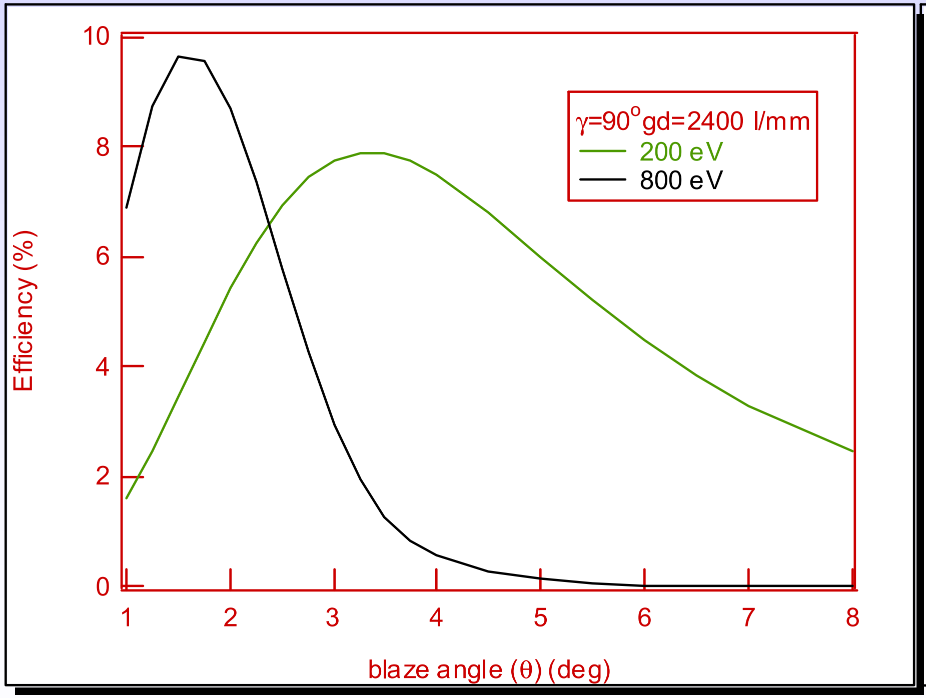
Gratings profiles (3)

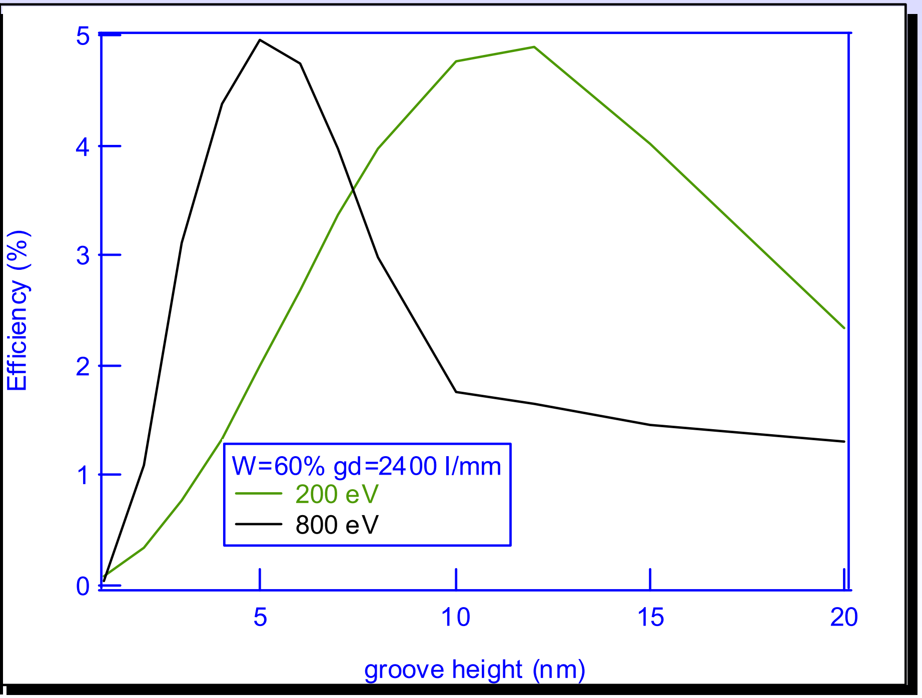


Blaze profile



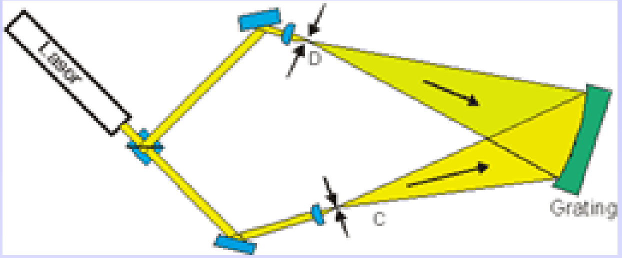
Laminar profile

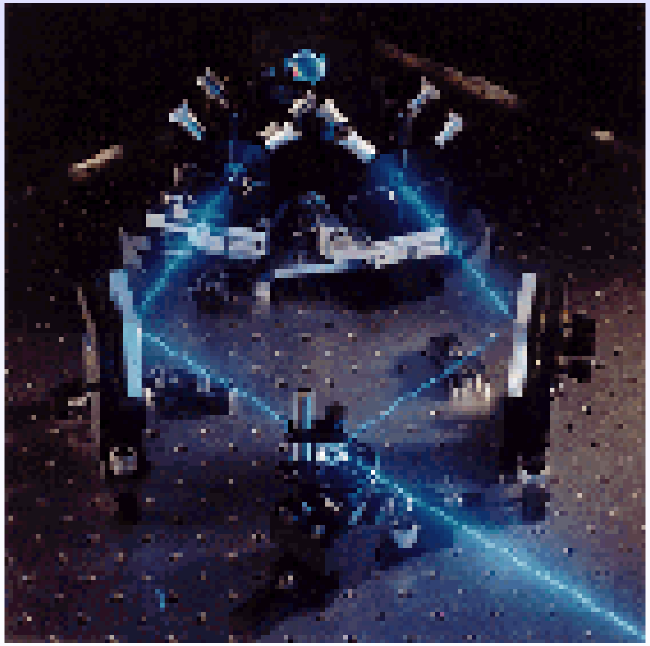


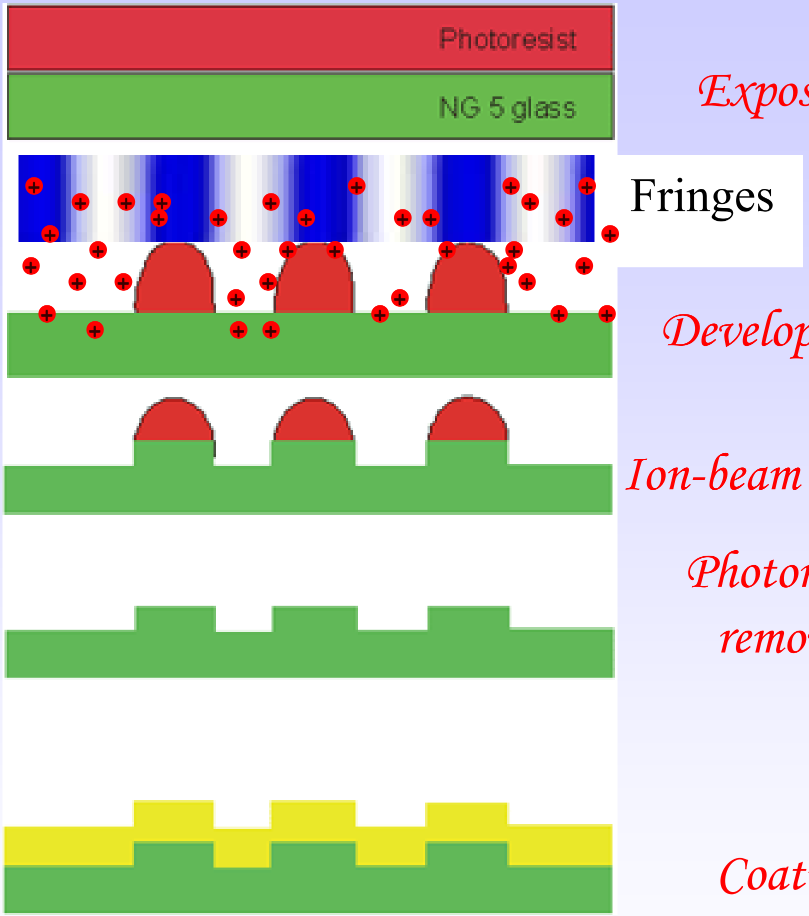


N=2400 g/mm (d=0.4 µm)

Holographically recorded grating







Exposure

Development

Ion-beam etching

Photoresist removal

Coating

Ruled and holographic gratings

Advantages and disadvantages

Efficiency:

holographic gratings usually have sinusoidal or nearly sawtooth profiles,

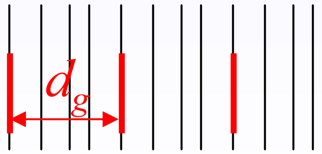
ruled gratings may have shallow blazed profiles

→ ruled gratings have usually higher efficiency

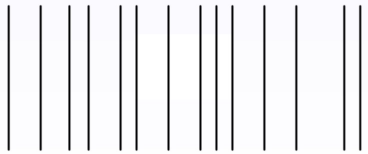
Scattered light:

a ruled grating is realized one groove after another → errors of ruling;
in an holographic grating all the grooves are formed simultaneously → the grating is free of periodic and random small displacements in the groove positions

→ holographic gratings have a much higher signal to noise ratio (no ghosts and much lower stray light)

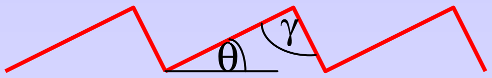


Periodic imperfections

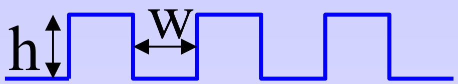


Random imperfections

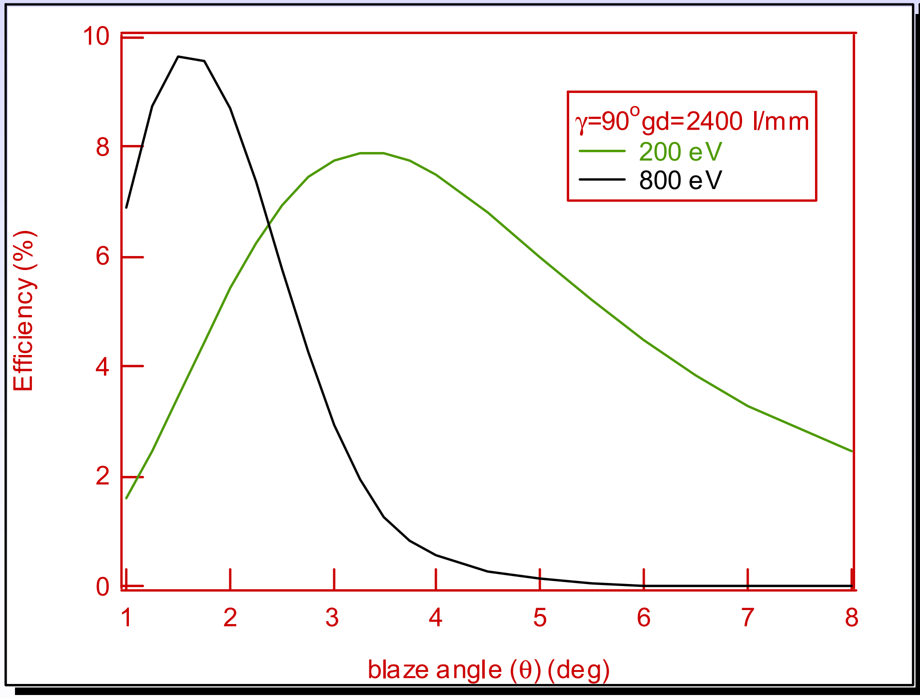
Gratings profiles (3)

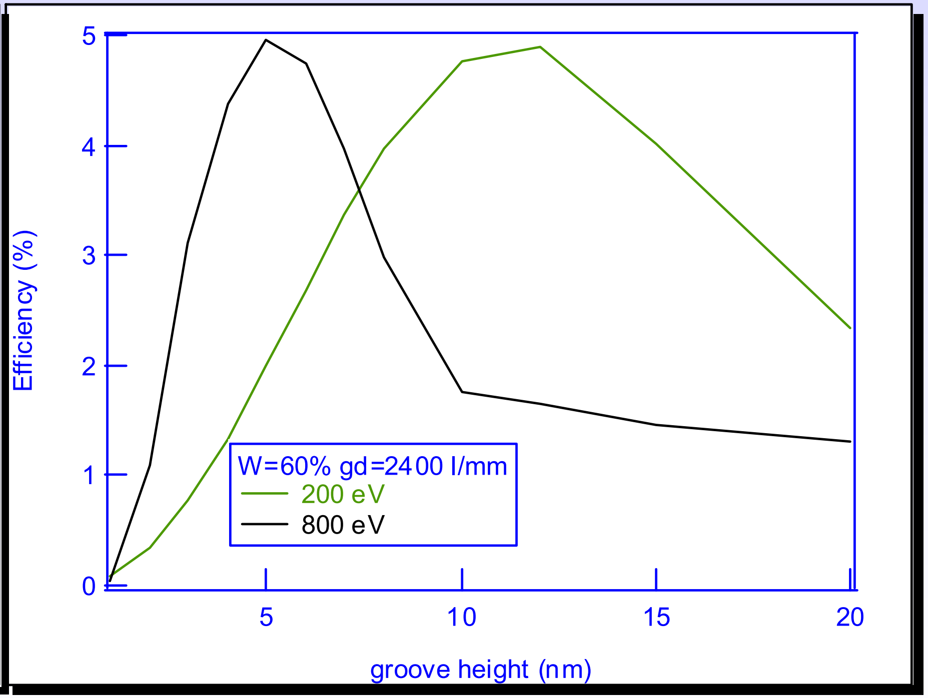


Blaze profile



Laminar profile





N=2400 g/mm (d=0.4 µm)

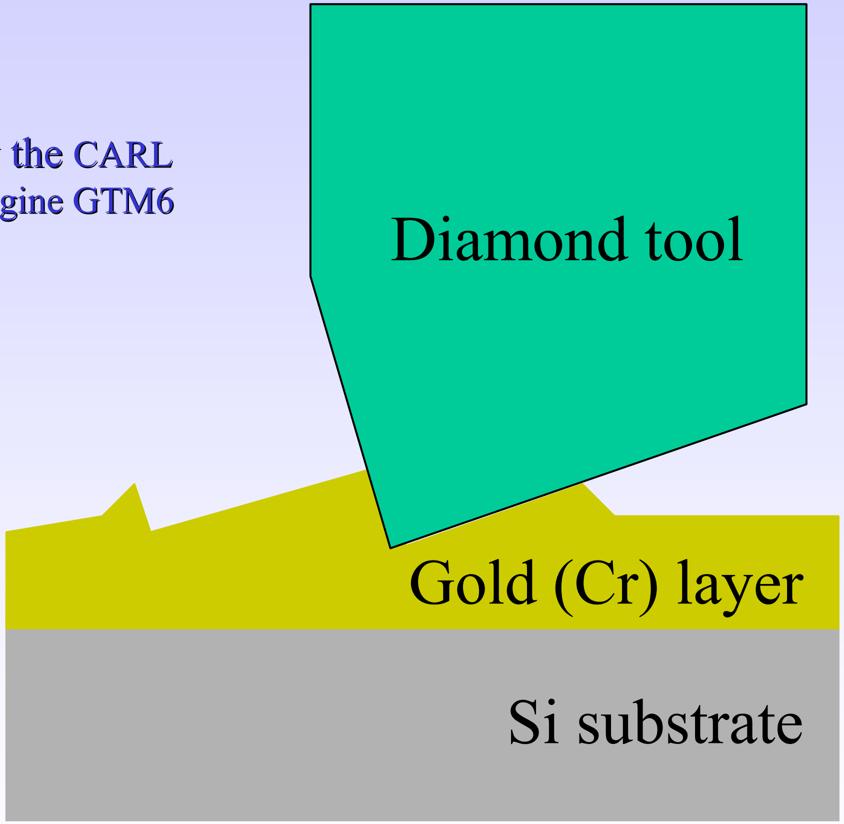
Shallow blaze angle grating production

- Thermal evaporation of Gold on the Si substrate (plus Cr binding layer)

Shallow blaze angle grating production

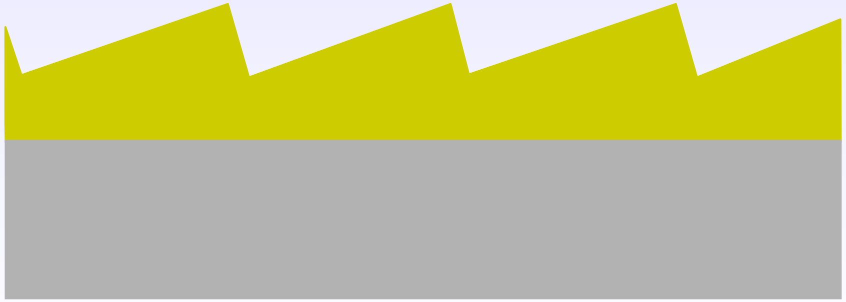
- Thermal evaporation of Gold on the Si substrate (plus Cr binding layer)
- Grooves formed by plastic deformation of the ruling layer

Mechanically ruled by the CARL ZEISS Grating Ruling Engine GTM6



Shallow blaze angle grating production

- Thermal evaporation of Gold on the Si substrate (plus Cr binding layer)
- Grooves formed by plastic deformation of the ruling layer
- Realization of low micro-roughness blaze grating with 20<gd<5000 l/mm and down to 1.5^o of blaze angle



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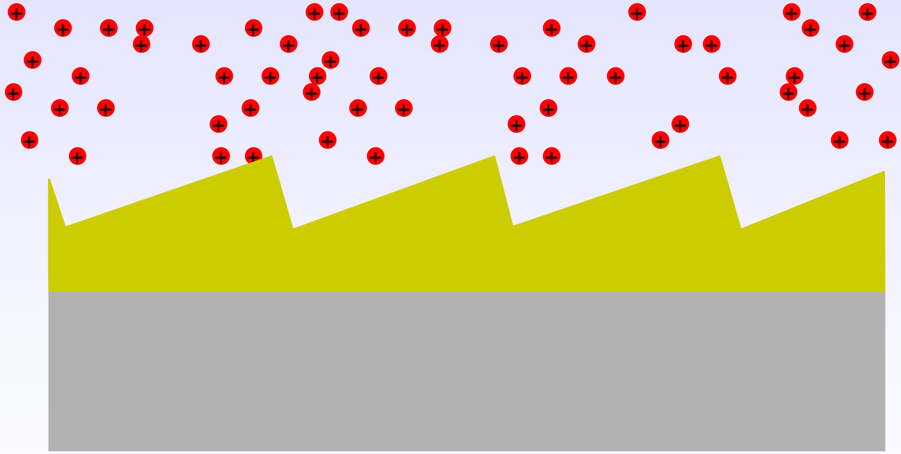

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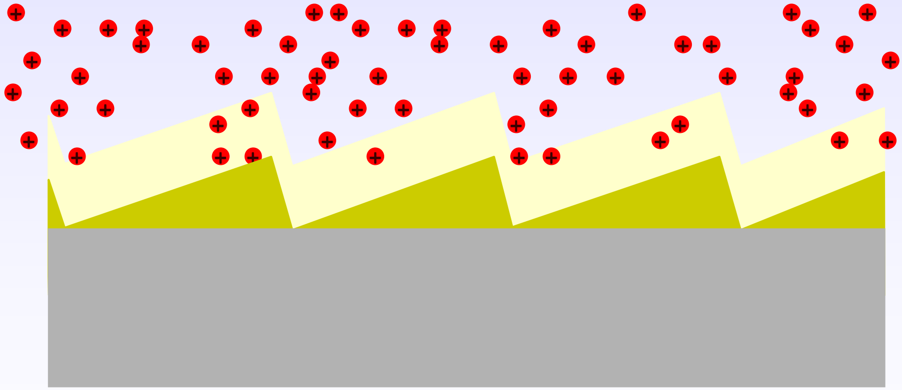

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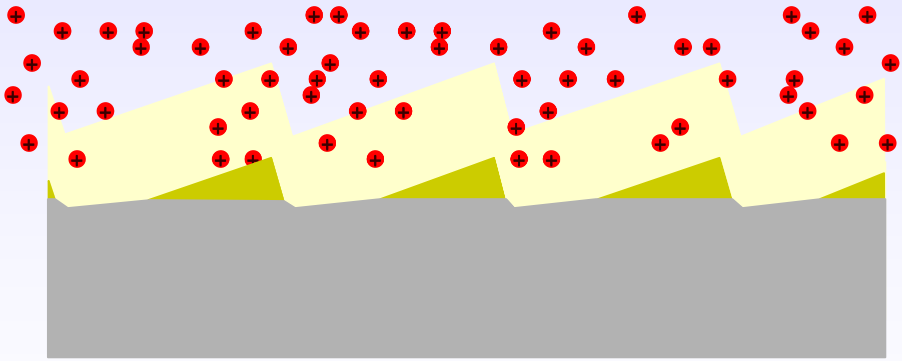

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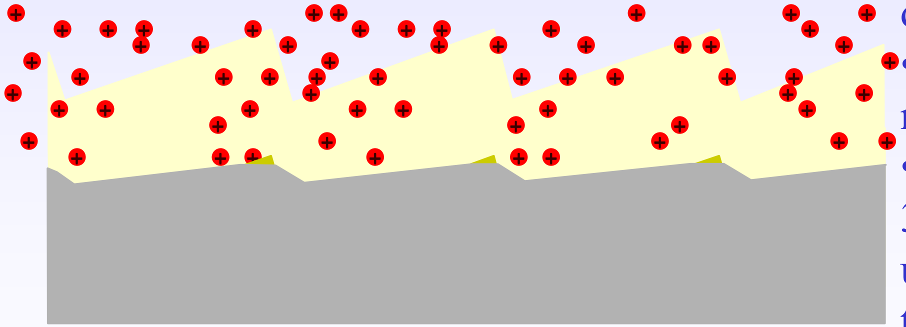
- **Ar^+ ion etching rate on gold much larger then on Silicon**

Shallow blaze angle grating production



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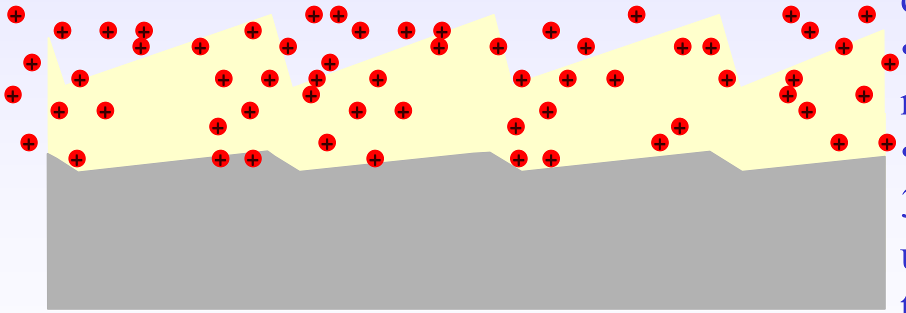
- Ar^+ ion etching (200 mm diameter collimated beam)
- Ar^+ ion etching rate on gold much larger then on Silicon
- An angle reduction of a factor 3 (even higher if $Ar^+ + O^+$ is used) can be achieved by this technique

Shallow blaze angle grating production



- Thermal evaporation of Gold on the Si substrate (plus Cr binding layer)
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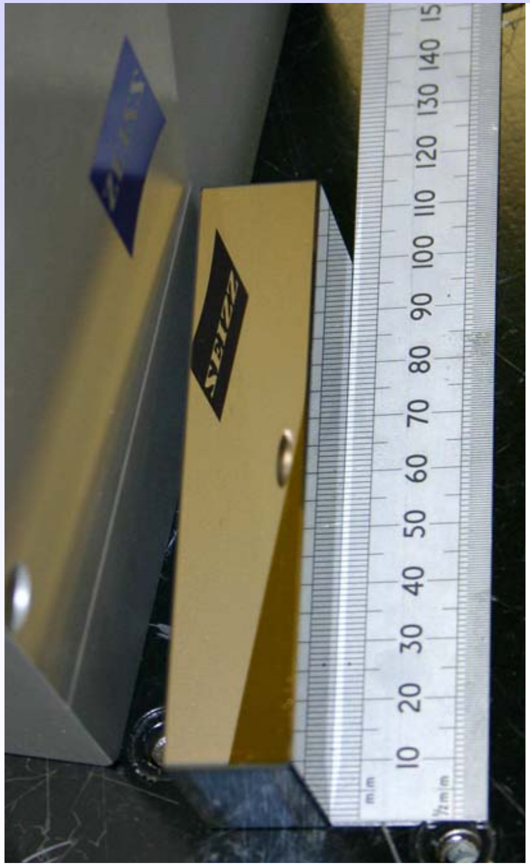
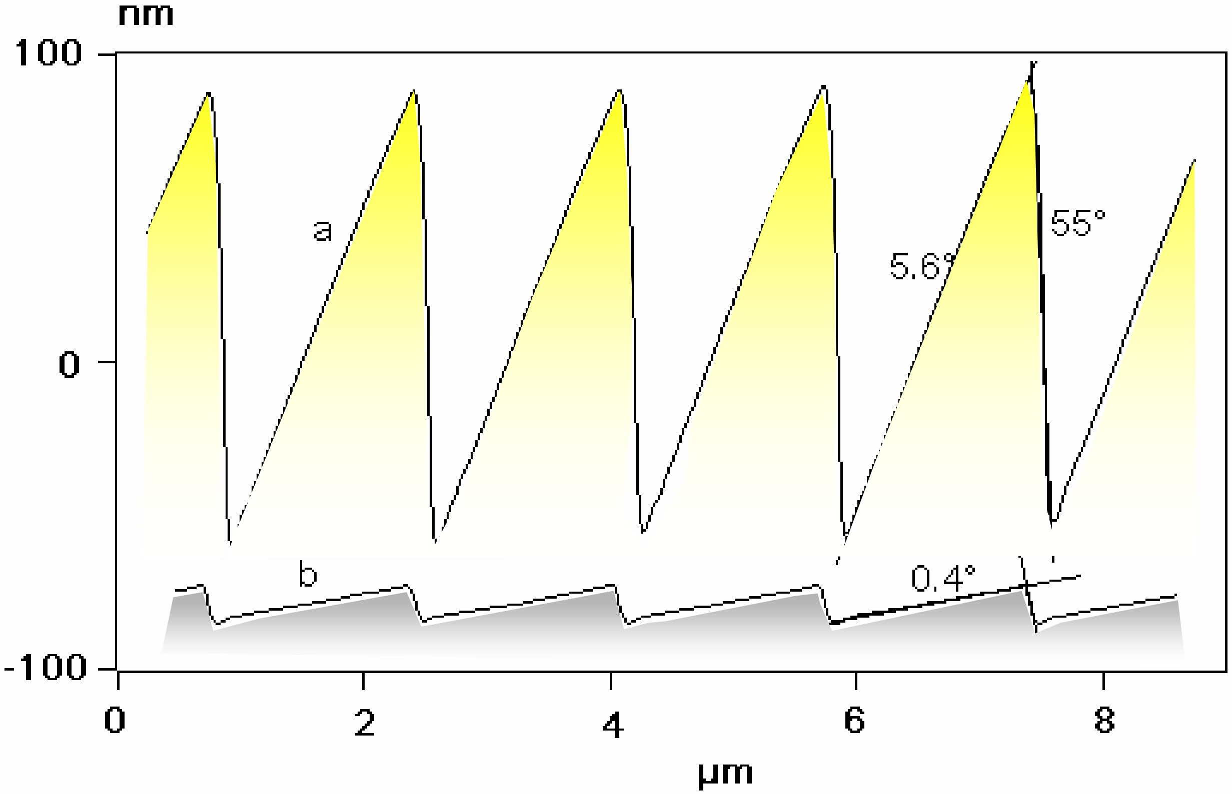
- Realization of low micro-roughness blaze grating with 20<gd<5000 l/mm and down to 1.5° of blaze angle
- Ar^+ ion etching (200 mm diameter collimated beam)
- Ar^+ ion etching rate on gold much larger then on Silicon
- An angle reduction of a factor 3 (even higher if $Ar^+ + O^+$ is used) can be achieved by this technique
- Roughness and anti blaze angle are also reduced.

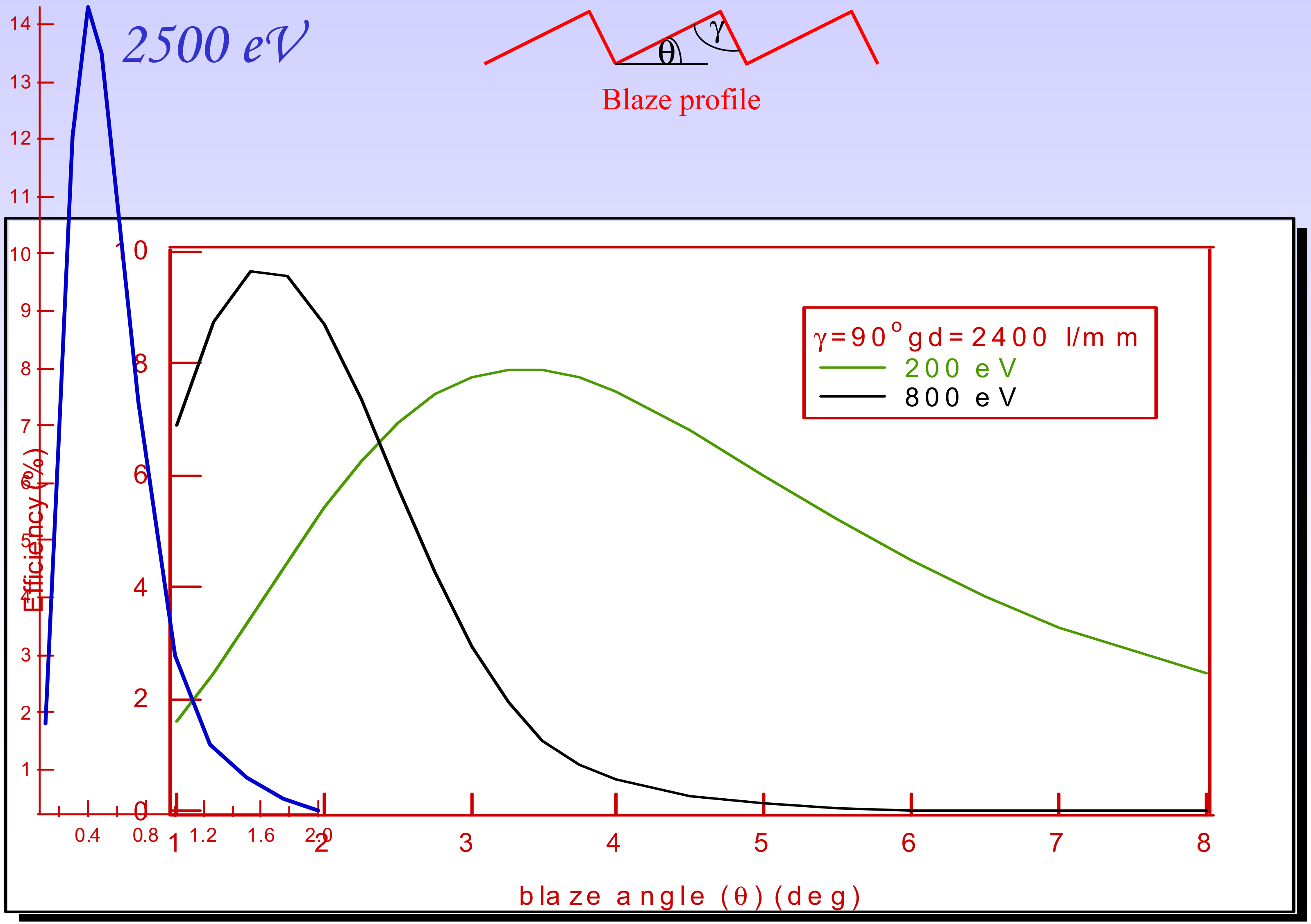
Shallow blaze angle grating production

Plane substrate, 600 l/mm, gold coated
80mm*5mm useful area, blaze angle 0.4°



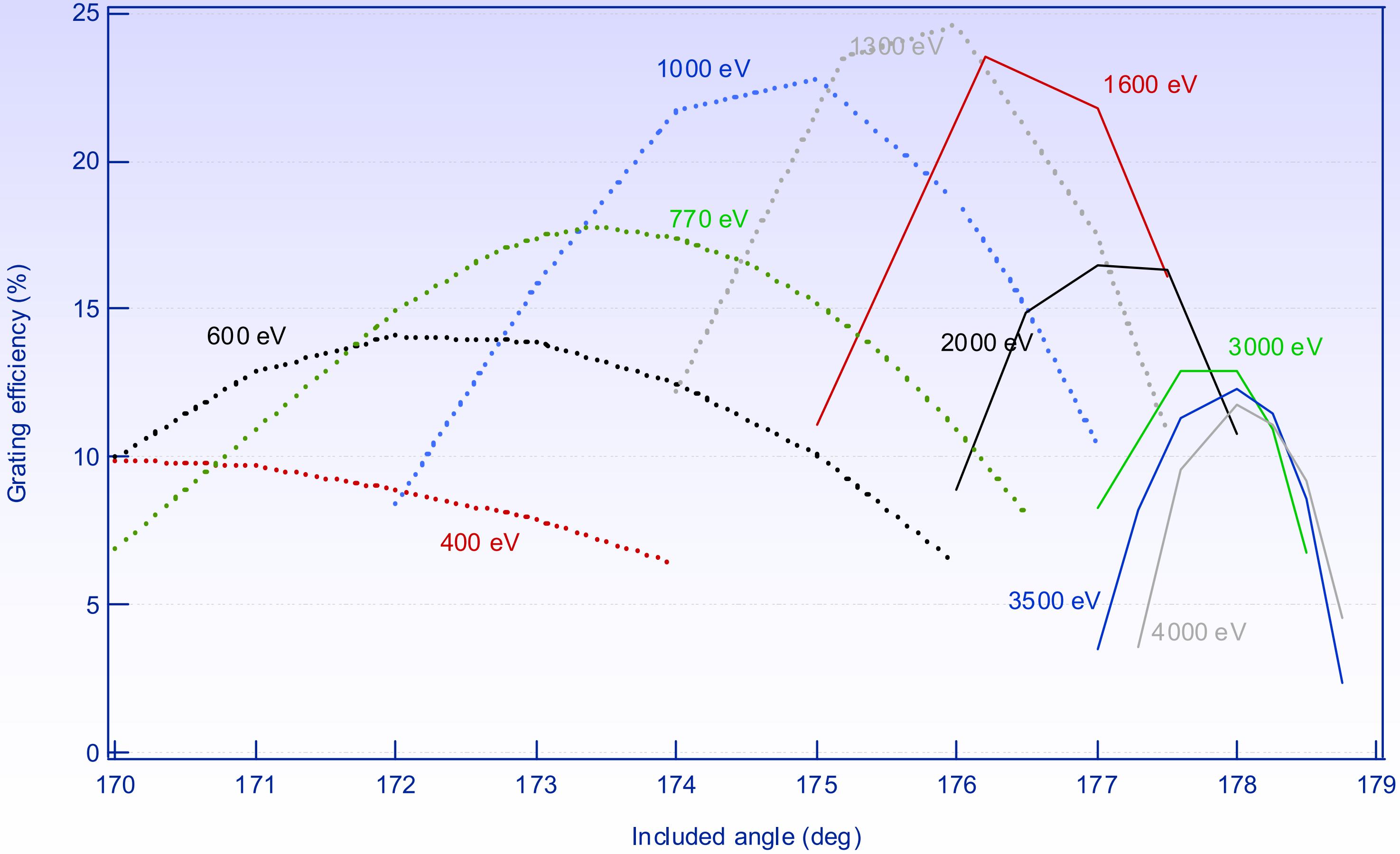


Blaze grating efficiency



Shallow blaze grating measured efficiency

Plane substrate, 600 l/mm, gold coated, blaze angle 0.4^{o}



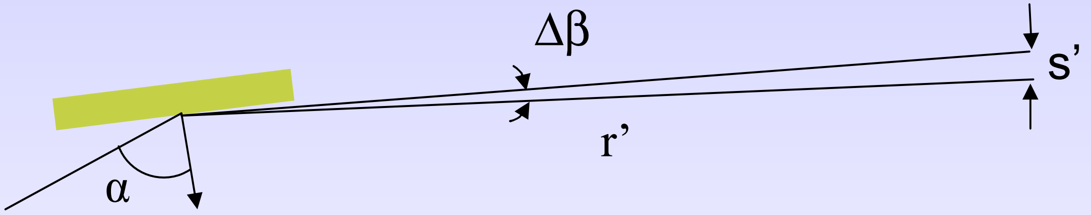
Grating resolving power (1)

Differentiating the grating equation: $\sin\alpha + \sin\beta = Nk\lambda$

the **angular dispersion** of the grating is obtained:

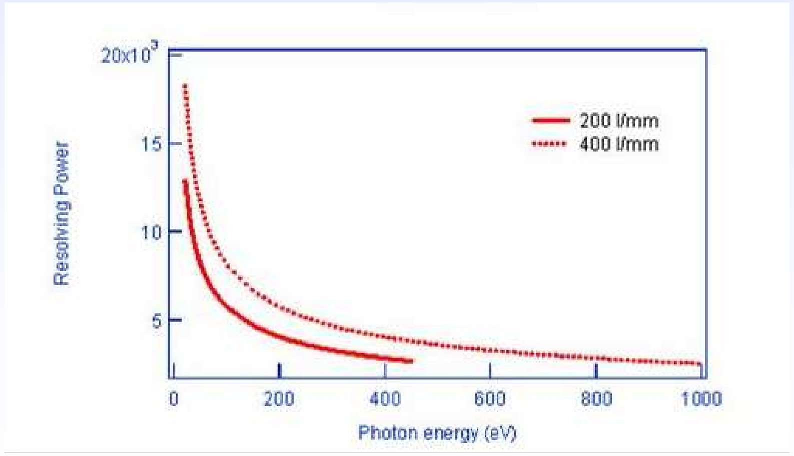
(higher groove density → higher angular dispersion)

$$\boxed{\Delta\lambda = \frac{\cos\beta}{Nk}\Delta\beta}$$



The **resolving power** is defined as:

$$\boxed{R = \frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda}}$$



R=10000 @100 eV → ΔE=100 eV/10000=10 meV

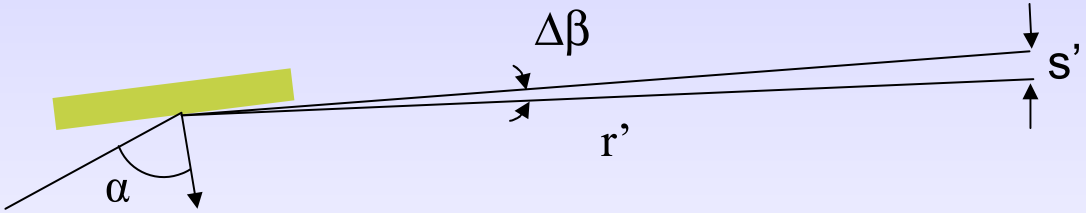
Grating resolving power (2)

Angular dispersion : $\Delta\lambda = \dfrac{\cos\beta}{Nk}\Delta\beta$

Resolving power: $R = \dfrac{E}{\Delta E} = \dfrac{\lambda}{\Delta\lambda}$

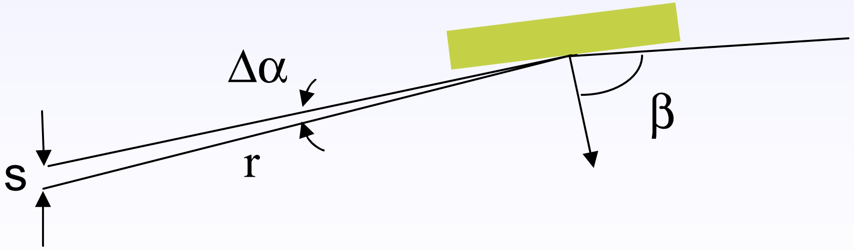
The main contribution is from the width s’ of the **exit slit**:

$$\boxed{\frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda} = \frac{\lambda\, N\, k\, r'}{(\cos\ \beta)s'}}$$



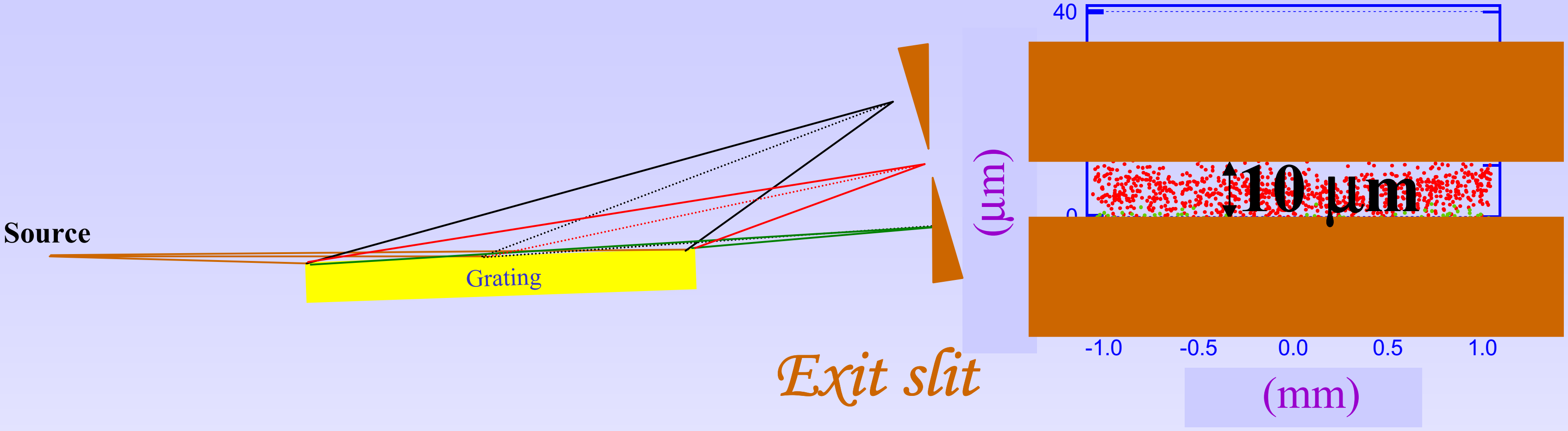
The **entrance slit** contribution is similar:

$$\boxed{\frac{E}{\Delta E} = \frac{\lambda}{\Delta\lambda} = \frac{\lambda\, N\, k\, r}{(\cos\ a)s}}$$



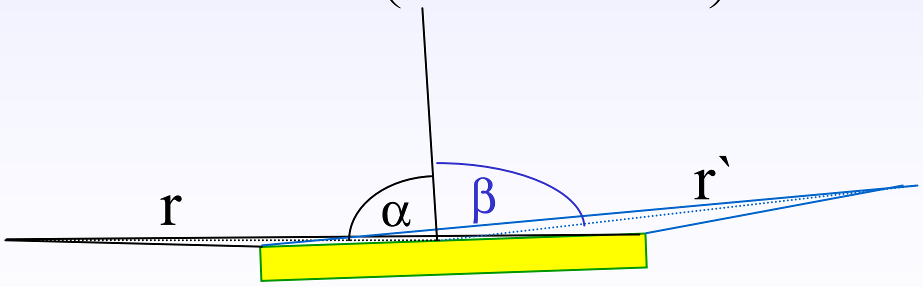
Smaller s and s’ → higher resolving power

Variable included angle spherical grating monochromator (1)



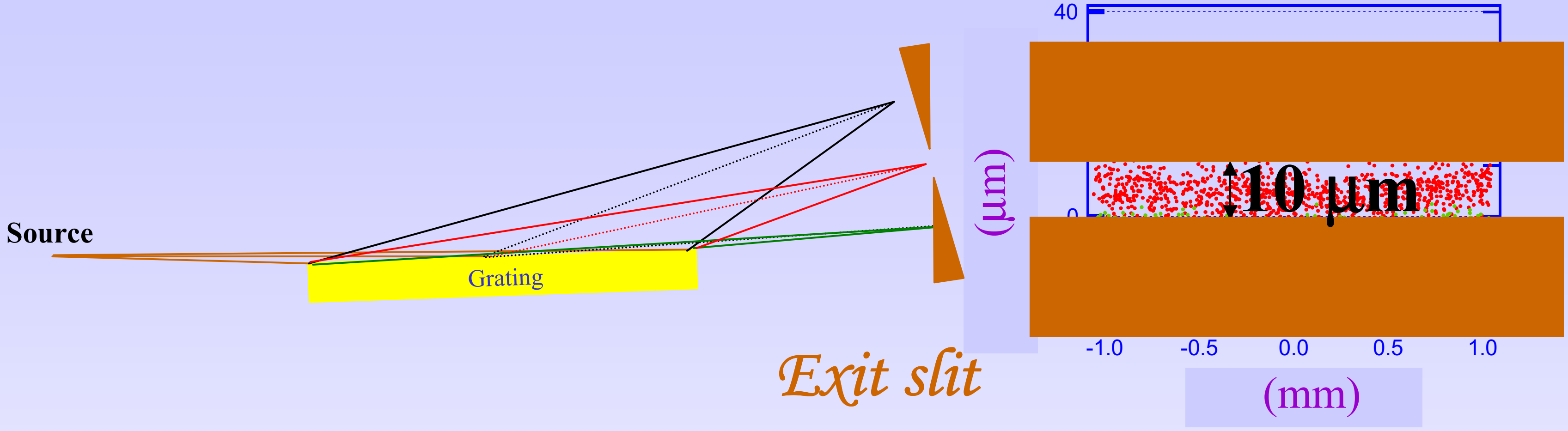
$F_{100} = 0 \Rightarrow \sin\alpha + \sin\beta = Nk\lambda$ grating equation

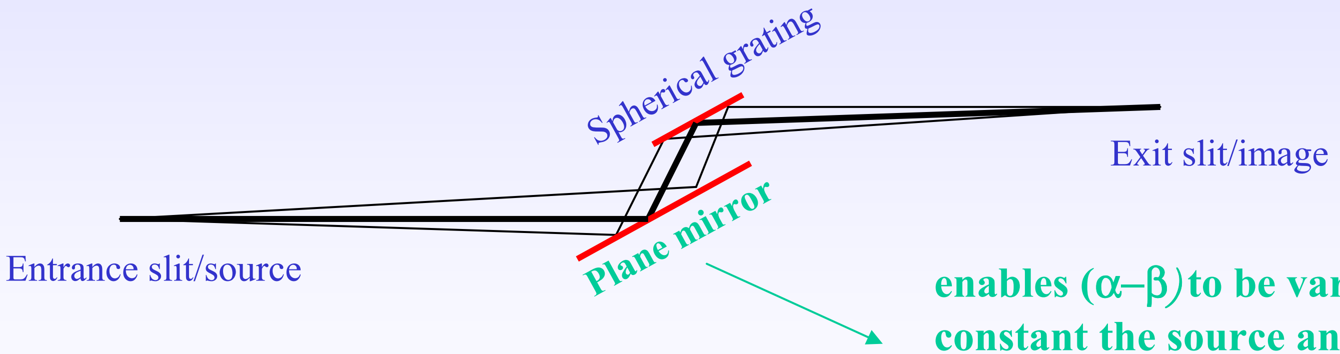
$F_{200} = 0 \Rightarrow \left(\frac{\cos^2\alpha}{r} + \frac{\cos^2\beta}{r'}\right) - \frac{(\cos\alpha + \cos\beta)}{R} = 0$ tangential focusing



Variable included angle=(α–β)

Variable included angle spherical grating monochromator (2)

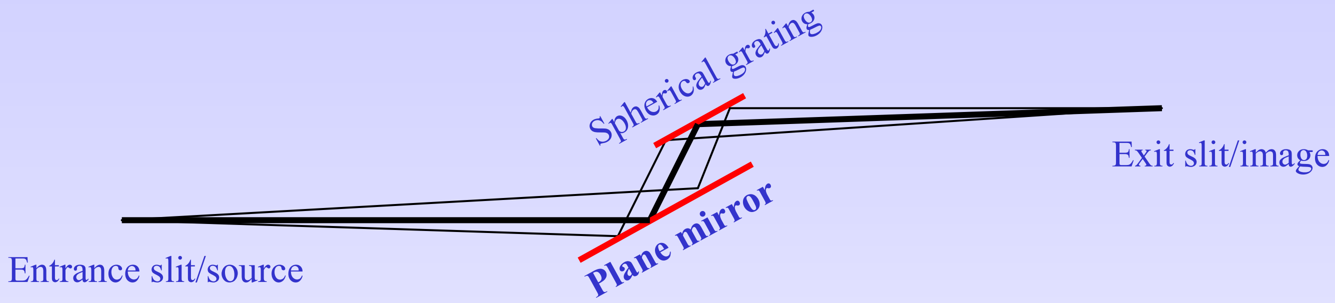




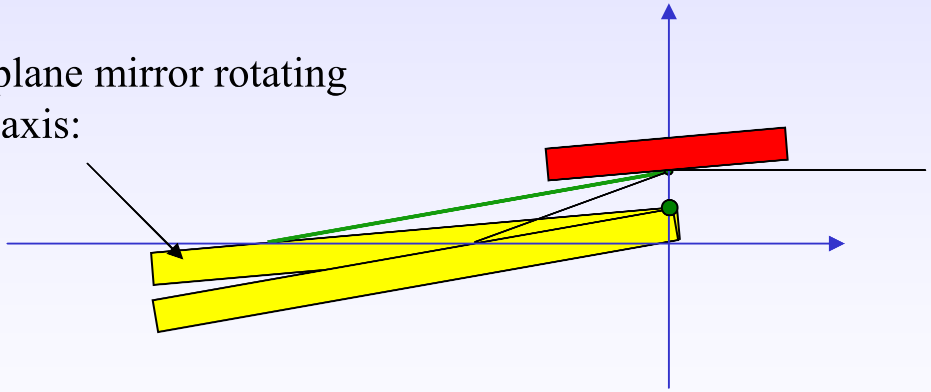
enables $(\alpha-\beta)$ to be varied keeping constant the source and the image in position and direction:

$i_{mirror}=(\alpha-\beta)/2$

Variable included angle spherical grating monochromator (3)

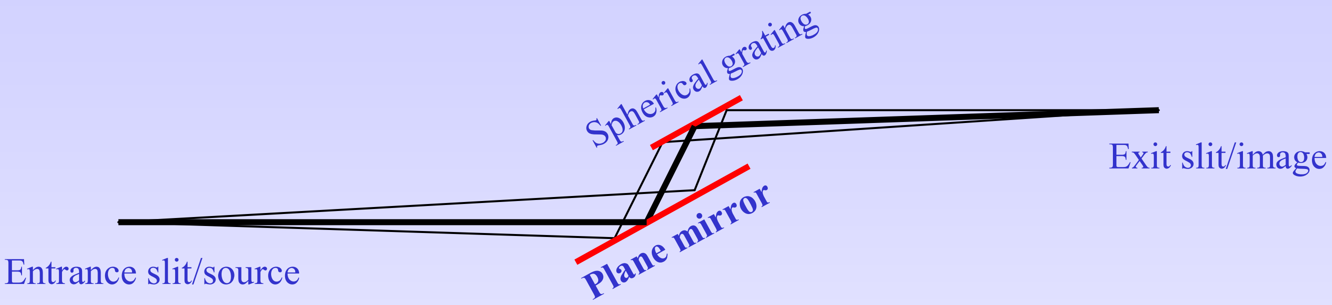


Sufficiently long plane mirror rotating about a particular axis:



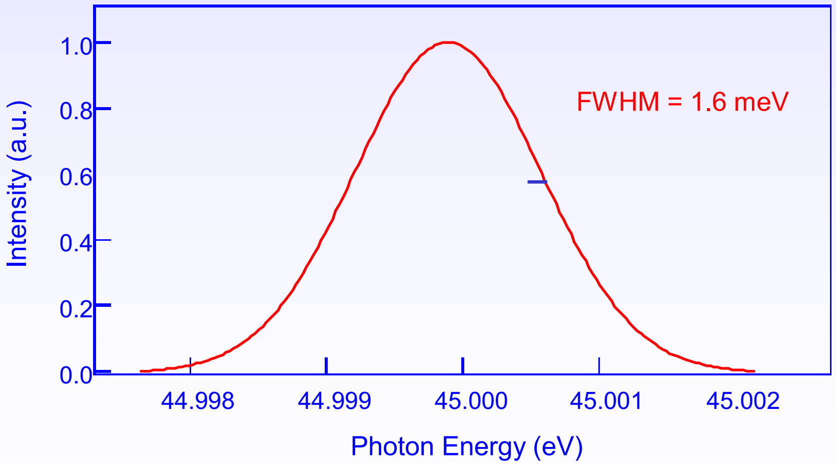
The light beam runs up and down the plane mirror as it is rotated

Variable included angle spherical grating monochromator (4)



resolving power:

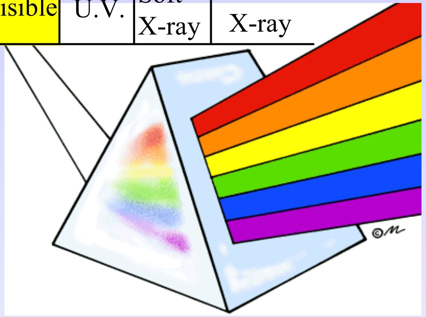
$$\frac{E}{\Delta E}=\frac{\lambda}{\Delta\lambda}=28000$$



Monochromators

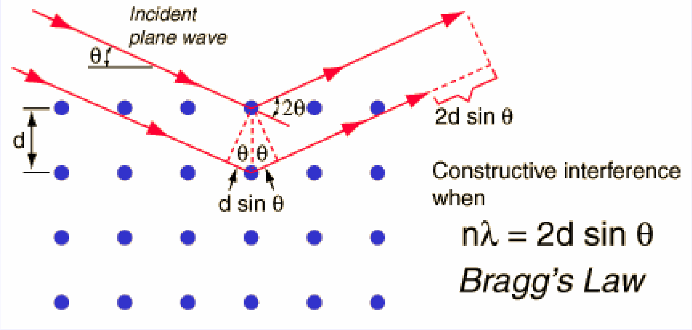
Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Prism

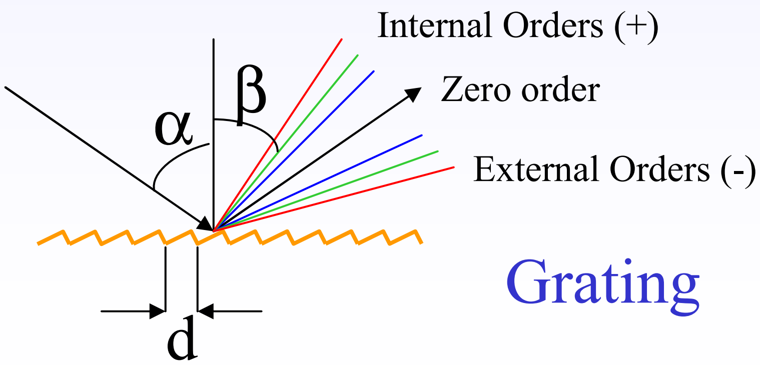


Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray

Crystal

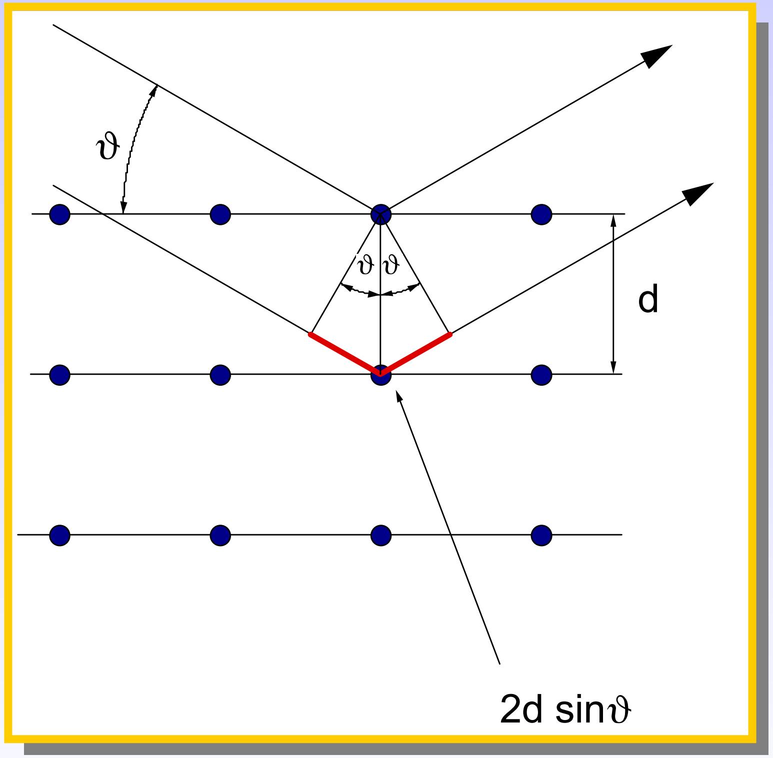


Micro wave	I.R.	Visible	U.V.	Soft X-ray	Hard X-ray



Grating

Bragg's law



Radiation of wavelength λ is reflected by the lattice planes. The outgoing waves interfere. The interference is constructive when the optical path difference is a multiple of λ:

$$\boxed{2d\sin\vartheta = n\lambda}$$

d is the distance between crystal planes.

$$\sin\vartheta \le 1 \;\Rightarrow\; \lambda \le \lambda_{\max} = 2d$$

The maximum reflected wavelength corresponds to the case of normal incidence: θ=90°

EXAMPLES:

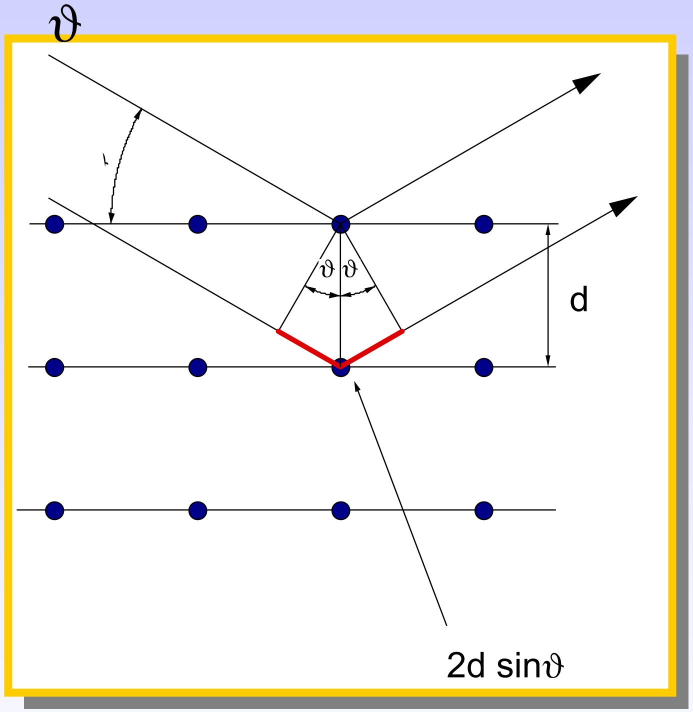
Si (111): d=3.13Å → Emin ≈ 2 keV

Si (311): d=1.64Å → Emin ≈ 3.8 keV

InSb (111): d=3.74Å → Emin ≈ 1.7 keV

Be $(10\underline{1}0)$*: d=7.98Å → Emin ≈ 0.8 keV*

Energy resolution



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

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta E}{E} = \Delta\vartheta \frac{\cos\vartheta}{\sin\vartheta}$$

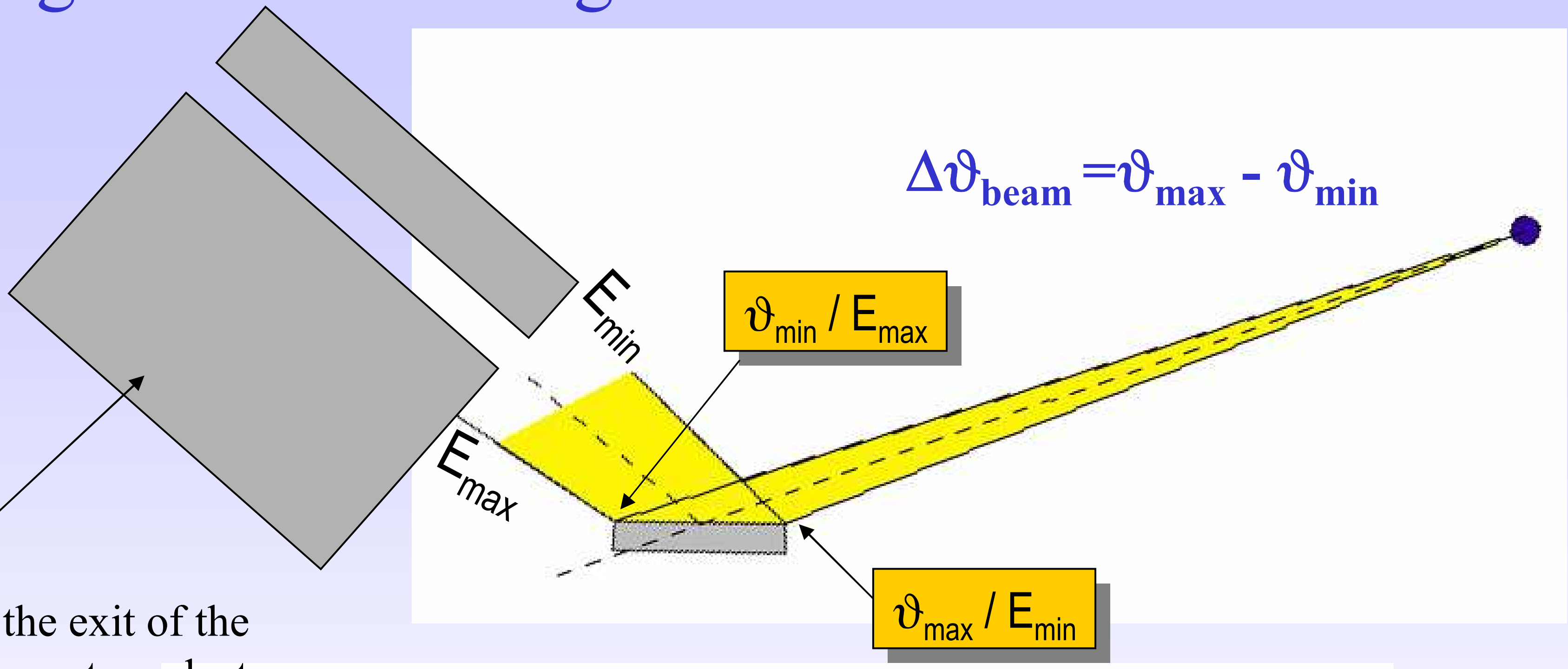
The energy resolution of a crystal monochromator is determined by the angular spread $\Delta\vartheta$ of the diffracted beam and by the Bragg angle ϑ

$\Delta\vartheta$ has two contributions :

$\Delta\vartheta_{\text{beam}}$: angular divergence of the incident beam

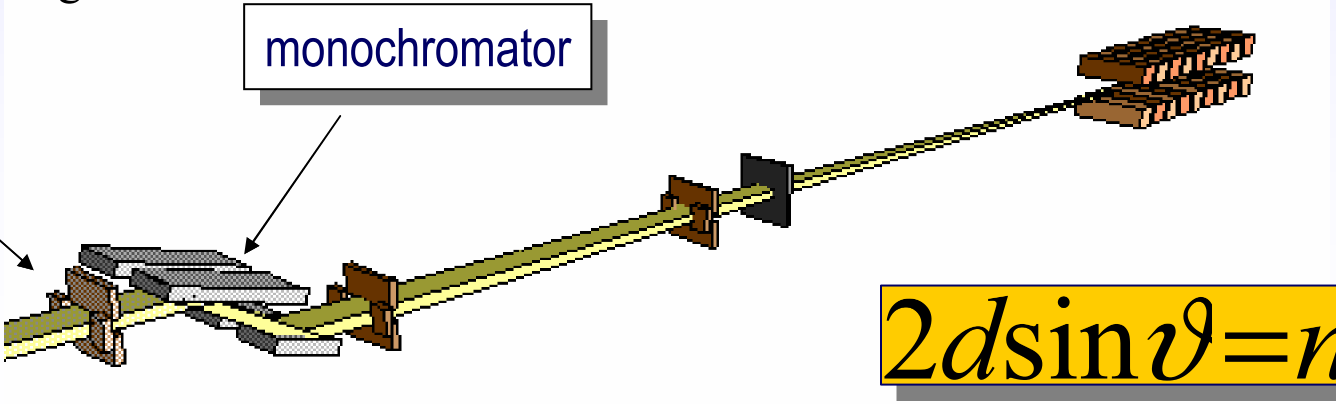
ω_{crystal} : intrinsic width of the Bragg reflection

Angular beam divergence



$$\Delta\vartheta_{beam} = \vartheta_{max} - \vartheta_{min}$$

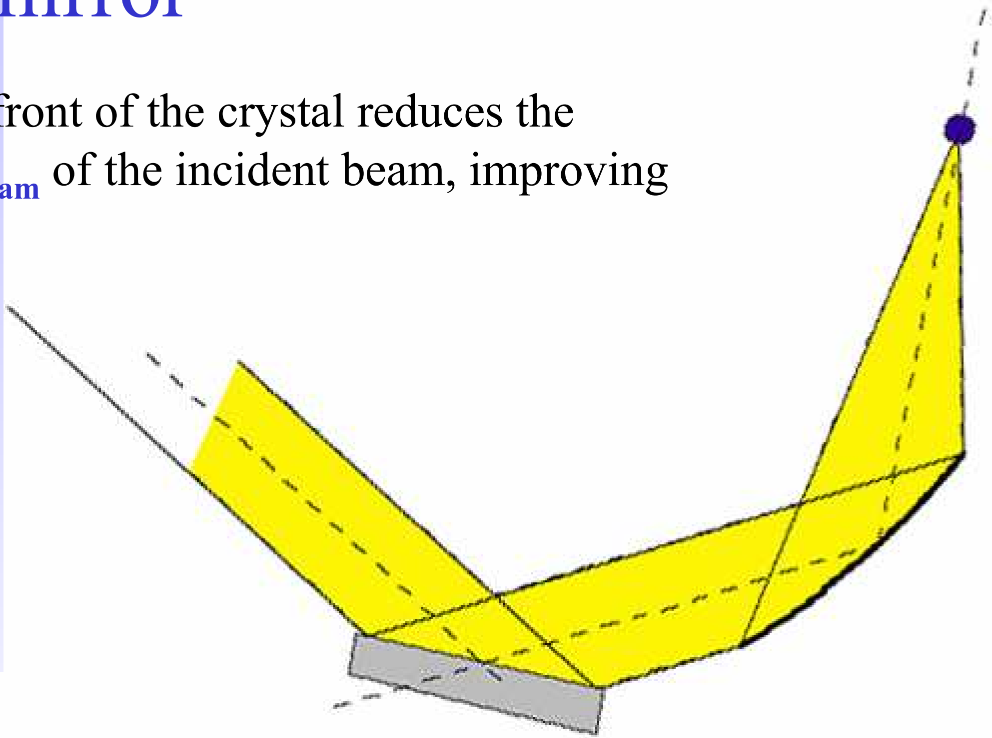
A slit at the exit of the monochromator selects a narrower energy range.

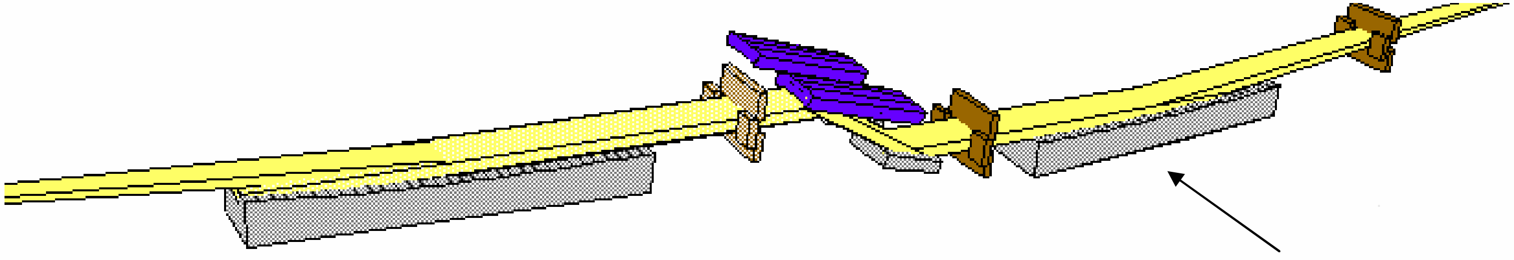


$$2d\sin\vartheta = n\lambda$$

Collimating mirror

A collimating mirror in front of the crystal reduces the angular divergence $\Delta\vartheta_{\mathrm{beam}}$ of the incident beam, improving the energy resolution.





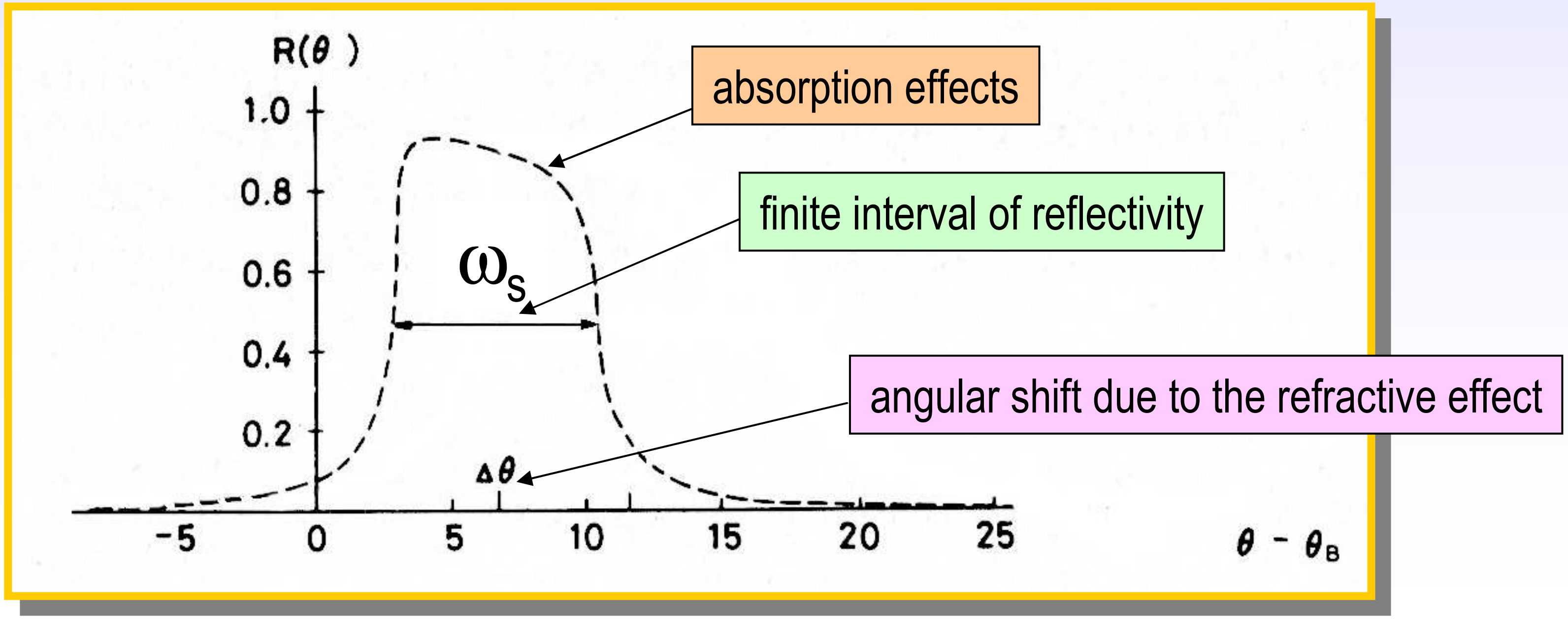
Collimating premirror

Darwin Curve

The intrinsic reflection width of the crystal, $\boldsymbol{\omega_s}$, can be obtained measuring the crystal reflectivity for a perfectly collimated monochromatic beam, as a function of the difference between the actual value of the incidence θ angle and the ideal Bragg value: $\Delta\theta = \theta - \theta_B$.

This reflectivity is derived by the dynamic diffraction theory, which includes multiple scattering → **Darwin curve:**

1. there is a finite interval of incidence angles for which the beam is reflected
2. the center of this interval does not coincide with the Bragg angle
3. R < 1 and has a typical asymmetric shape

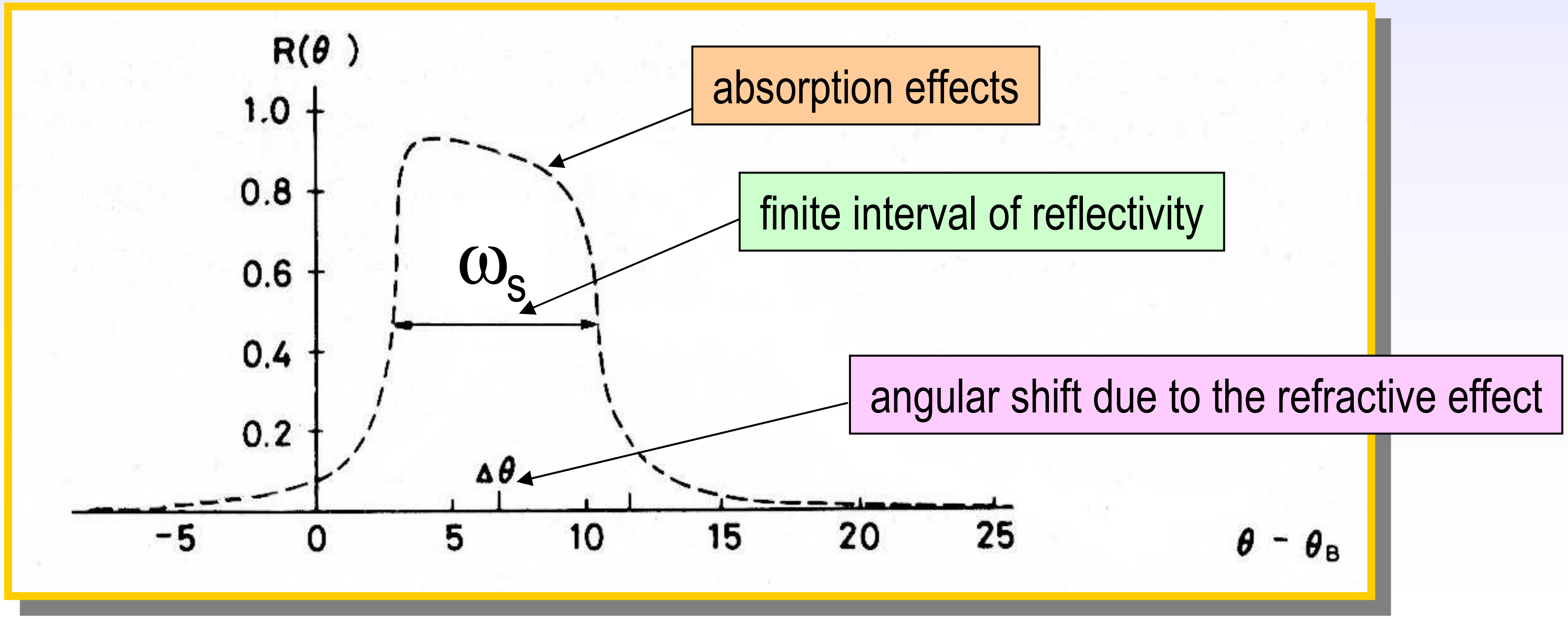


Intrinsic width of the Bragg reflection

$$\omega_S = \frac{2}{\sin(2\vartheta_B)} \frac{r_e \lambda^2}{\pi V} C \left| F_{hr} \right| e^{-M}$$

Dynamic diffraction theory

θ_B	**Bragg angle**
λ	**wavelength of radiation**
r_e	radius of the electron e^2/mc^2
V	volume of the unit cell
C	polarization factor
$\lvert F_{hr} \rvert$	amplitude of the **crystal structure factor F_r related to the (hkl) diffraction**
e^{-M}	temperature factor



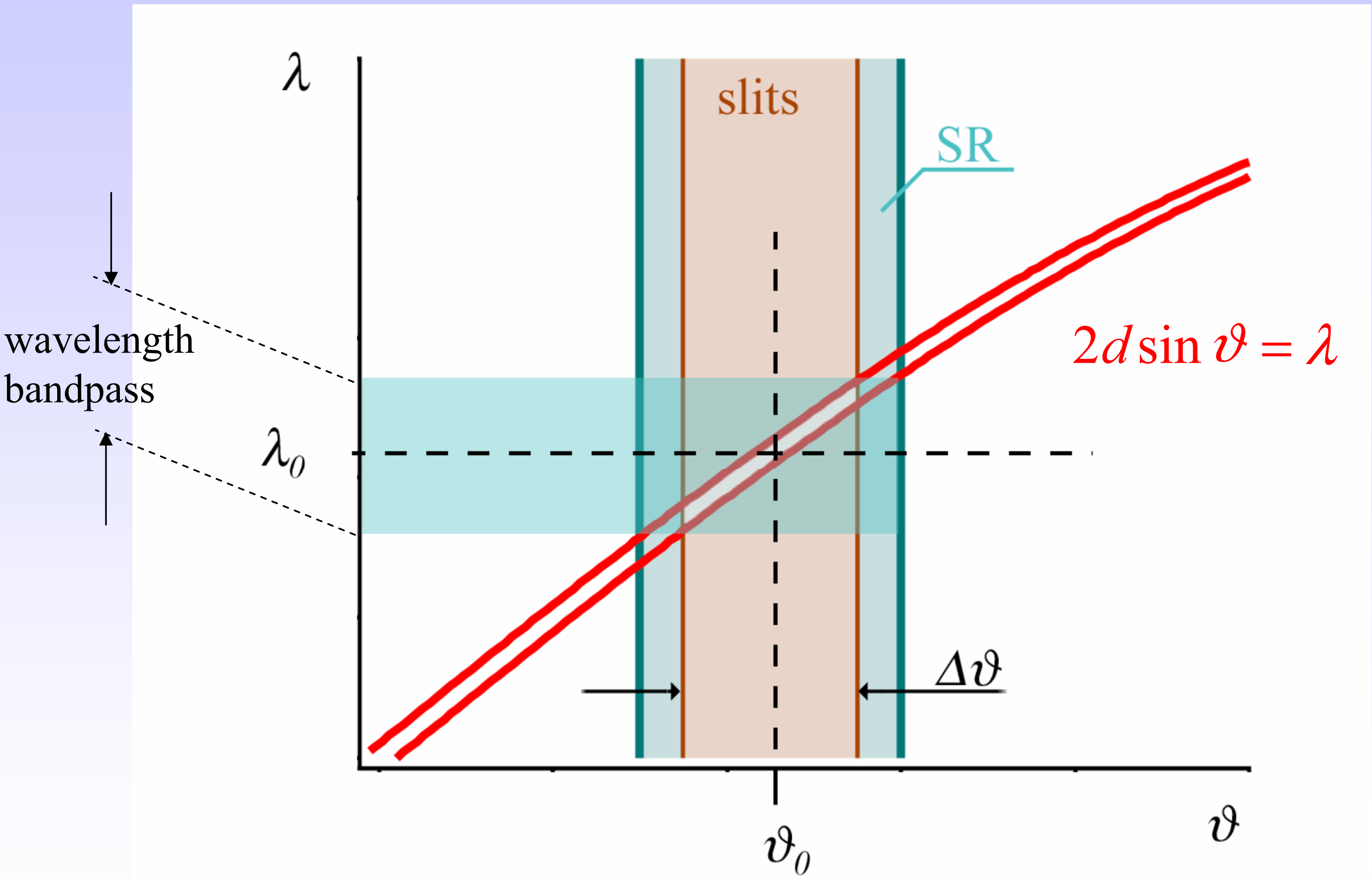
absorption effects

finite interval of reflectivity

angular shift due to the refractive effect

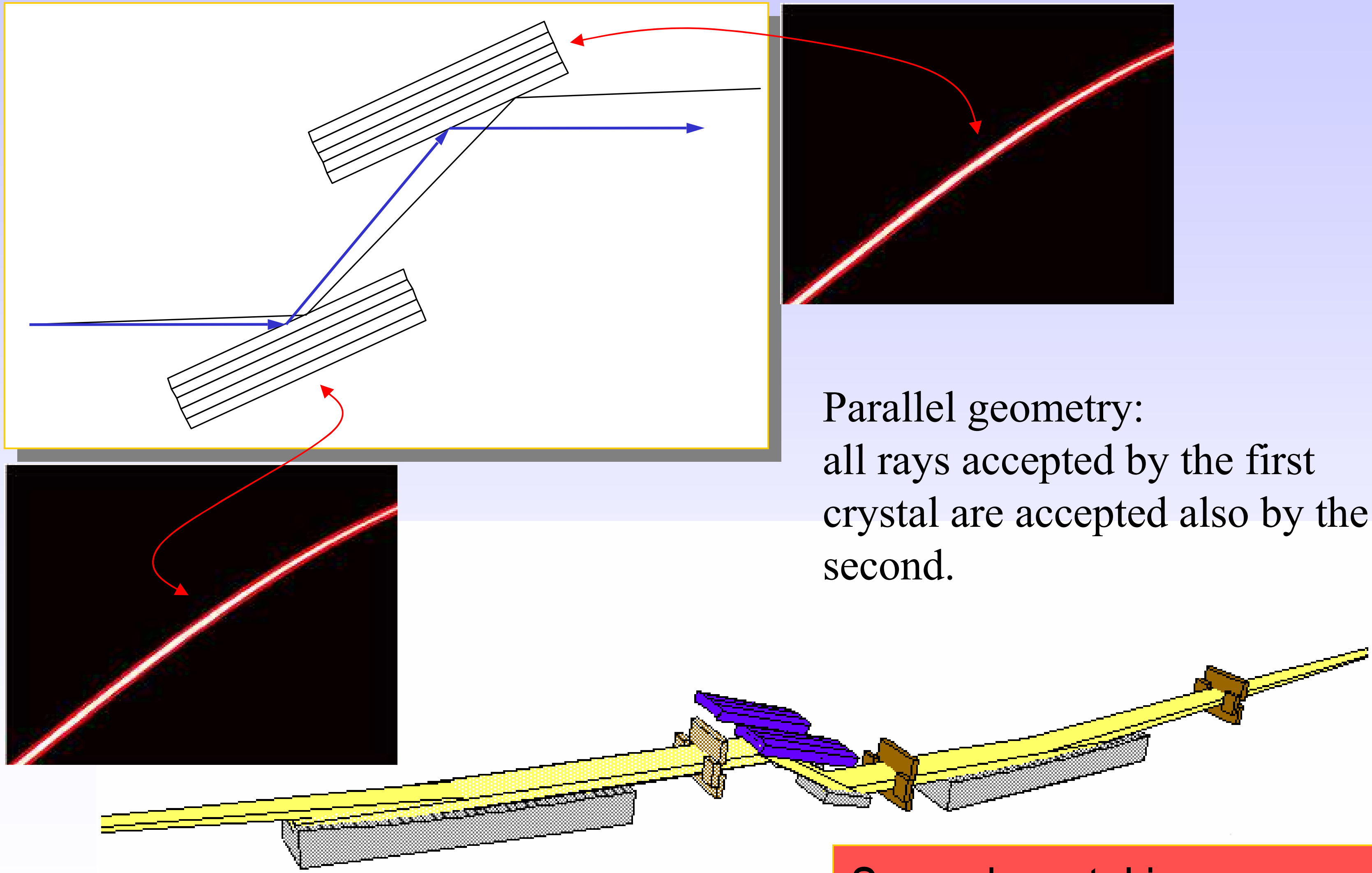
Du Mond diagram

$\Delta\vartheta$= angular acceptance of the slit



The Du Mond diagram describes the reflection of radiation by the crystal in the $\vartheta - \lambda$ space.

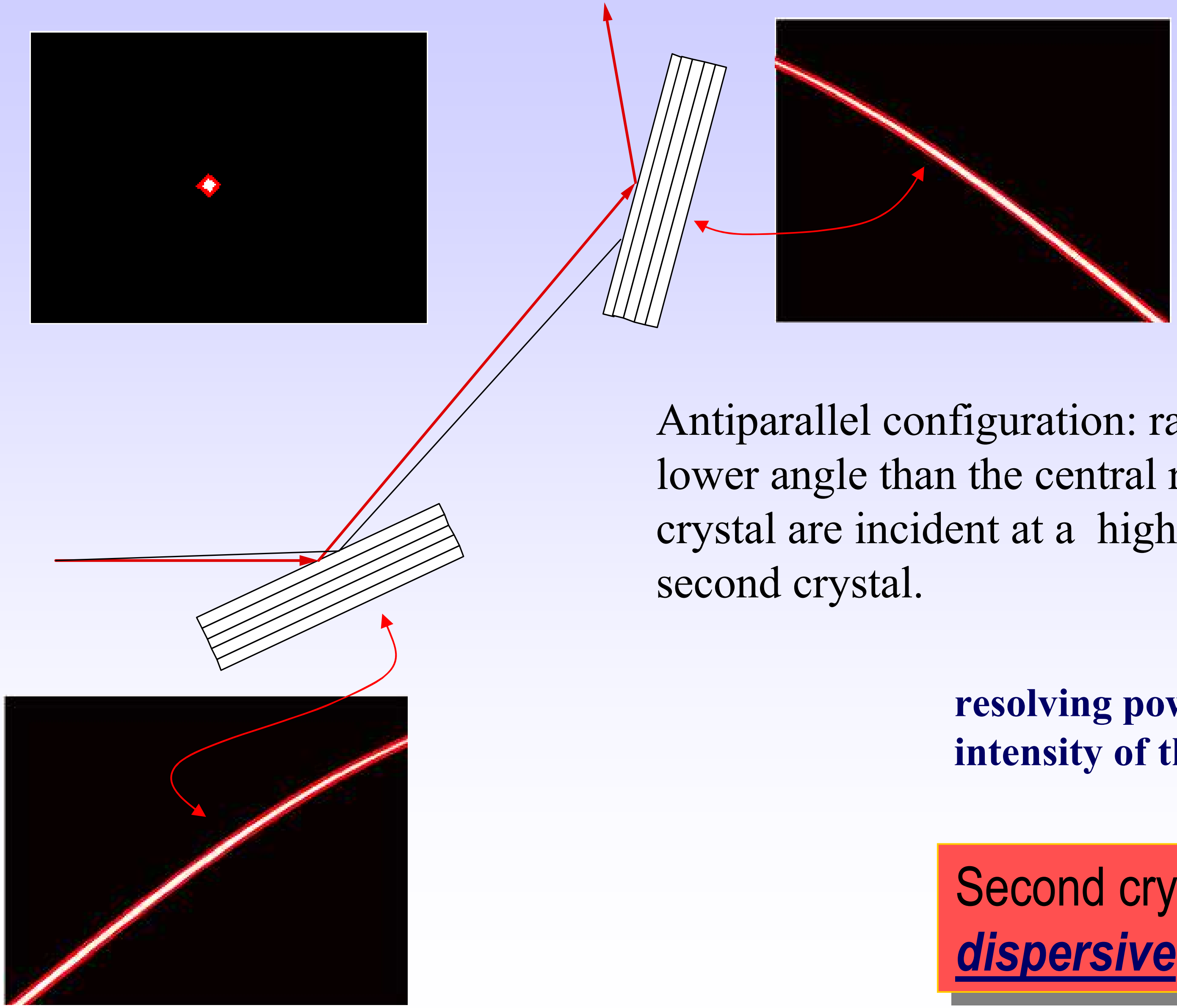
Crystal Monochromators



Parallel geometry:
all rays accepted by the first crystal are accepted also by the second.

Second crystal in
non dispersive configuration

Crystal Monochromators

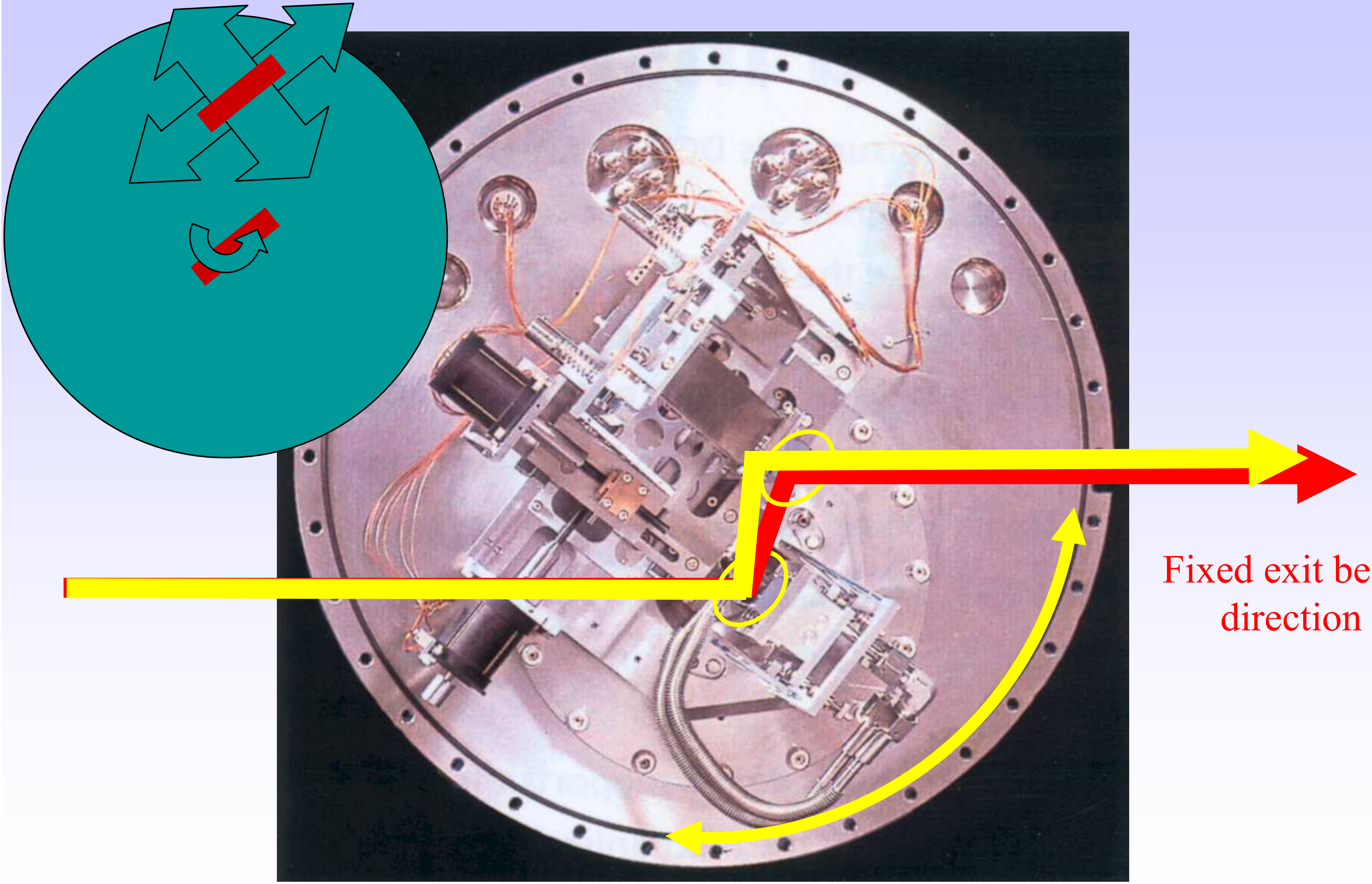


Antiparallel configuration: rays incident at a lower angle than the central ray on the first crystal are incident at a higher angle on the second crystal.

resolving power ↑
intensity of the reflection ↓

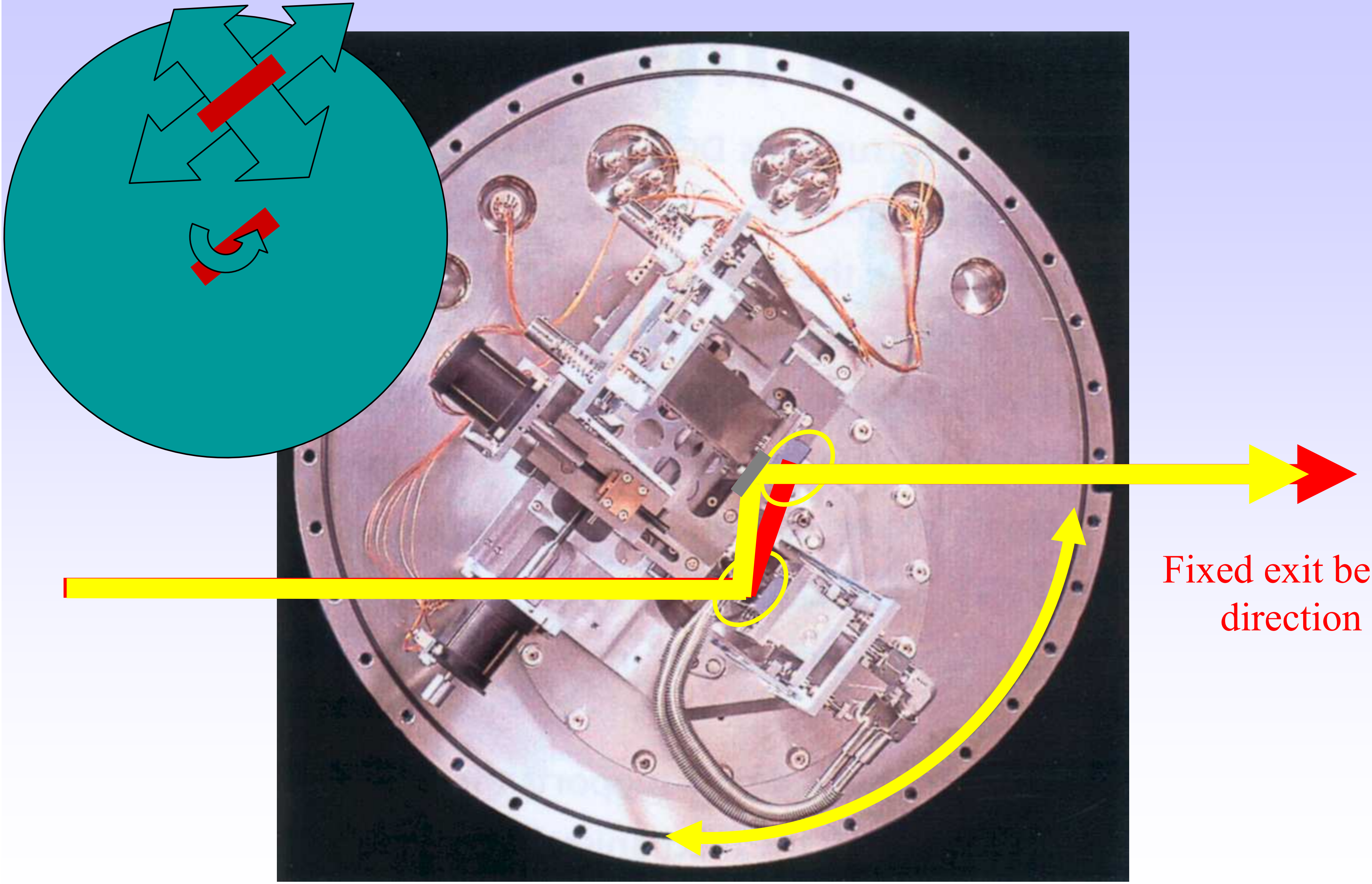
Second crystal in ***dispersive*** configuration

Double Crystal Monochromator



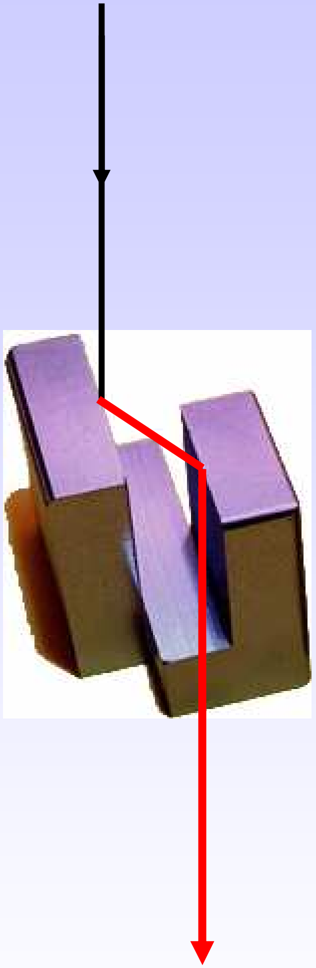
Fixed exit beam direction

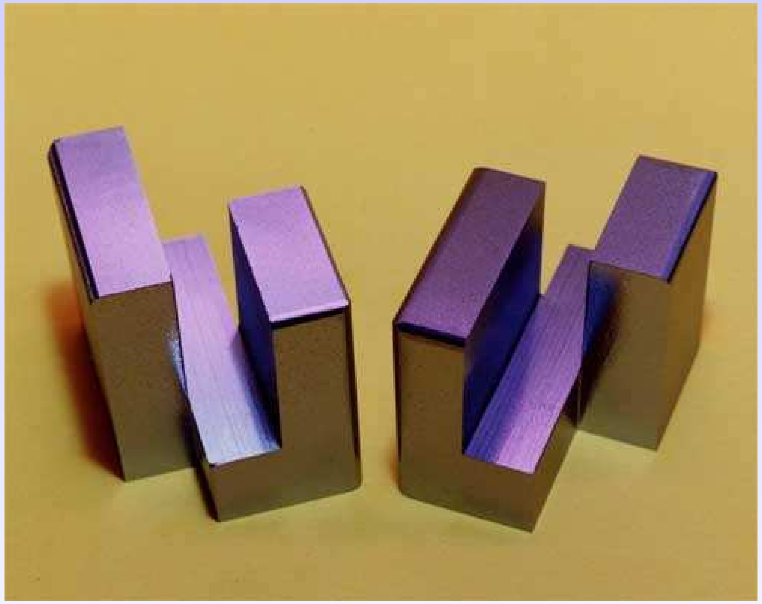
Double Crystal Monochromator



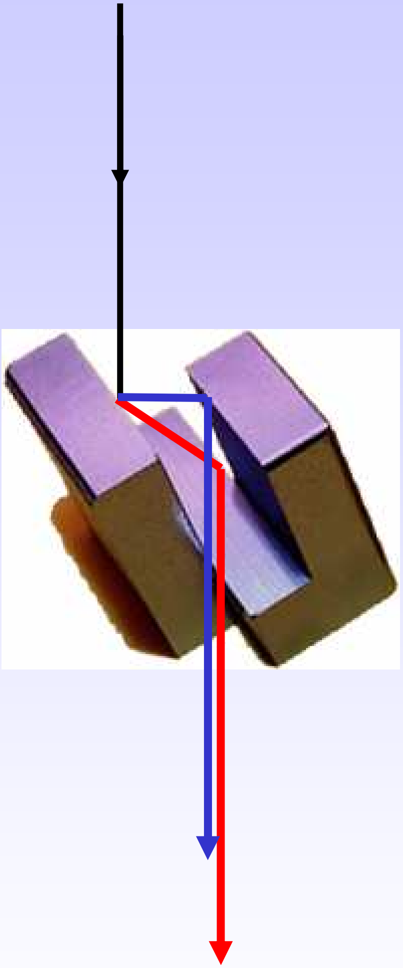
Fixed exit beam direction

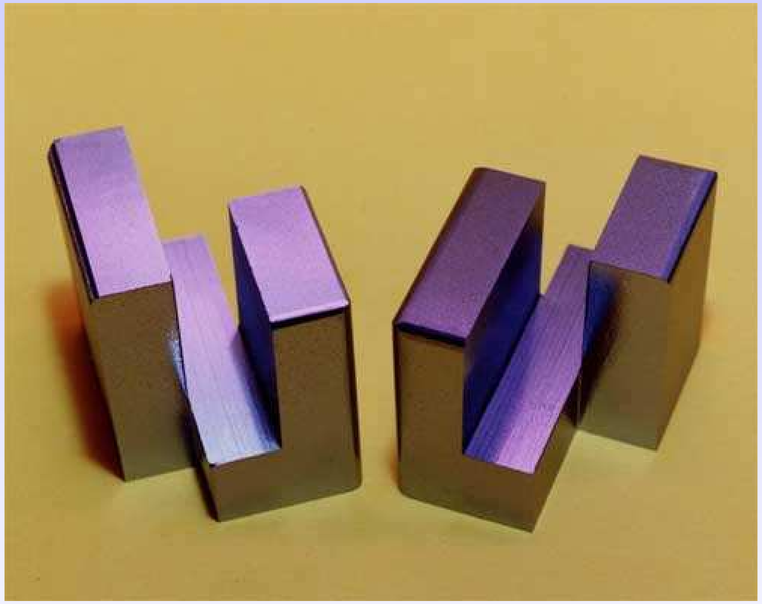
Channel-cut



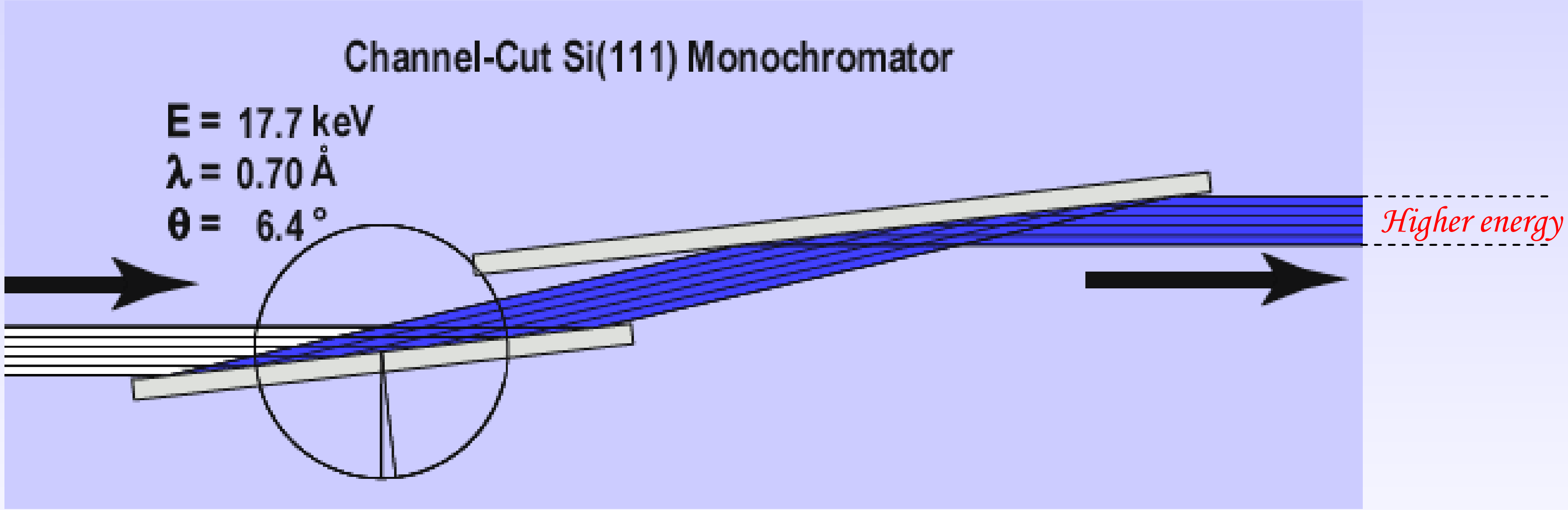


Channel-cut





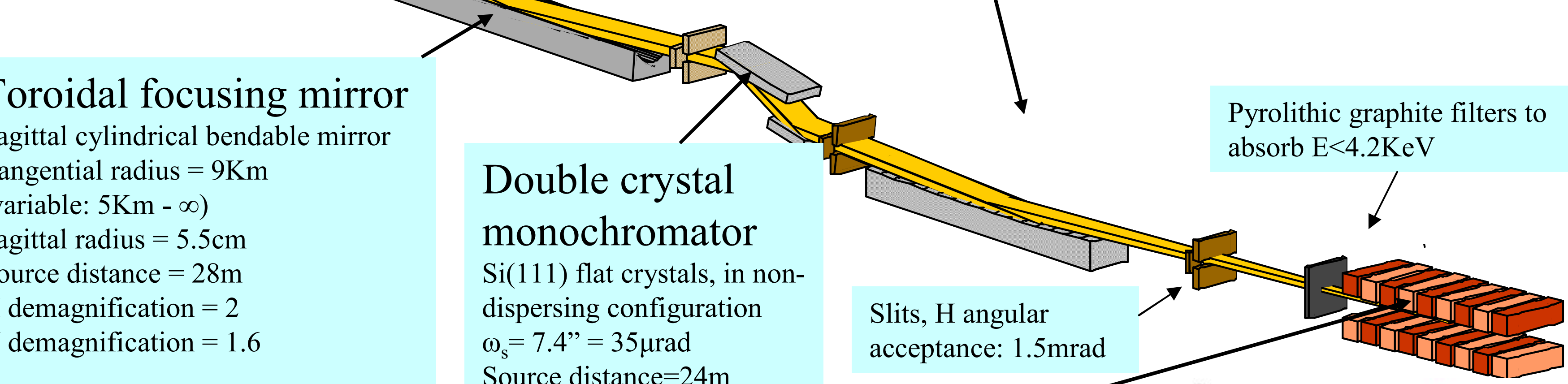
Channel-cut



Much easy to align

Exit beam displacement

Example: the ELETTRA X-ray Diffraction beamline

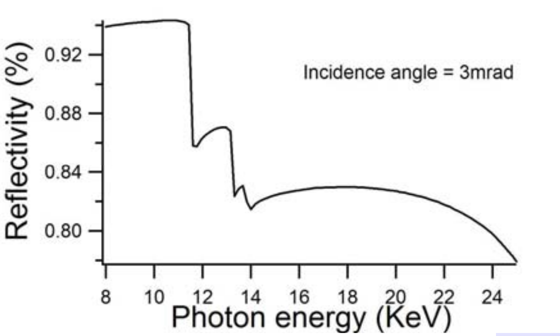


Experiment

Source distance = 41.5m
Energy range: 4-21KeV
spot size: 0.7x0.2mm^2
Photon flux: 10^{12}ph/s (at λ=1Å)
Resolving power: 3-4000

Cylindrical mirror for vertical collimation

Silicon with 50nm Platinum coating
Mirror length=1.4m
i=3mrad; Vertical angular acceptance =180µrad
Radius=14Km
Source distance d=22m
Collimated beam vertical divergence <10µrad



Toroidal focusing mirror

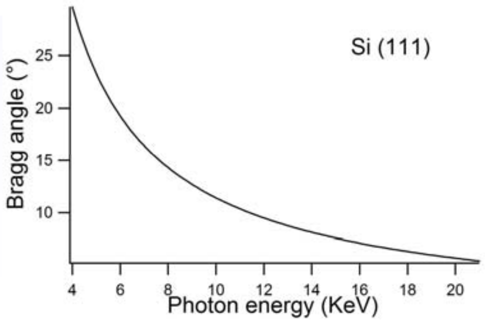
Sagittal cylindrical bendable mirror
Tangential radius = 9Km
(variable: 5Km - ∞)
Sagittal radius = 5.5cm
Source distance = 28m
H demagnification = 2
V demagnification = 1.6

Double crystal monochromator

Si(111) flat crystals, in non-dispersing configuration
ω_s= 7.4" = 35µrad
Source distance=24m

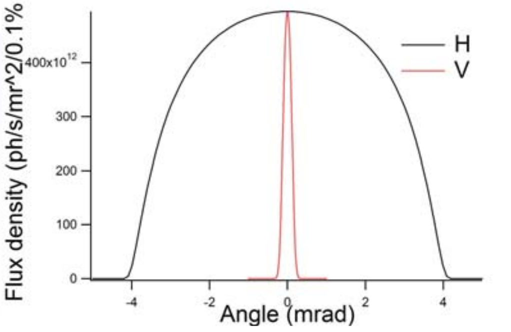
Slits, H angular acceptance: 1.5mrad

Pyrolithic graphite filters to absorb E<4.2KeV



Multi-pole wiggler

57 poles, 1.5T magnetic field,
14cm period length,
5.8KeV critical energy @2.4GeV
5 kW total power @140mA



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- “Selected Papers on VUV Synchrotron Radiation Instrumentation: Beam Line and Instrument Development”, D.L.Ederer Editor, SPIE vol. MS 152, 1998

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- R.L. Johnson, “Grating Monochromators and Optics for the VUV and Soft-X-Ray Region” in “Handbook on Synchrotron Radiation”, Vol.1, E.E.Koch, Editor, North Holland, 1983, chapter 3

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- G.P.Williams, “Monocromator Systems”, in “Synchrotron Radiation Research: Advances in Surface and Interface Science”,Vol.2, R.Z.Bachrach, Editor, Plenum Press, 1992, chapter 9

Programs

- **Shadow** http://www.nanotech.wisc.edu/CNT_LABS/shadow.html
  (ray tracing)

- **XOP** http://www.esrf.eu/computing/scientific/xop2.1/intro.html
  (general optical calculations)

- **SPECTRA** http://radiant.harima.riken.go.jp/spectra/index_e.html
  (optical properties of synchrotron radiation emitted from bending magnets, wigglers and undulators)

Useful link: http://www-cxro.lbl.gov/index.php?content=/tools.html/
(general information and on line software)