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School on Synchrotron Radiation

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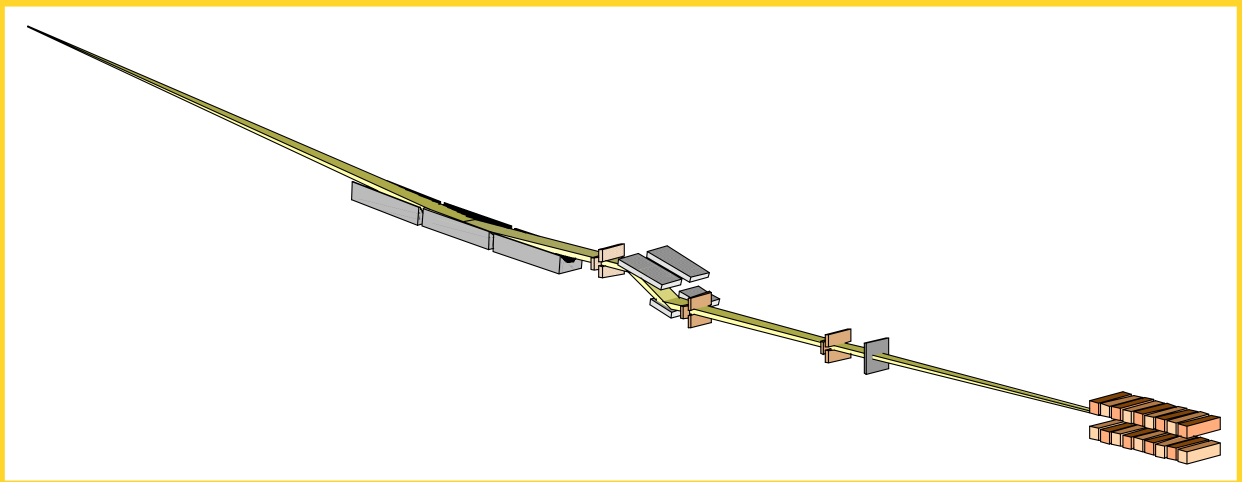
Optical components for hard x-ray beamlines

Edoadro Busetto



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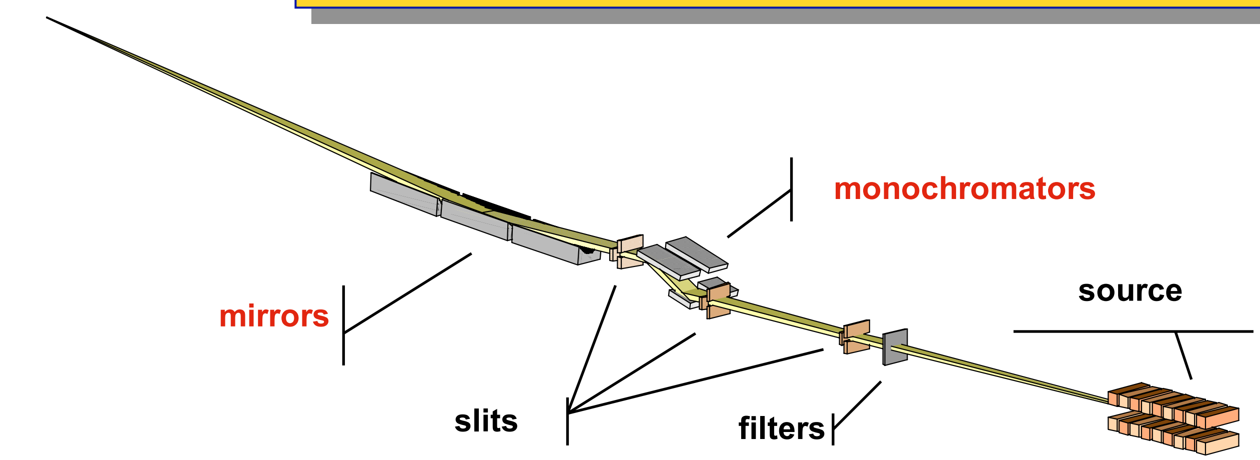
Optical components for hard x-ray beamline

High brilliance and small electron beam emittance mean X-ray beams of high quality

" ...The finite quality and the fundamental limits of the optical components increase the emittance of the beam…….

The main aim of the optical design consists on minimizing the inevitable beam degradation…"

Jean Susini *"Design parameters for hard x-ray mirrors: the ESRF case"*
OPTICAL ENGINEERING/February 1995/Vol. 34 2/361



Most important optical elements:

- sources
- filters
- slits and pinholes
- mirrors
- monochromators
- detectors

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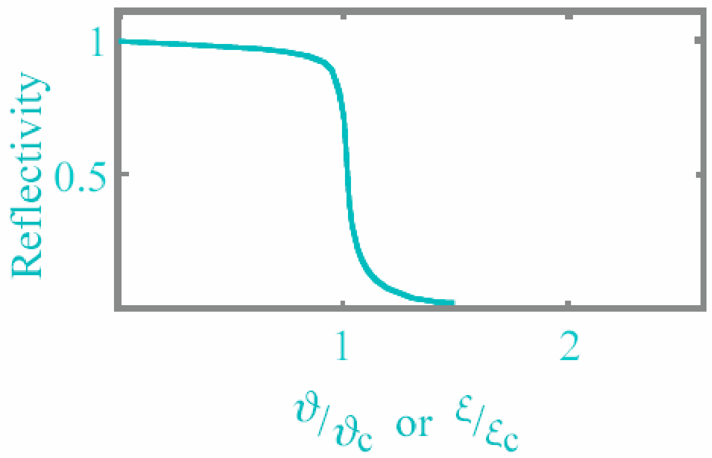
Mirrors 1: total reflection

For x-rays the refractive index is $\mathbf{n} = 1 - \delta$
with $0 < \delta << 1$, therefore is $0 < \mathbf{n} < 1$

If we consider ϑ as the angle that the incoming radiation does with the mirror surface (*grazing angle*), the photons will be totally reflected if $\vartheta < \vartheta_c$



$\vartheta < \vartheta_c$

$\vartheta = \vartheta_c$

$\vartheta > \vartheta_c$

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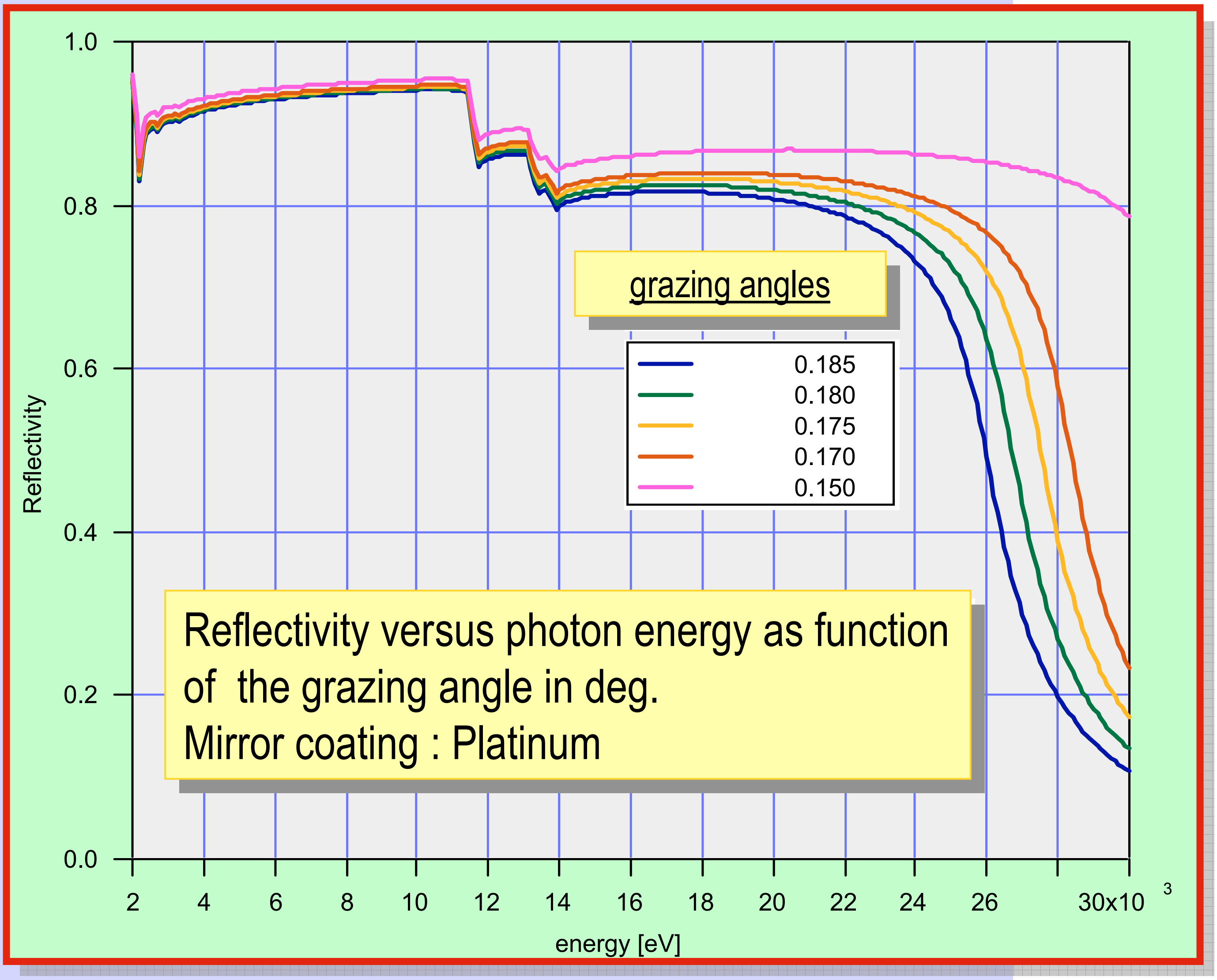

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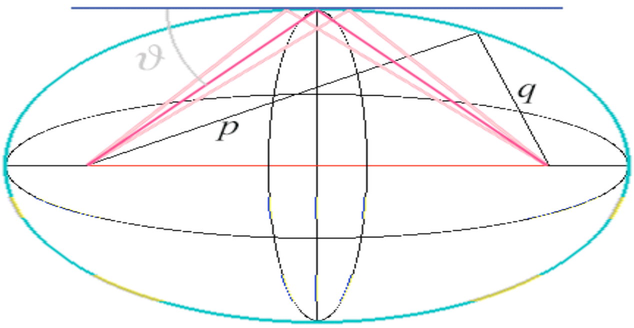
Mirrors 2: focussing

In the ideal mirror device all rays from one particular **point** are reflected and focused into another **point** according to $1/q + 1/p = 1/f$

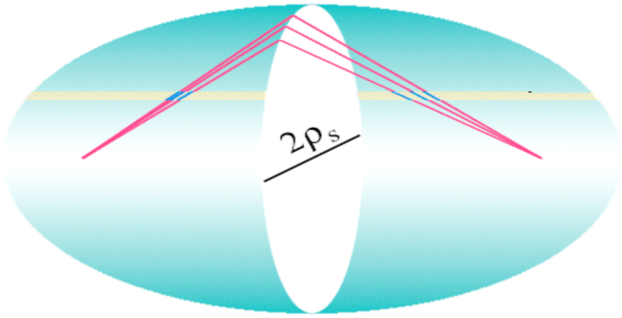
ELLIPSOIDAL SURFACE

best approximation circle



$$\rho_{tangential} = 2f / \sin\vartheta$$

Tangential focussing



$$\rho_{sagittal} = 2f \sin\vartheta$$

Sagittal focussing

** the bending magnet case*

** the extended source case*

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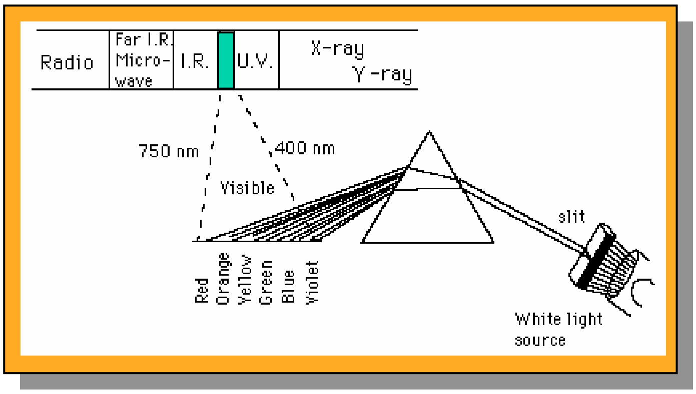

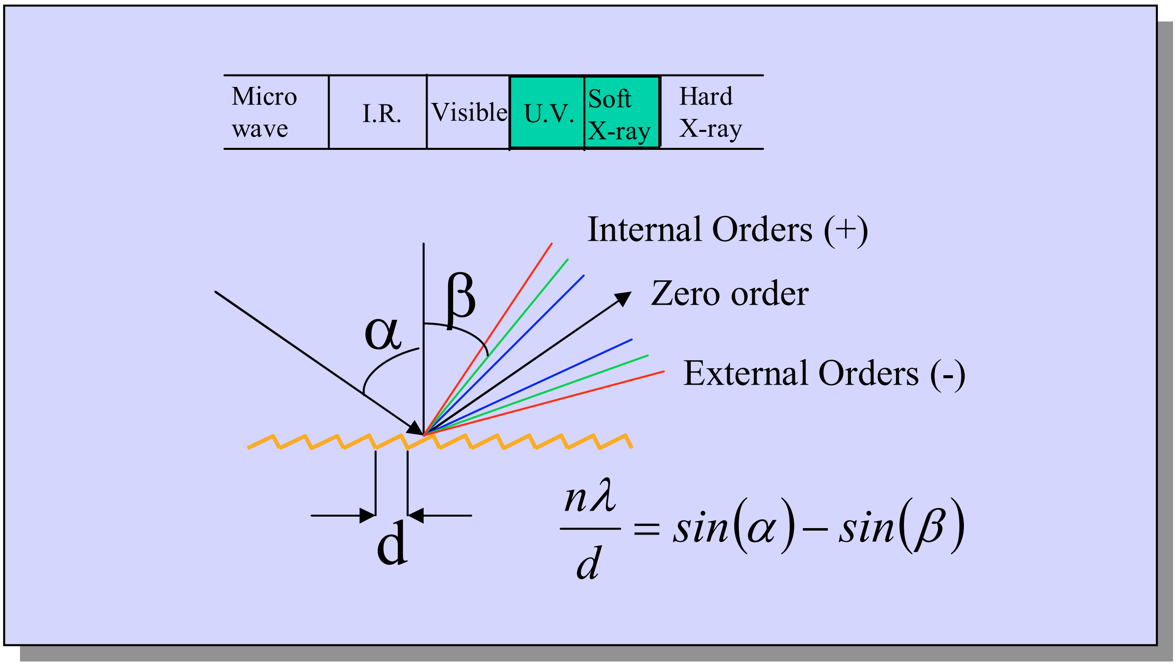

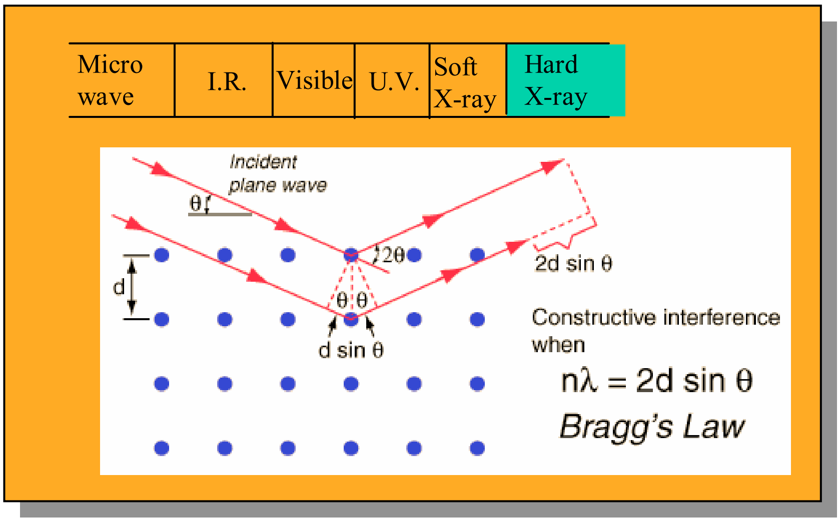

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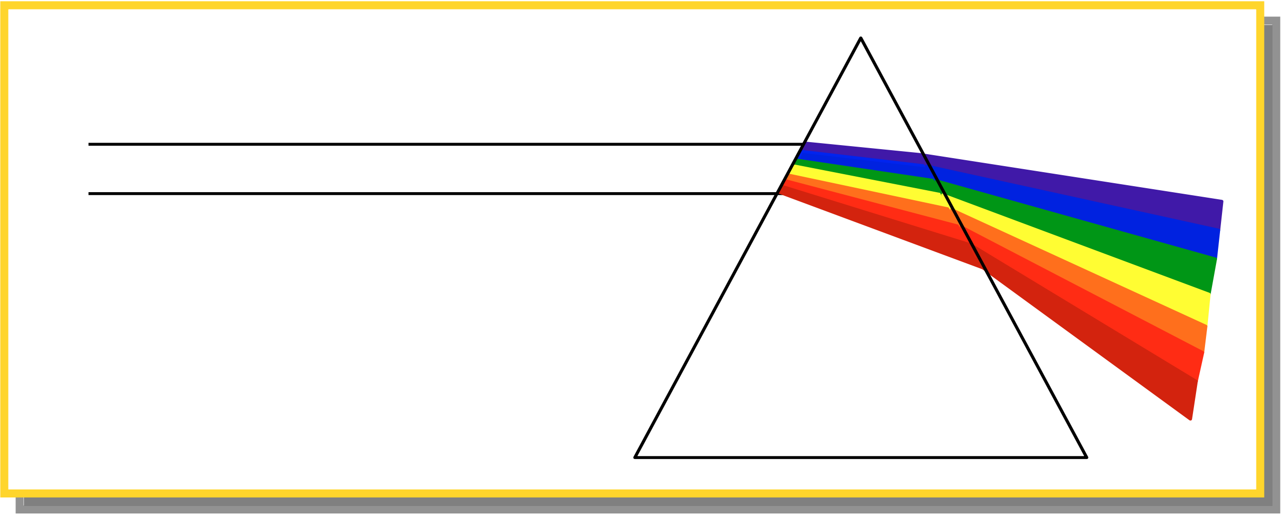

the optical prism is used to separate the components of the white visible light

sampling the out-coming light with a couple of slits it is possible to select a part of the spectrum with a spectral purity which depends on the slits distance and aperture.

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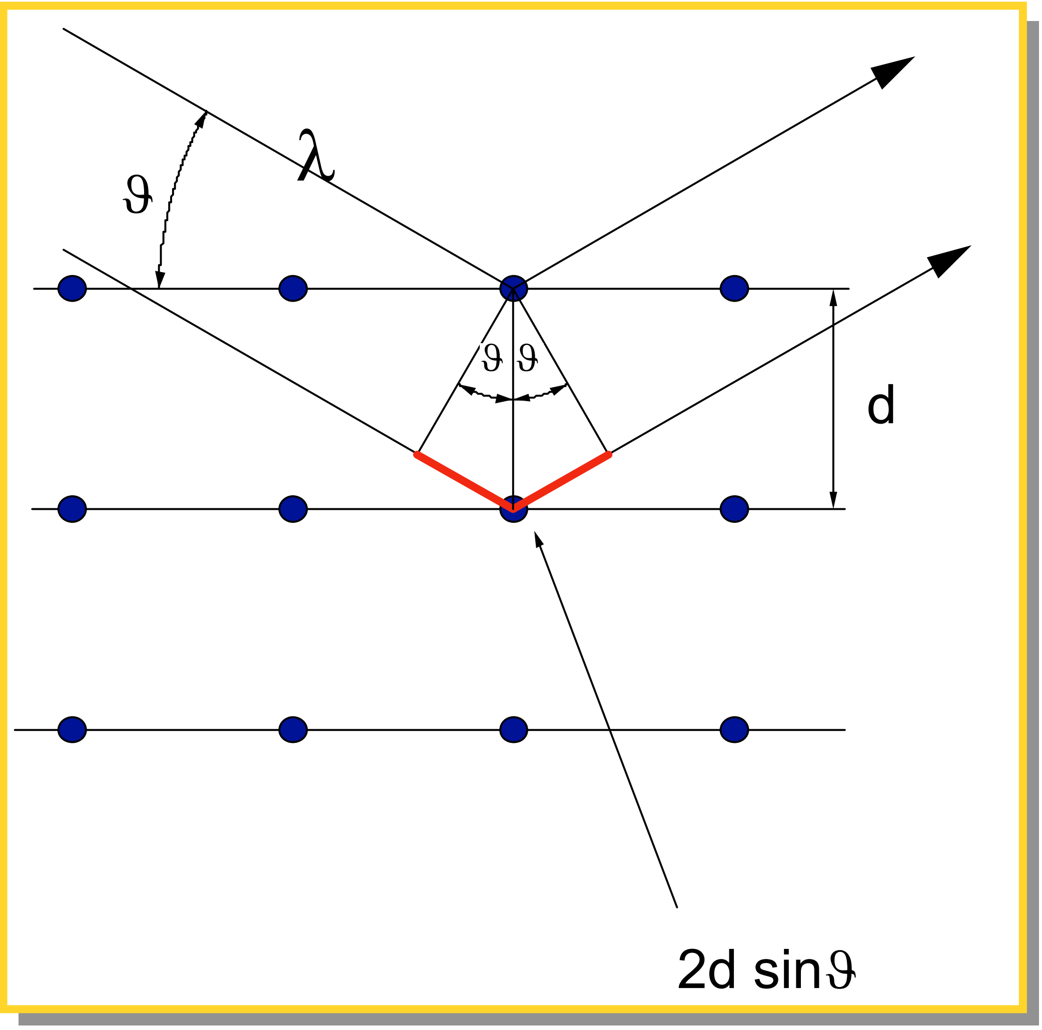

the Bragg's law

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

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

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

from the Bragg law

$$\sin\vartheta = 1 \;\Rightarrow\; \lambda_{\text{max}}$$

therefore

$$\lambda_{\text{max}} = 2\text{d}$$

and the Bragg angle is 90°

important properties for the x-ray monochromators

\- *ENERGY RESOLUTION*

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta E}{E} = \Delta\vartheta \cot g(\vartheta_B)$$

$\Delta\vartheta$ has two contribution :

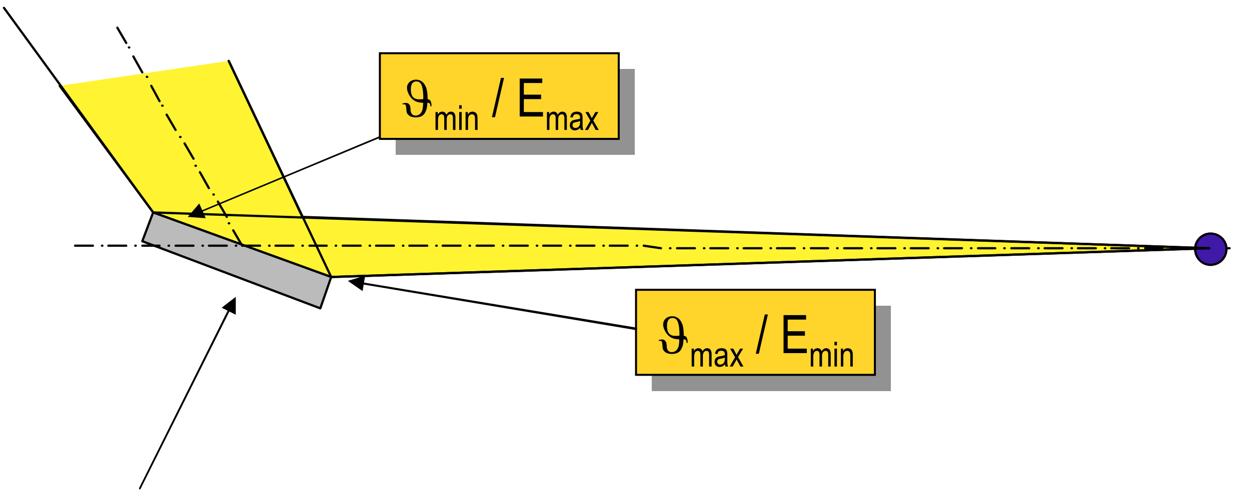
$\Delta\vartheta_{beam}$ - beam angular spread (optics)

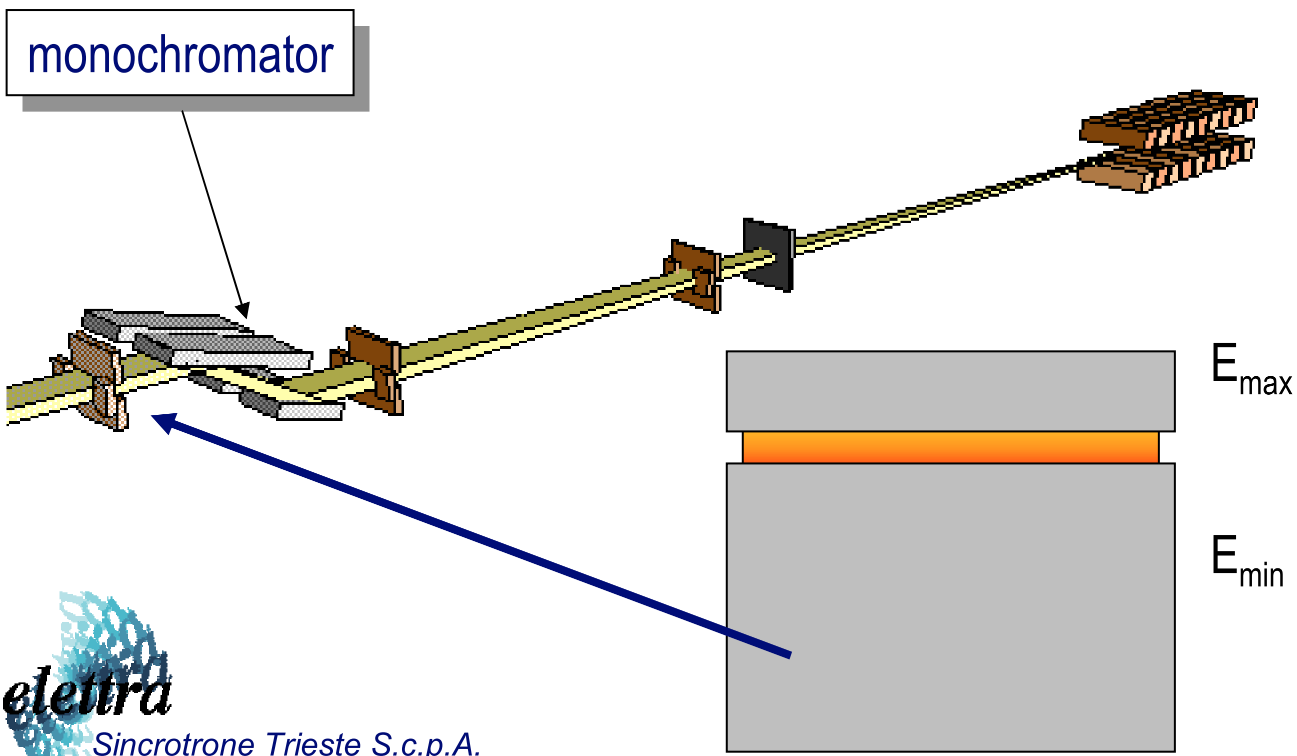
$\omega_{crystal}$ - intrinsic reflection width of the monochromator

Case of $\Delta\vartheta_{beam} >> \omega_{crystal}$

white beam with divergence in the plane of scattering

The crystal accepts all the rays with $\vartheta_{min} \leq \vartheta_B \leq \vartheta_{max}$





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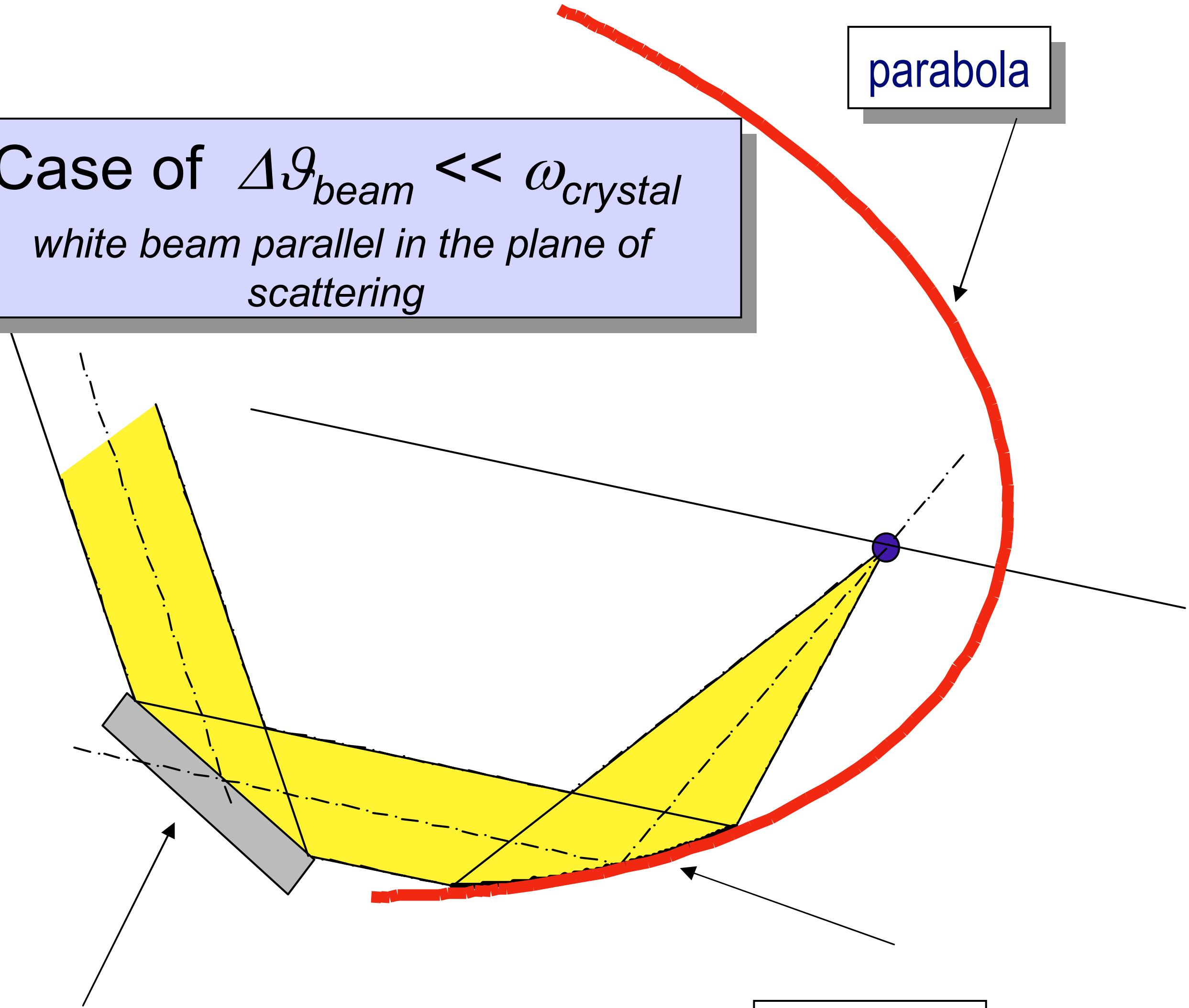
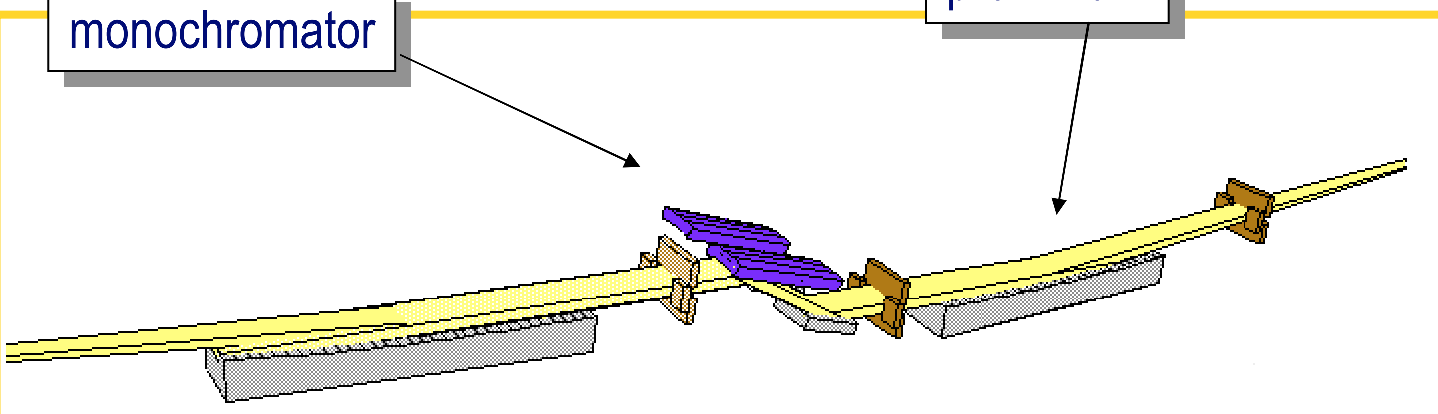
Case of $\Delta\vartheta_{beam} << \omega_{crystal}$

white beam parallel in the plane of scattering





The energy bandwidth is determined by the derivative of the Bragg's law

$$\Delta E = \omega_{crystal} \, \mathrm{cotg}(\vartheta_B) \; E$$

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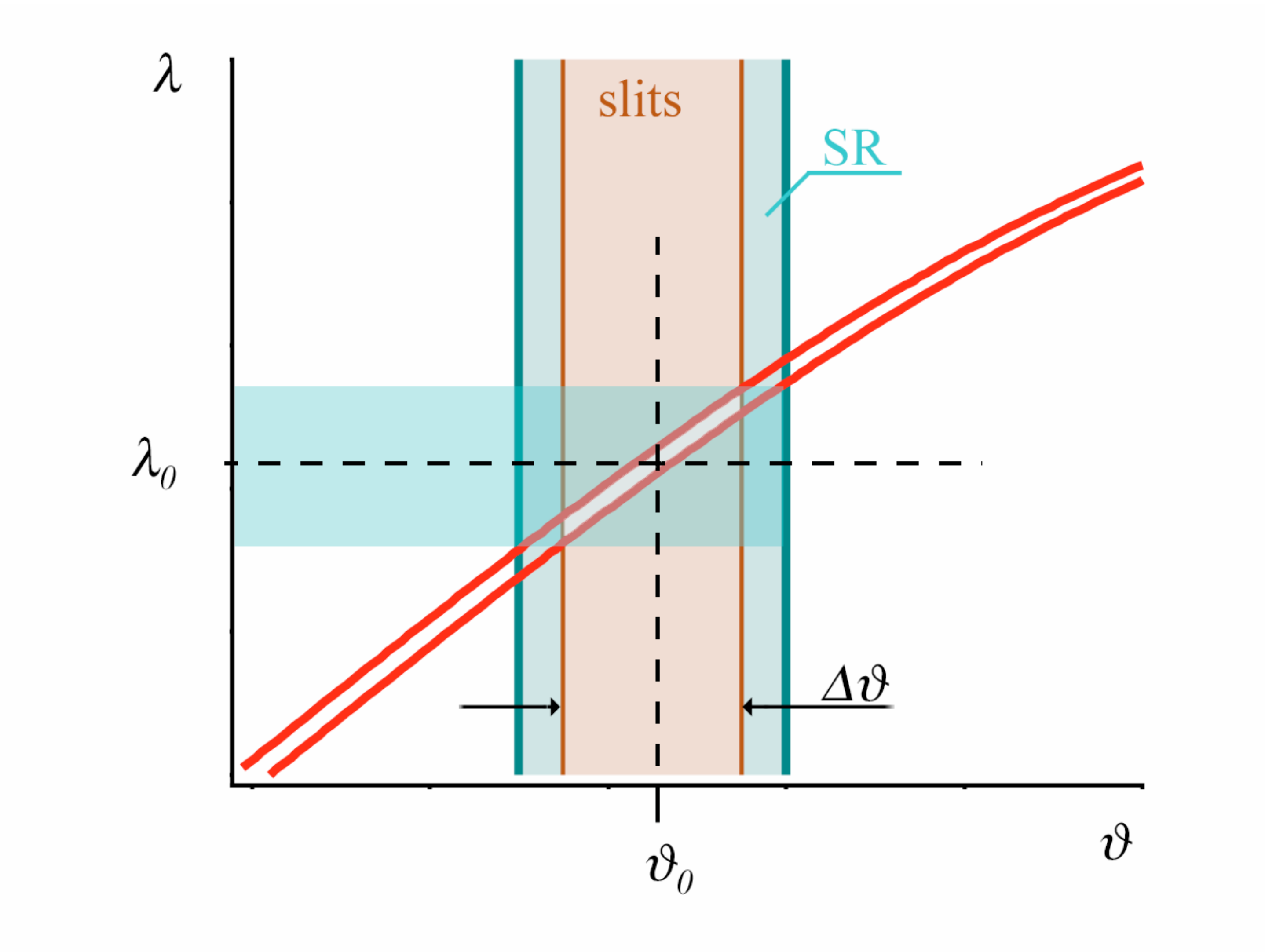
Dumond diagrams



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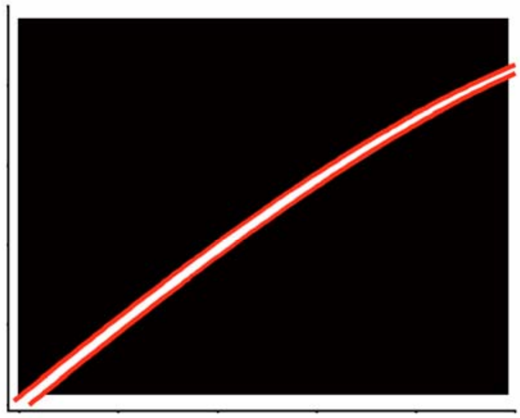
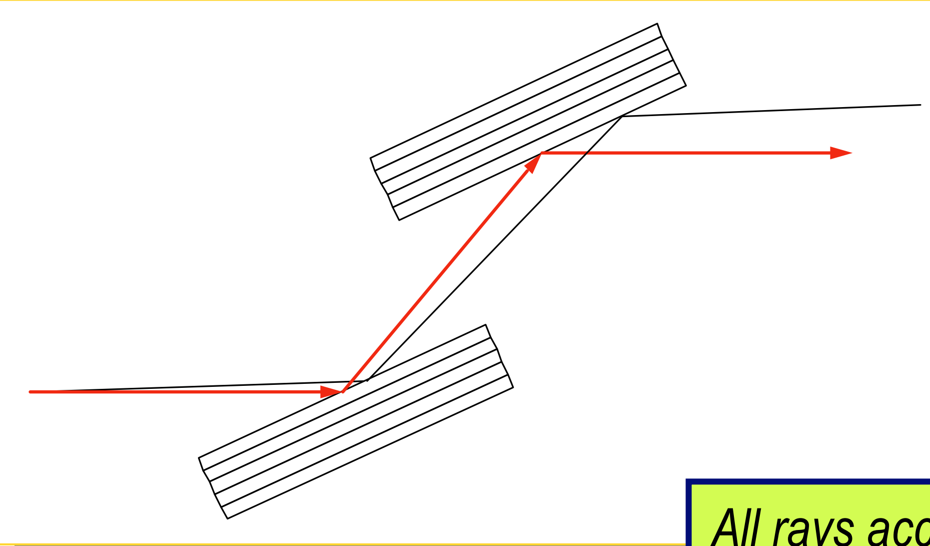
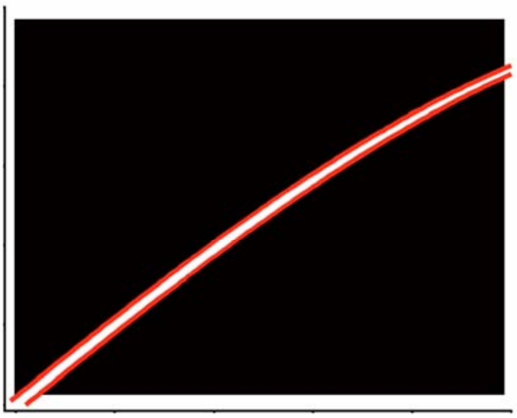
Second crystal in *__non dispersive__* configuration





All rays accepted by the first crystal are accepted also at the second.



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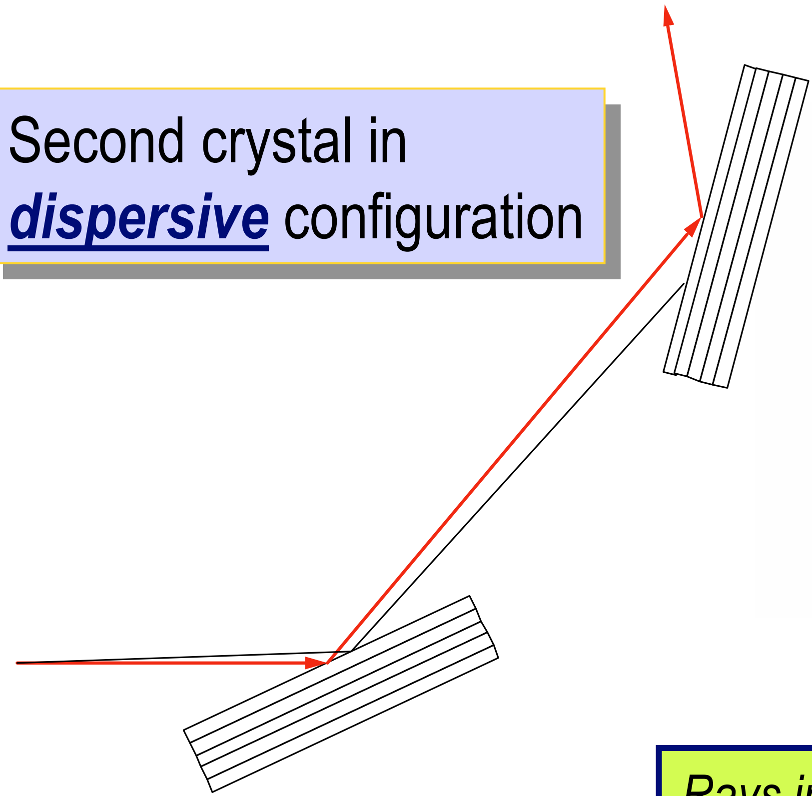
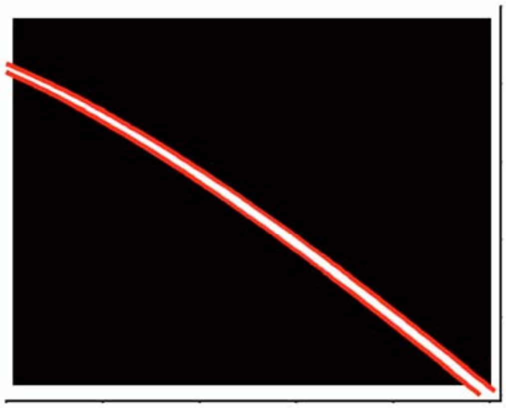
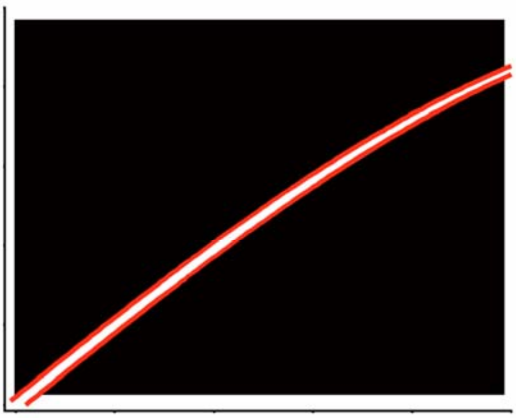
Second crystal in ***dispersive*** configuration

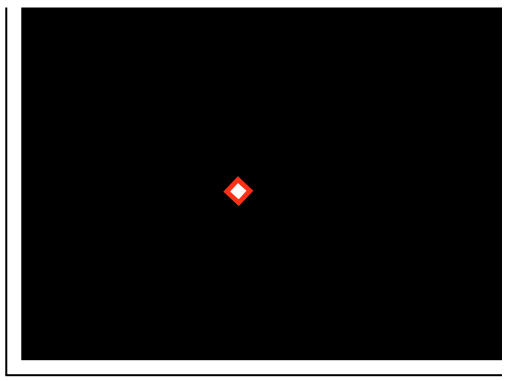






Rays incident at a lower angle than the central ray on the first crystal are incident at a higher angle on the second crystal.

energy resolution ↑
intensity of the reflection ↓



two models for the x-ray diffraction in single crystals

kinematical model

apply this model for:

- **thin perfect crystals**
- **distorted or mosaic crystals**

according with Darwin model (1922) the mosaic crystal is defined by two general conditions:

- crystallites have to be **misoriented** more than the Darwin with of the perfect crystal (loss of the phase condition)
- their dimensions have to be smaller than the **extintion length** of the considered radiation (no second interaction)

dynamical model

apply this model for:

- **thick and perfect crystal**

a) we can't longer consider single interaction. (extinction length)

b) we can't neglect, as well as in the kinematical model, the effect of the radiation absorption

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INTENSITY OF THE REFLECTION

- reflectivity or peak reflectivity
- integral reflecting power

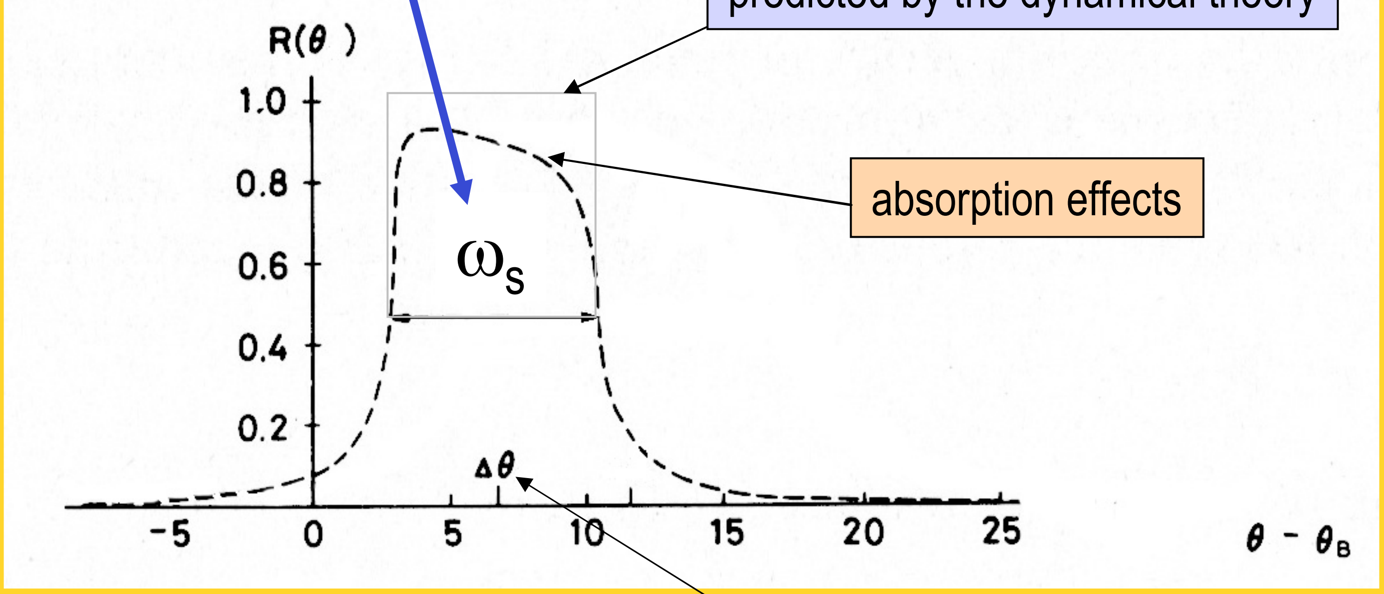
The Darwin curve

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

n	order of the reflection
λ_1	wavelength of the fundamental
$\mathbf{e}^{-M(n)}$	temperature factor
V	volume of the unit cell
ϑ_B	Bragg angle
$\mathbf{R_e}$	radius of the electron $\mathbf{e^2/mc^2}$

$\mathbf{F_{hr}}$ real part of the structure factor related to the diffracted direction **h**(h,k,l)

predicted by the dynamical theory



angular shift due to the refractive effect

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the **b** parameter defined as :

$$b = \frac{\sin(\alpha - \vartheta_B)}{\sin(\alpha + \vartheta_B)}$$

α is the angle between the Bragg plane and the crystal surface

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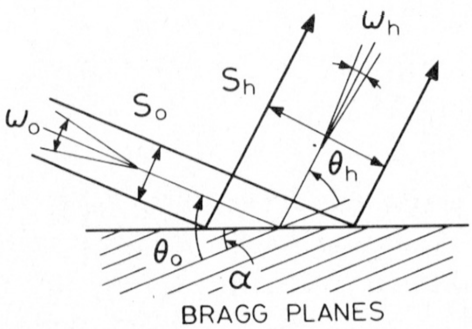

Fig. 3. Geometry of X-ray reflection by a perfect single crystal. θ_0: incidence angle; θ_h: reflection angle. For a non-zero asymmetry angle α $(0 < |\alpha| < \theta_B)$, the angular width ω_0 for acceptance is not equal to the angular width ω_h for emergence. The figure is drawn for $b < 1.0$, where $\omega_0 > \omega_s > \omega_h$. Note also the change of beam cross sections, S_0 and S_h.

$$\omega_0 = \frac{\omega_s}{\sqrt{b}}$$

the angular acceptance as function of the intrinsic width and the **b** parameter:

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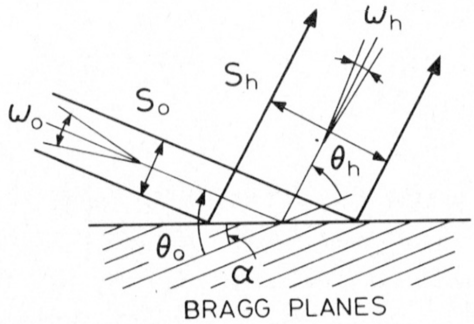

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Bragg reflection width in case of asymmetric cut crystal is defined by:

$$\omega_h = \omega_s \sqrt{b}$$

$$\omega_h = b\omega_o$$

the angular acceptance as function of the Bragg reflection width

also for the beams sections

$$S_h = \frac{S_o}{b}$$

combining the two formulas we have the well known Liouville’s theorem

$$\omega_h S_h = \omega_o S_o$$

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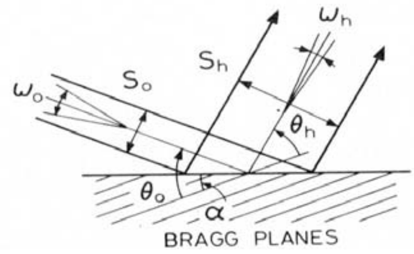

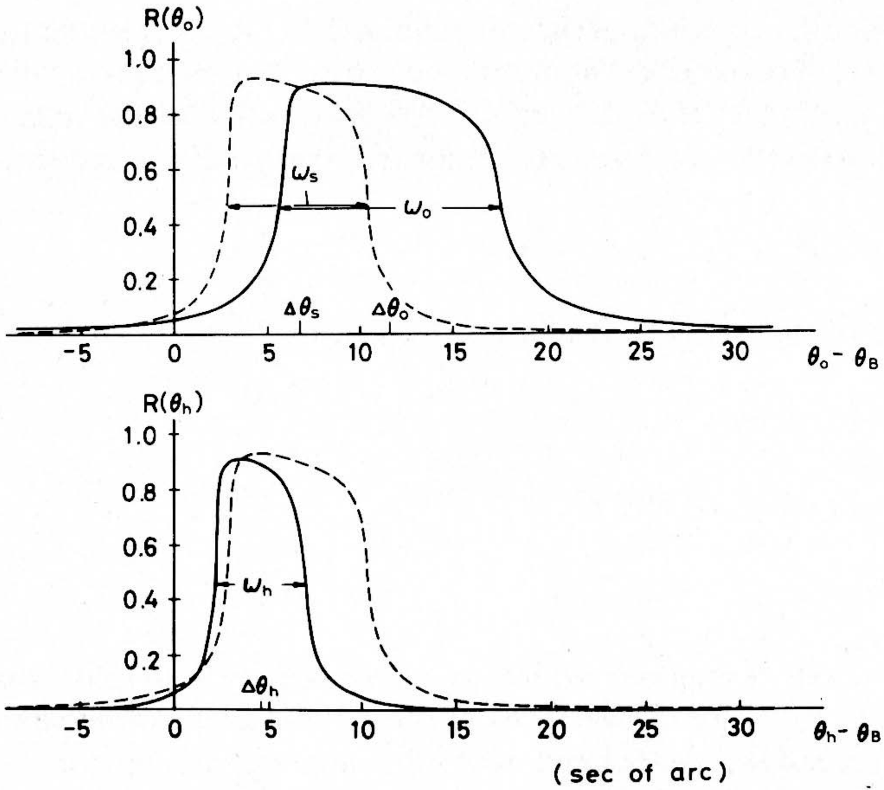

Fig. 4. Perfect-crystal reflection curves for the (111) reflection of silicon at 1.6 Å. $R(\theta_0)$ shows the reflectivity for the ideal plane wave as a function of the incidence angle θ_0, while $R(\theta_h)$ represents the intensity reflected at a reflection angle θ_h for a plane wave incident at θ_0, θ_0 and θ_h being related by $(\theta_h - \theta_B) = b(\theta_0 - \theta_B)$. The solid curves are calculated for an asymmetric case of $b = 0.4$, while the broken curves for the symmetric case ($b = 1.0$) where $R(\theta_0) \equiv R(\theta_h)$.

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Handbook on Synchrotron Radiation, Vol. 1, edited by E.E. Kock
North-Holland Publishing Company, 1983

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Table 2
Intrinsic Bragg reflection widths ω_s, energy resolutions $\Delta E/E$ and integral reflecting powers I of perfect crystals of silicon, germanium and α-quartz at 1.54 Å.

Crystal	*hkl*	ω_s (second or arc)	$\Delta E/E$ ($\times 10^5$)	I ($\times 10^6$)
Silicon	111	7.395	14.1	39.9
	220	5.459	6.04	29.7
	311	3.192	2.90	16.5
	400	3.603	2.53	19.3
	331	2.336	1.44	11.8
	422	2.925	1.47	15.5
	333 (511)	1.989	0.88	9.9
	440	2.675	0.96	14.0
	531	1.907	0.60	9.3
Germanium	111	16.338	32.64	85.9
	220	12.449	14.46	67.4
	311	7.230	6.92	37.1
	400	7.951	5.94	42.3
	331	5.076	3.34	25.4
	422	6.178	3.34	32.4
	333 (511)	4.127	2.00	20.2
	440	5.339	2.14	27.5
	531	3.719	1.33	17.7
α-quartz	100	3.798	10.00	18.8
	101	7.453	15.26	40.9
	110	2.512	3.69	12.2
	$10\bar{2}$	2.488	3.36	12.9
	200	2.252	2.81	11.5
	112	2.927	3.03	15.5
	202	2.072	1.93	10.6
	212	2.042	1.47	10.7
	$20\bar{3}$	2.430	1.74	12.9
	301	2.368	1.69	12.6

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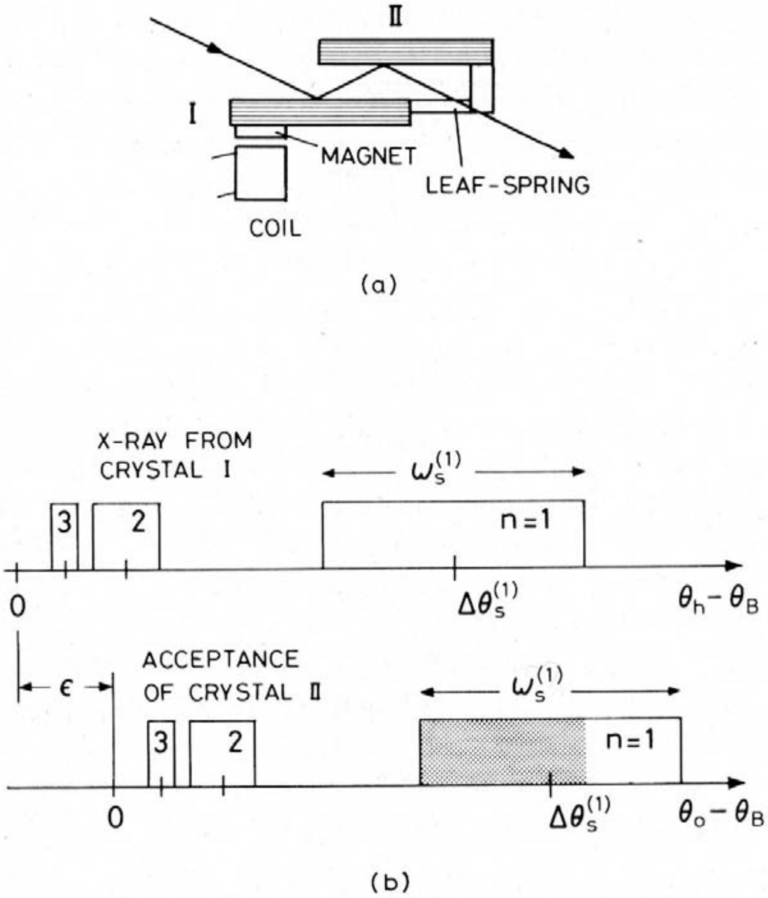

Fig. 33. An off-set harmonics-rejection monochromator. (a) Geometry of the monochromator. (b) The principle of harmonics rejection. Perfect-crystal reflection curves for the fundamental ($n = 1$) and the harmonics ($n = 2, 3$) are approximated by rectangular boxes. ε: off-set or misalignment angle. The shaded area represents delivered X-rays (Hart and Rodrigues 1978).

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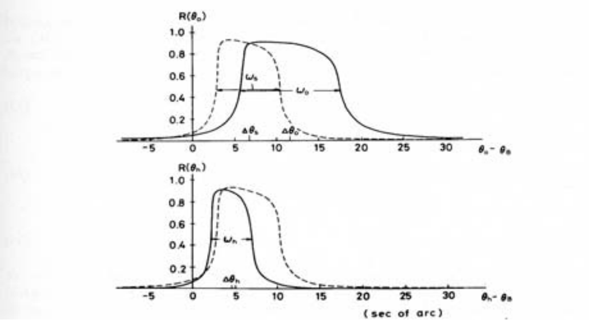

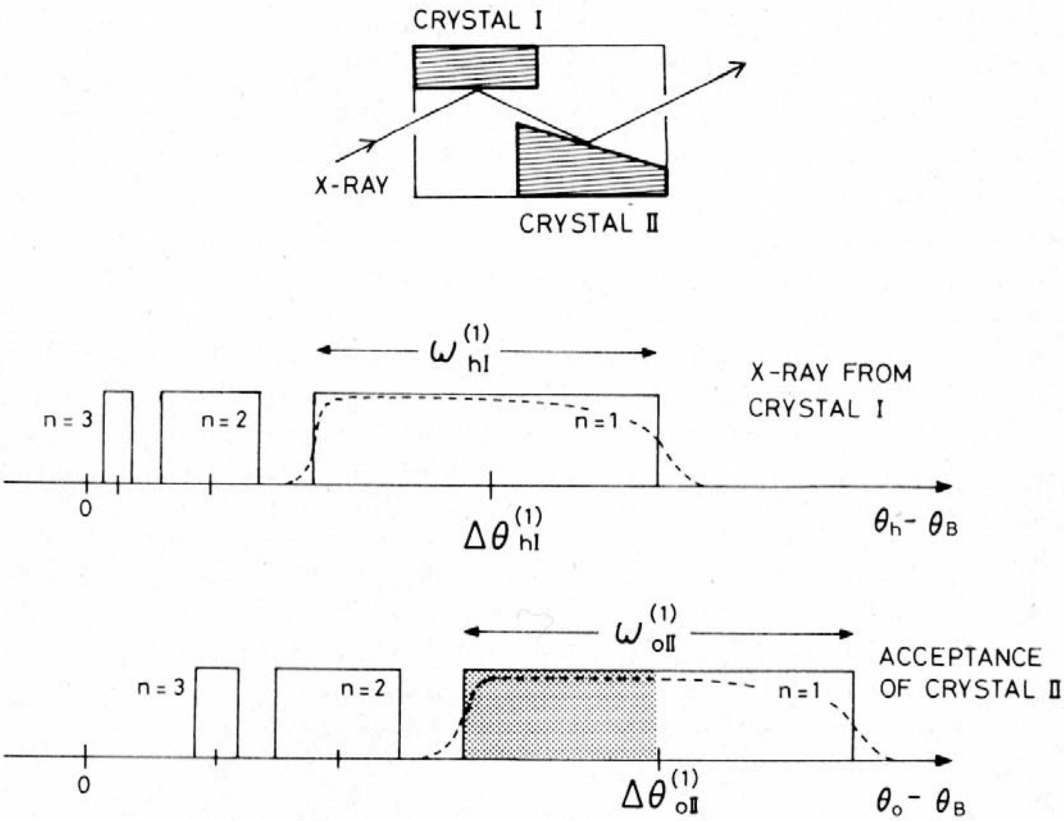

Fig. 34. A monolithic harmonics-rejection monochromator. (a) Crystals I and II of unequal asymmetry factors are built as two outstanding parts of a perfect single crystal. (b) The principle of harmonics rejection. Perfect-crystal reflection curves for the fundamental ($n = 1$) and the harmonics ($n = 2, 3$) are approximated by rectangular boxes. The broken curves show the real reflection curves for the fundamental. The shaded area represents delivered X-rays.

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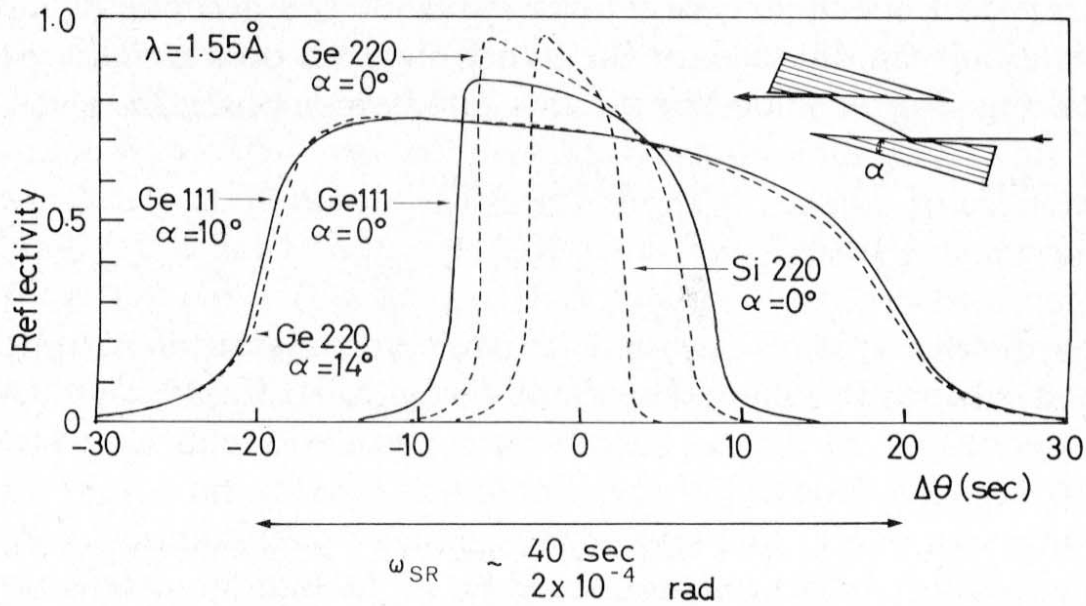

Calculated reflectivity curves of grooved monochromators using various asymmetric reflections of silicon and germanium for 1.55 Å X-rays (Kohra et al. 1978).

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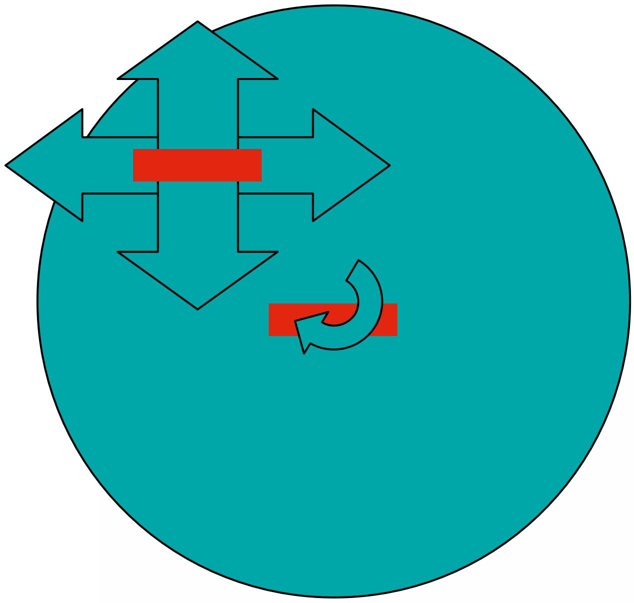
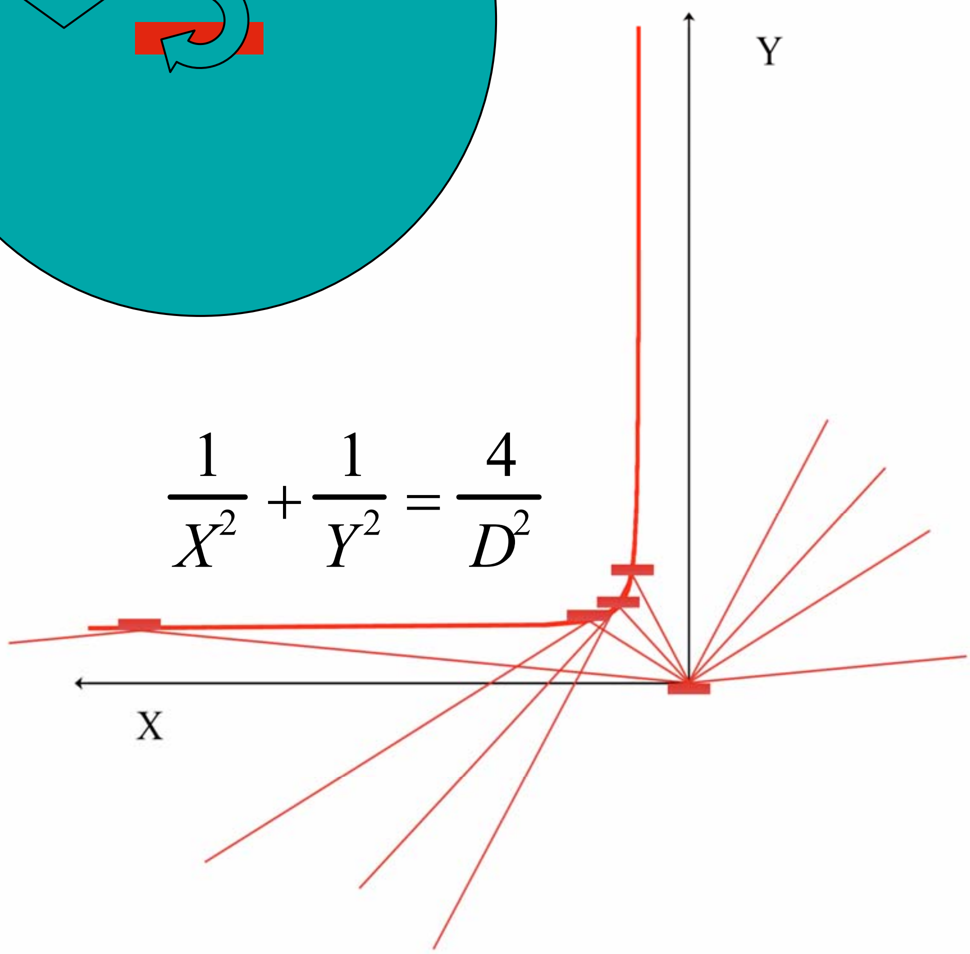
Note as the refractive effect on the first crystal has been totally compensated by the second one

Double crystal monochromator





$$\frac{1}{X^2} + \frac{1}{Y^2} = \frac{4}{D^2}$$