

SOS - WORKSHOP

Simulating Hard X-ray beamline
optics by ray-tracing using
ShadowOui

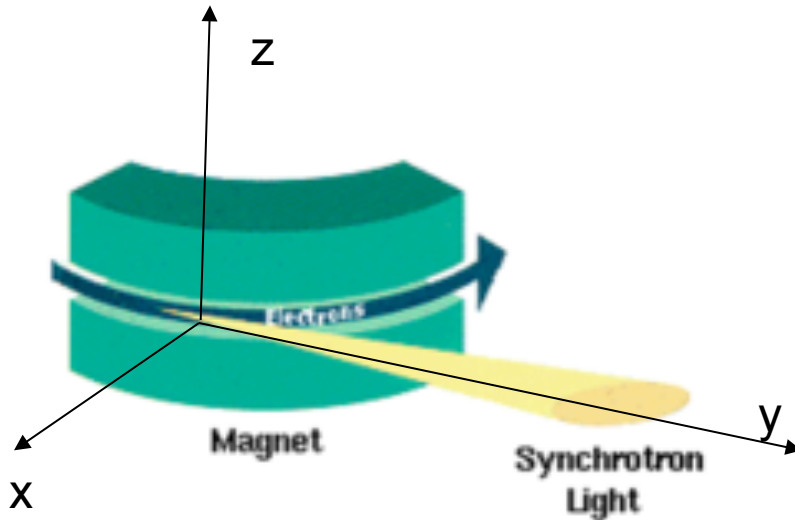
Manuel Sánchez del Río

AAM, ISDD, ESRF

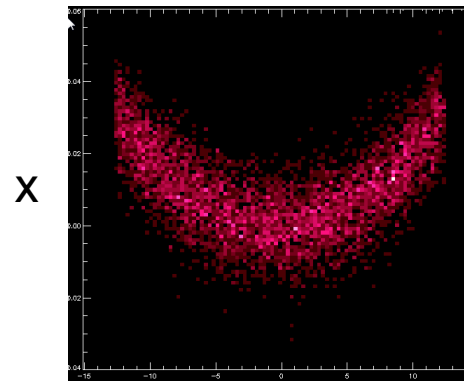
Oasys+ShadowOui

- Install Oasys+ShadowOui:
 - <https://github.com/srio/oasys-installation-scripts/wiki>
- Download Tutorial Examples:
 - <https://github.com/srio/ShadowOui-Tutorial>

BM – Emission by N incoherent e^-

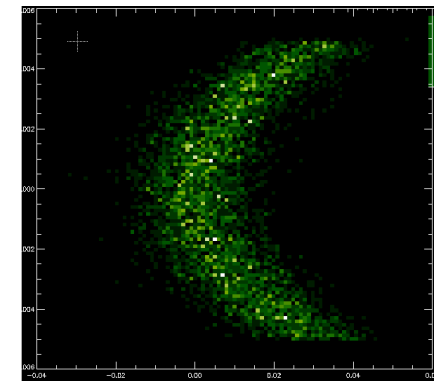


Real Space (top)



y

Phase Space (H)



x

- Monte Carlo (SHADOW)
 - Energy (and polarisation) sampled from spectrum
 - Angular Distribution ($1e^-$, σ'_x , σ'_z)
 - Geometry (along the arc, σ_x , σ_z)
 - Limitation: Computer time and memory
 - Typically: 10^3 - 10^9 rays
 - Desirable: one ray per photon, i.e., 10^{14} - 10^{20}

Wiggler: Like BM, but a bit more complex

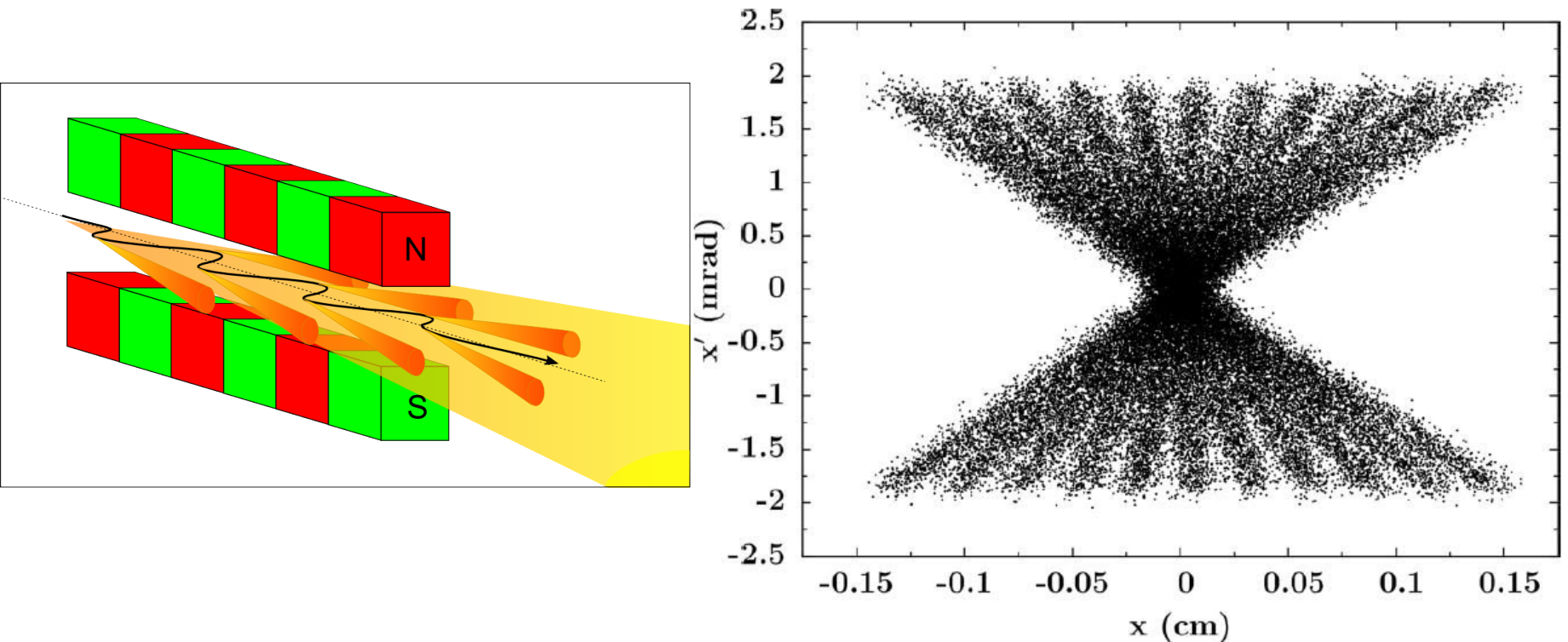
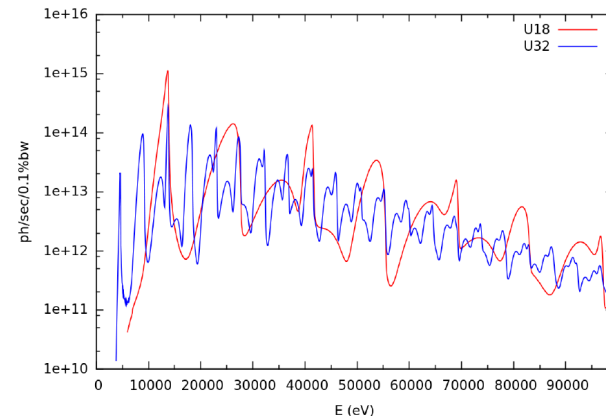
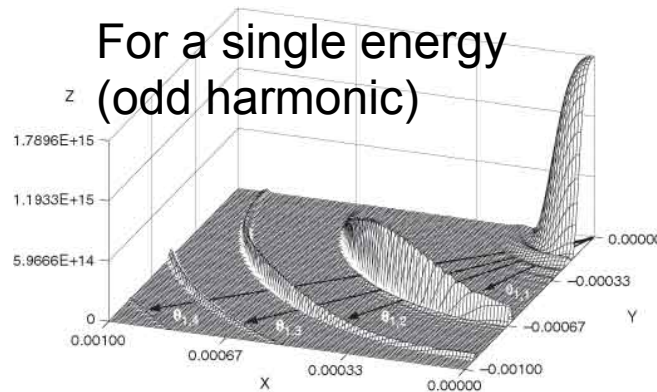
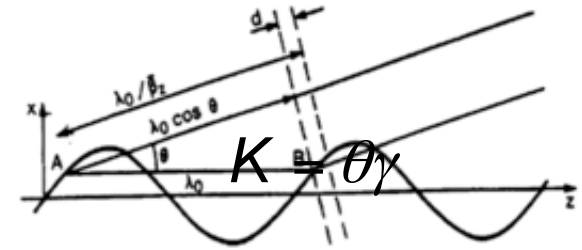
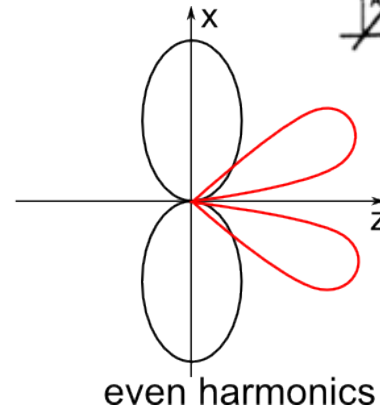
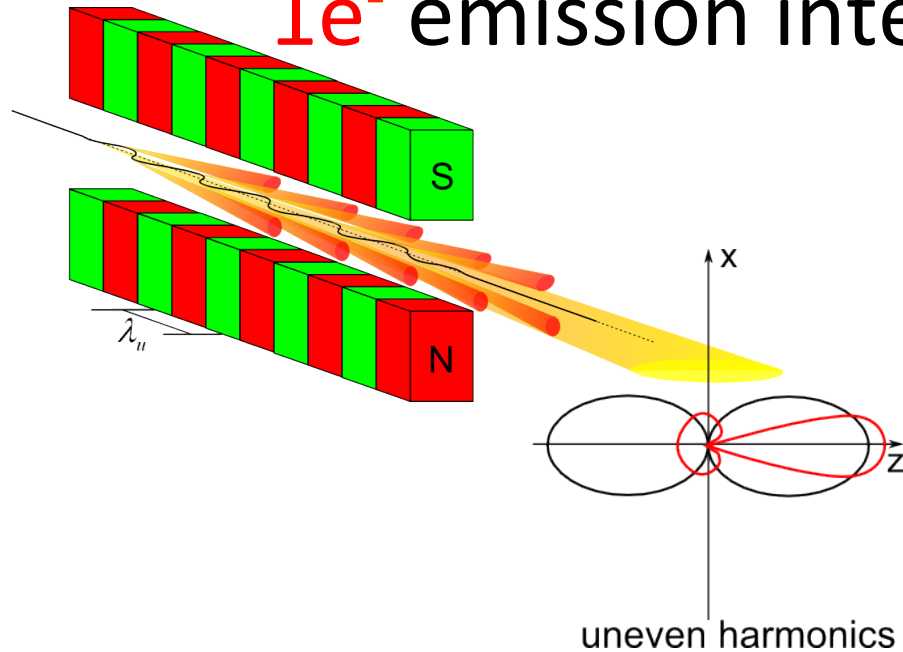


Figure 5

Plot of the horizontal phase space for a wiggler (ID17 at the ESRF) with 11 periods of 0.15 m length, $K = 22.3$ and electron beam energy of 6.04 GeV.

Undulator: Much more complex:

$1e^-$ emission interferes with itself



Onuki & Elleaume Undulators, Wigglers and their applications, CRC press, 2002

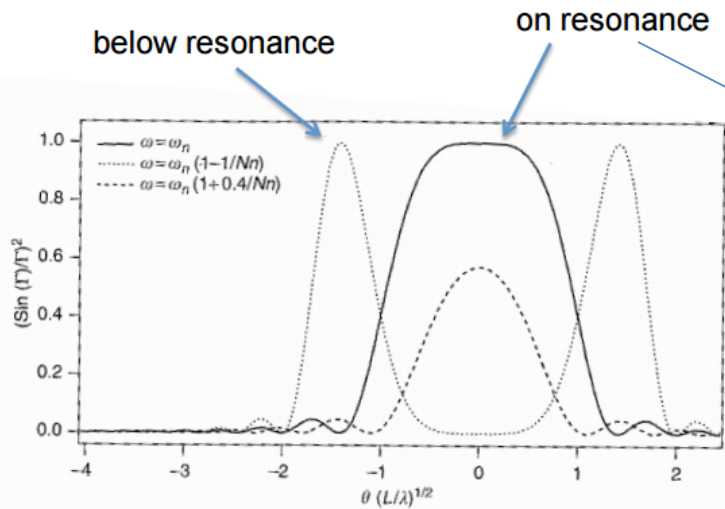


Figure 3.3 Graph of $(\sin(\Gamma)/\Gamma)^2$ as a function of the angle $\theta = \sqrt{\theta_x^2 + \theta_z^2}$ for three different frequencies. ω_n is an abbreviation for $n\omega_1(0, 0)$.

78 P. Elleaume

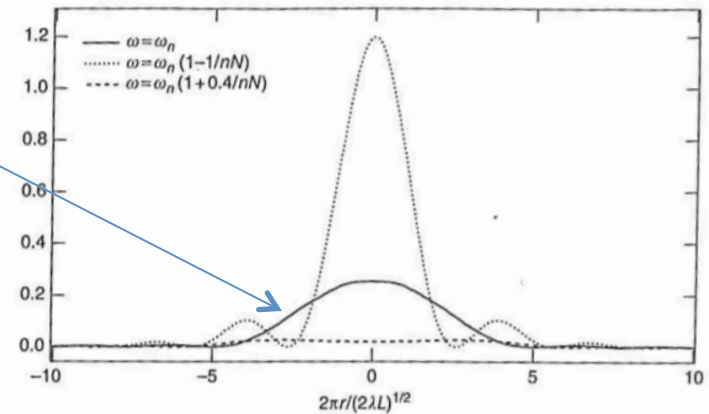


Figure 3.4 Spectral flux per unit surface in the middle of the undulator for three frequencies close to the on-axis resonant frequency $\omega_n = n\omega_1(0, 0)$.

Even on resonance, beam is not fully Gaussian
But for resonance, can be reasonably approximated as Gaussian

$$\sigma_{r'} = 0.69 \sqrt{\frac{\lambda}{L}} \approx \sqrt{\frac{\lambda}{2L}}$$

$$\sigma_r = \frac{2.704}{4\pi} \sqrt{\lambda L} \approx \sqrt{\frac{\lambda L}{2\pi^2}}$$

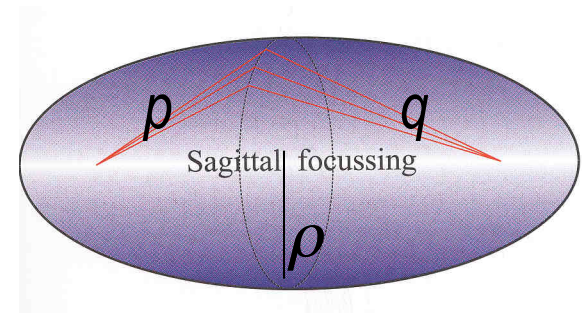
$$\sigma_r \sigma_{r'} = \frac{1.89\lambda}{4\pi} \approx \frac{\lambda}{2\pi}$$

- Undulator beams have not Gaussian profiles (even at resonances)
- BY NOW, WE APPROXIMATE UNDULATORS BY GEOMETRIC SOURCES WITH GAUSSIAN SIZES AND DIVERGENCES

Non-imaging system:

BL as a concentrator: which shape (in reflection)?

- Point to point focusing (ellipsoid)
- Collimating (paraboloid)
- Focalization in two planes
 - Tangential or Meridional (ellipse or parabola)
 - Sagittal (circle)
- Demagnification: $M=p/q$
- Easier manufacturing:
 - 2D: Ellipsoid => Toroid
 - Only one plane: cylinder Ellipsoid (ellipse)=> cylinder (circle)
 - Sagittal radius: non-linear (ellipsoid) => constant (cylinder) or linear (cone),
- Aberrations

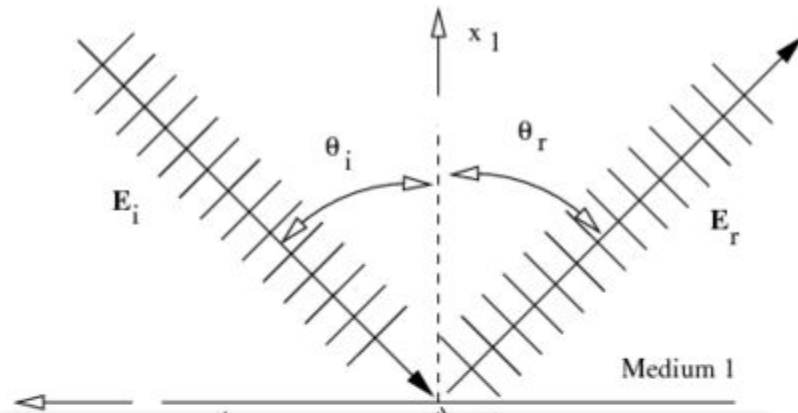


$$\frac{1}{p} + \frac{1}{q} = \frac{2}{R \sin \theta}$$

$$\frac{1}{p} + \frac{1}{q} = \frac{2 \sin \theta}{\rho}$$

Mirrors

Geometrical model

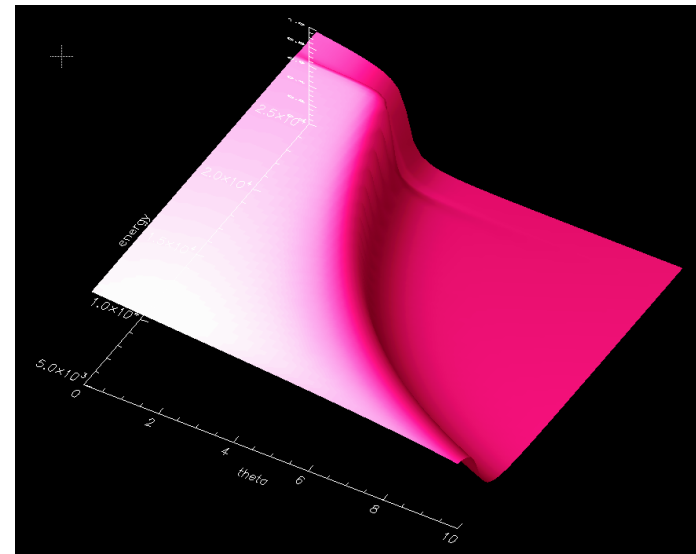


$$\hat{\mathbf{d}}_s = 2 (\hat{\mathbf{d}}_n \cdot \hat{\mathbf{d}}_i) \hat{\mathbf{d}}_n - \hat{\mathbf{d}}_i,$$

Physical model

Fresnel equations give the reflectivity as a function of angle and photon energy. As a consequence, one gets the critical angle:

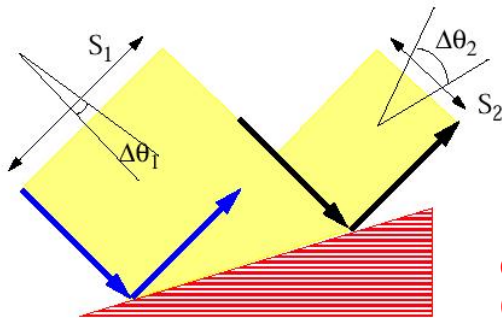
$$1 = \left(\frac{n_1}{n_2} \right)^2 \cos^2 \theta_c \Leftrightarrow \sin \theta_c = \sqrt{2\delta - \delta^2} \approx \sqrt{2\delta}$$



Crystals

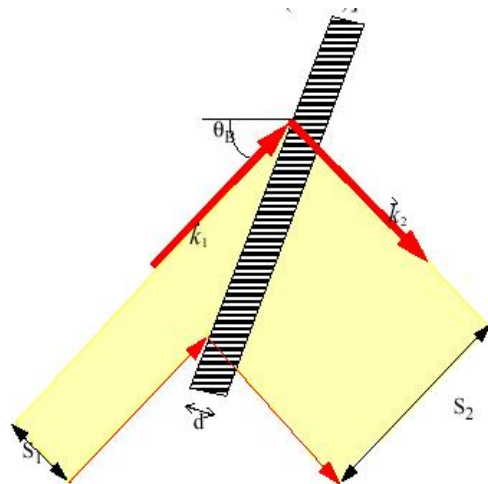
Geometrical model

like a grating originated by the truncation of the Bragg planes with the crystal surface. Crystals are dispersive elements, except for the most used case of Bragg-Symmetric reflection.



BRAGG or reflection

[ex17_sagittalfocusing.ows](#)
[OTHER_EXAMPLES/crystal_analyzer_diced.ows](#)
[OTHER_EXAMPLES/crystal_asymmetric_backscattering.ows](#)

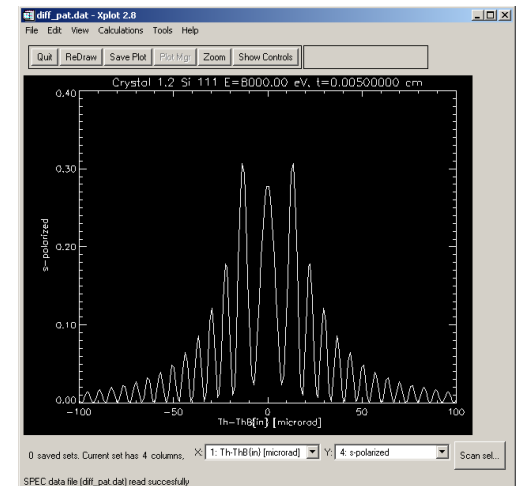
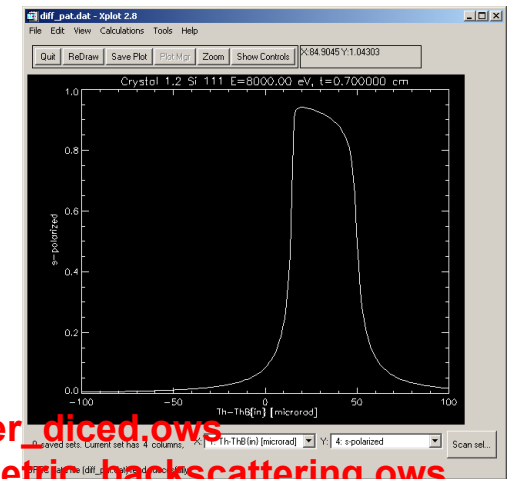


LAUE or transmission

([ex23_crystal_laue.ows](#))

Physical model

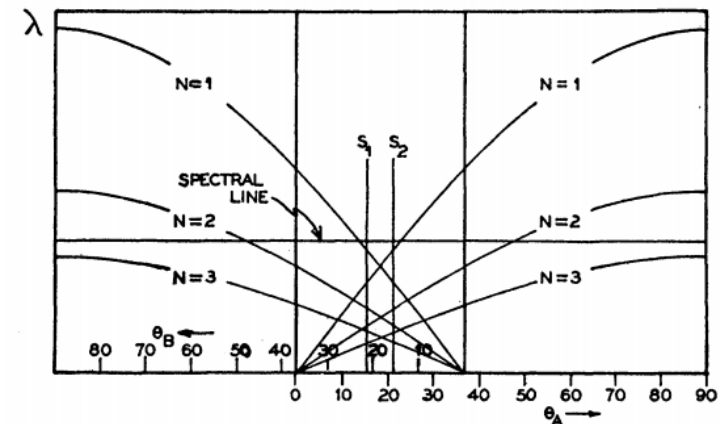
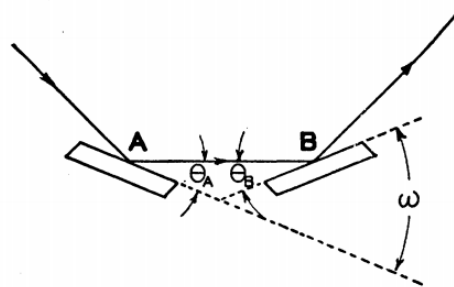
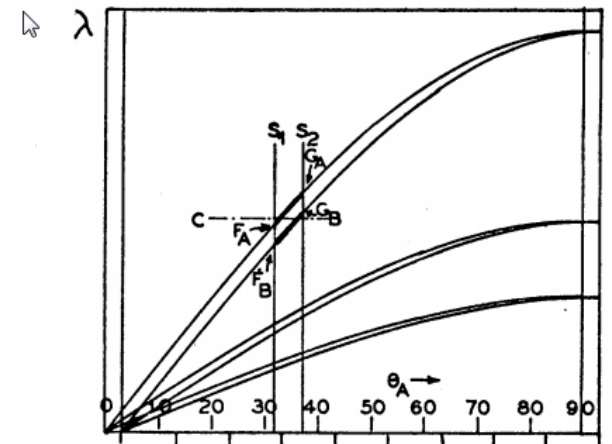
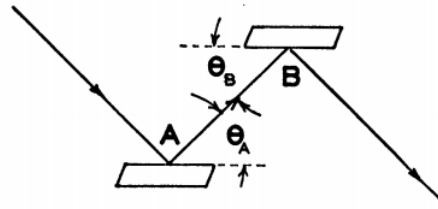
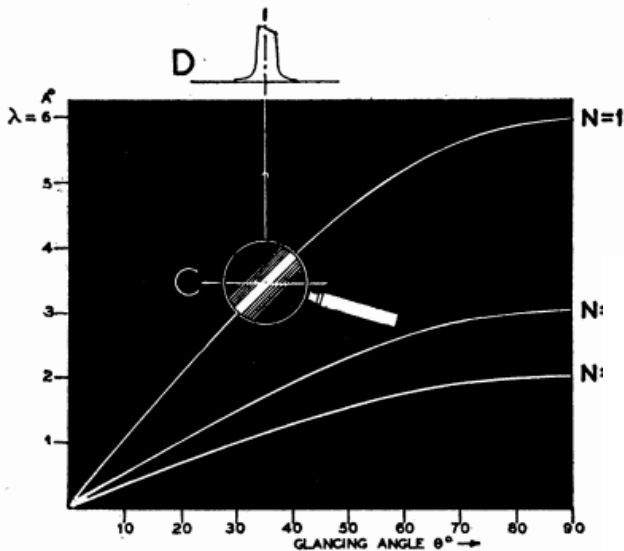
(crystal reflectivity) is given by the Dynamical Theory of Diffraction and gives the “Darwin width”



Theory of the Use of More Than Two Successive X-Ray Crystal Reflections to Obtain Increased Resolving Power

J W. M. DuMond Phys. Rev. **52**, 872 – (1937)

<http://dx.doi.org/10.1103/PhysRev.52.872>



LENSE = TWO INTERFACES

Geometrical model

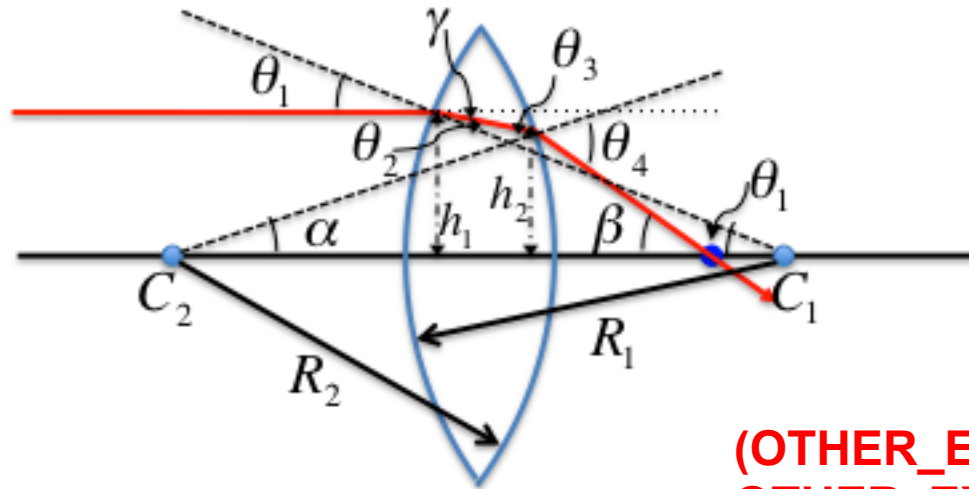
Physical model

Law of Refraction (Snell's Law)

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$

absorption in media

$$I/I_0 = \exp(-\mu t)$$

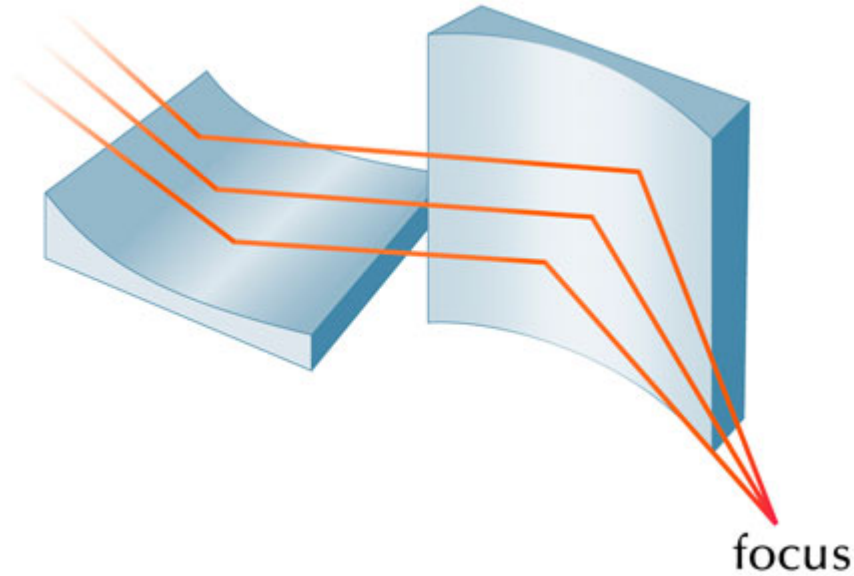


(OTHER_EXAMPLES/lens_elliptical.ows)
OTHER_EXAMPLES/CRL_Snigirev_1996.ows
ex24_transfocator.ows

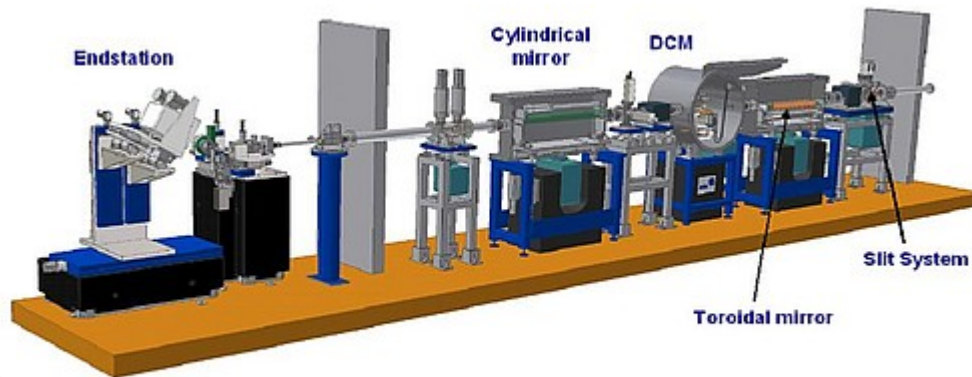
CRL = n identical Lenses

TRANSFOCATOR = m different CRLs

Other



ex16_kb.ows



ex19_beamline.ows