

HERCULES 2019

Simulating beamline optics by ray-tracing using ShadowOui

Manuel Sánchez del Río

AAM, ISDD, ESRF

2019 March 27th

Goals

Calculate main characteristics of synchrotron sources (dipoles and IDs)

Simulating beamline optics by ray-tracing to obtain main parameters of beam size, energy resolution and flux

Understand basic principles of x-ray optics: Reflective (aberrations, slope errors), Diffractive (dispersion) and Refractive (chromatic aberrations)

A few words (only) about coherence

The OASYS Project



Manuel Sanchez del Rio

Luca Rebuffi

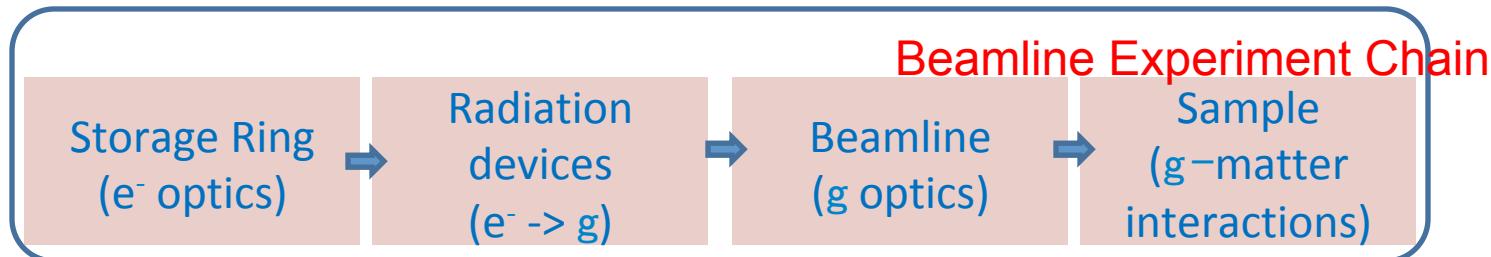
- ✓ OASYS = OrAnge SYnchrotron Suite
- ✓ A common platform to build synchrotron-oriented User Interfaces ***that communicate***
- ✓ The upper layer of the application presented to the user
- ✓ Open Source & Python technology

Luca Rebuffi, Manuel Sanchez del Rio (2017)

OASYS (OrAnge SYnchrotron Suite) : an open-source graphical environment for x-ray virtual experiments

Proc. SPIE 10388: 10388-10388. <http://dx.doi.org/10.1117/12.2274263>

Synchrotron Virtual Experiments

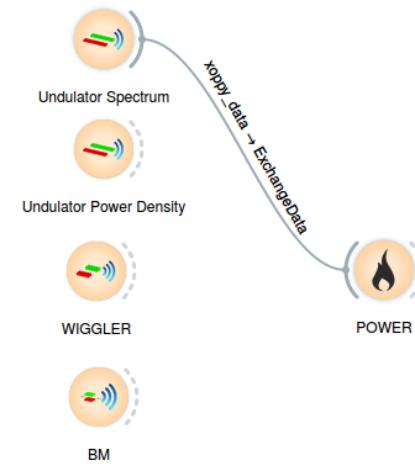
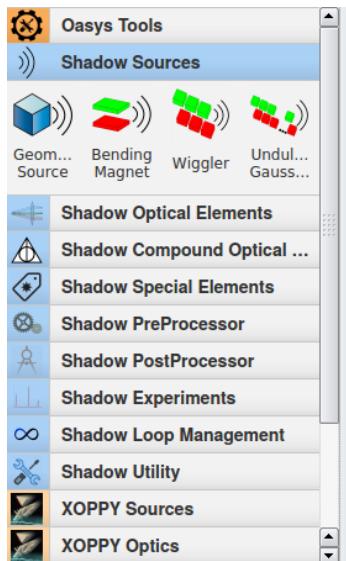


Suite of Add-ons



Source emission (XOPPY)

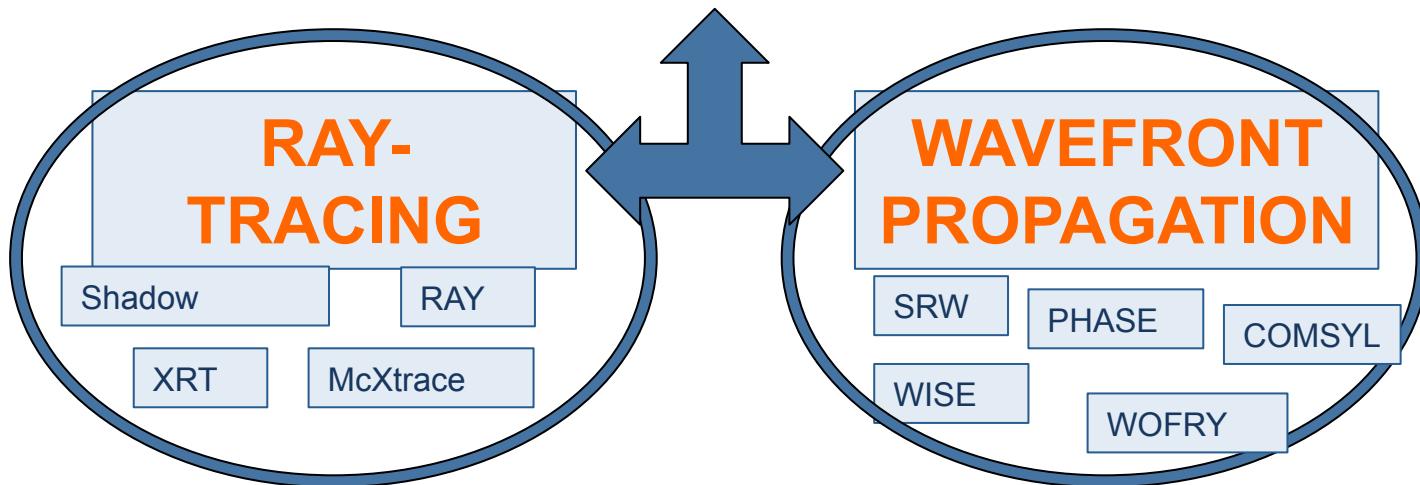
- Undulator spectrum – power
- Undulator power density
- Wiggler spectrum
- BM



Computer simulation of light sources and optical components is a mandatory step in the design and optimization of synchrotron and FEL radiation beamlines

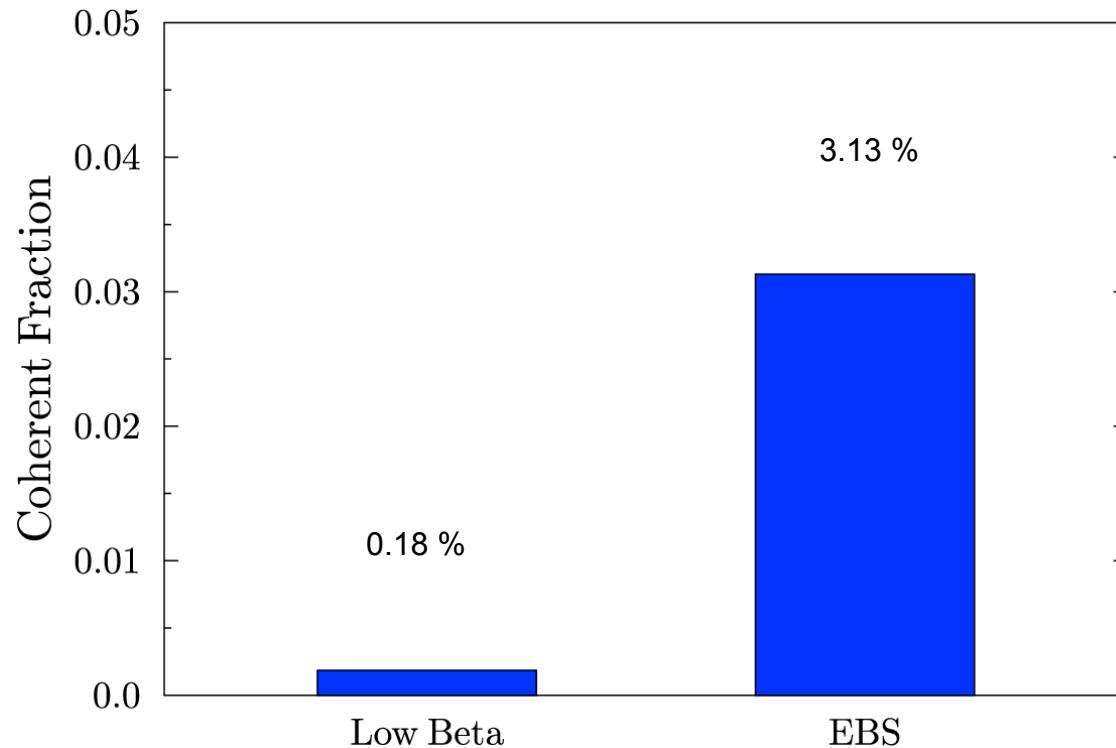


different codes for numerical simulations are available, implementing different physical approaches



AT HIGH ENERGIES, WE ARE FAR FROM DIFFRACTION-LIMIT (=FULLY COHERENCE)
U17 2m @ 17 keV ($K=0.4842$) $L=2\text{m}$ Coherent Fraction

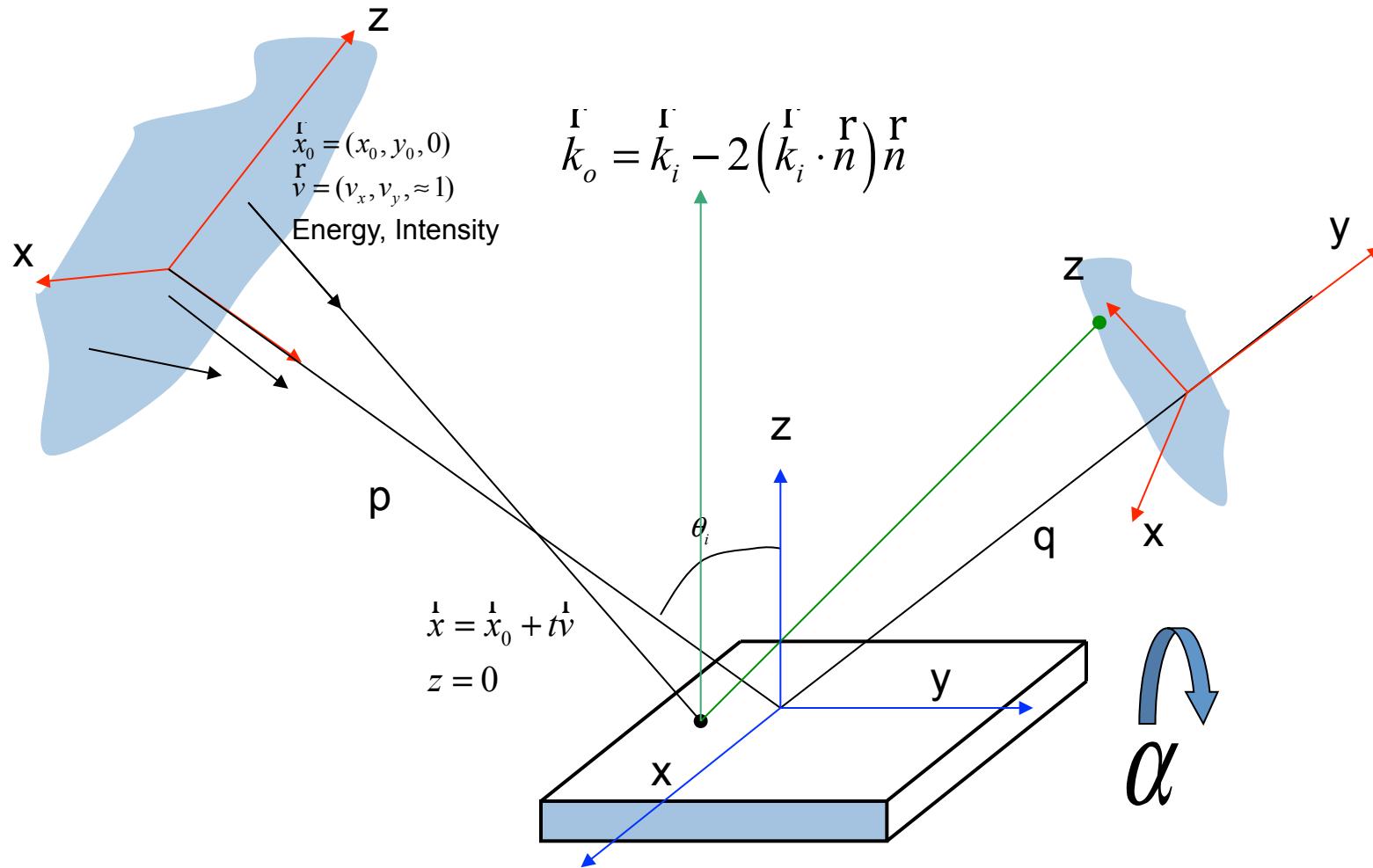
THEREFORE, ANY BEAMLINE SIMULATION MUST START WITH RAY
TRACING (INCOHERENT BEAMS)



Oasys+ShadowOui

- Install Oasys+ShadowOui:
 - <https://github.com/oasys-kit/oasys-installation-scripts/wiki>
- Today: Use rnice.
- Download Tutorials:
 - `export all_proxy=http://proxy.esrf.fr:3128/`
 - `git clone https://github.com/srio/ShadowOui-Tutorial`
- Start OASYS:
 - `oarsub -I -l nodes=1/cpu=1/core=8,walltime=10:00:00`
 - `/scisoft/XRayOptics/OASYS1.1d_RNICE8/start_oasys.sh`

Trace (the beamline)



Compute e⁻ beam sizes

$$\Sigma = \begin{pmatrix} \langle x^2 \rangle & \langle xx' \rangle \\ \langle xx' \rangle & \langle x'^2 \rangle \end{pmatrix} = \begin{pmatrix} \beta_x \mathcal{E}_x & -\alpha_x \mathcal{E}_x \\ -\alpha_x \mathcal{E}_x & \gamma_x \mathcal{E}_x \end{pmatrix} + \eta^2 \sigma_\delta^2 I_{2x2}$$

With e the emittance (constant), and Twiss parameters:

$$\alpha = -\frac{1}{2} \frac{d\beta}{ds}; \quad \gamma = \frac{1+\alpha^2}{\beta}$$

At **s** (any point of the trajectory):

$$\sigma_x = \sqrt{\langle x^2 \rangle} = \sqrt{\beta_x \mathcal{E}_x}; \quad \sigma_{x'} = \sqrt{\langle x'^2 \rangle} = \sqrt{\gamma_x \mathcal{E}_x}; \quad \sigma_x \sigma_{x'} = \mathcal{E}_x \sqrt{1+\alpha_x^2}$$

At **waist** (zero correlation, $r=a=0$, b is minimum):

$$\sigma_x = \sqrt{\langle x^2 \rangle} = \sqrt{\beta_x \mathcal{E}_x}; \quad \sigma_{x'} = \sqrt{\langle x'^2 \rangle} \Big|_w = \sqrt{\frac{\mathcal{E}_x}{\beta_x}}; \quad \boxed{\sigma_x \sigma_{x'} = \mathcal{E}_x}$$



ShadowOui asks for s and e at waist (plus distance from waist to center of device)

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

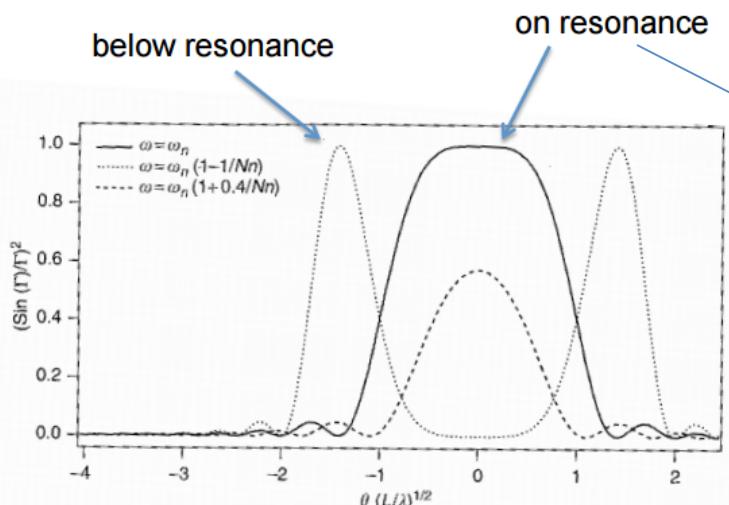


Figure 3.3 Graph of $(\sin(\Gamma)/\Gamma)^2$ as a function of the angle $\theta = \sqrt{\theta_x^2 + \theta_z^2}$ for three different frequencies. ω_n is an abbreviation for $n\omega_1(0, 0)$.

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

$$\sigma_r = 0.69 \sqrt{\frac{\lambda}{L}} \approx \sqrt{\frac{\lambda}{2L}}$$

78 P. Elleaume

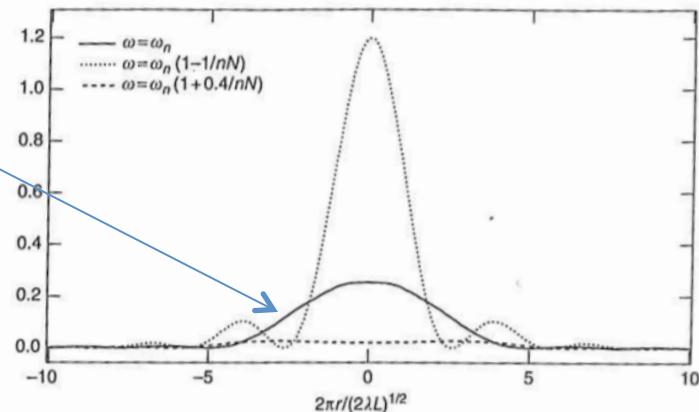


Figure 3.4 Spectral flux per unit surface in the middle of the undulator for three frequencies close to the on-axis resonant frequency $\omega_n = n\omega_1(0, 0)$.

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

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

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

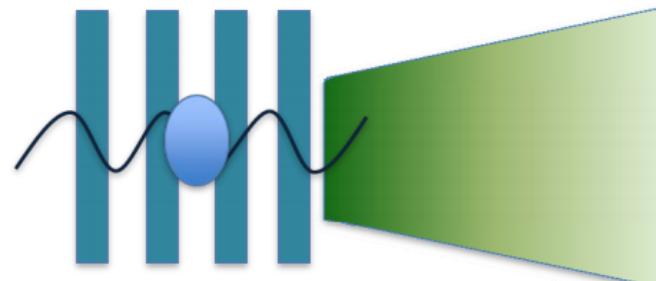
Photon beam size and divergence is determined by a combination of electron beam and single electron emission

$$\Sigma_x^2 = \sigma_{x,elec}^2 + \sigma_{x,photon}^2$$

$$\Sigma_{x'}^2 = \sigma_{x',elec}^2 + \sigma_{x',photon}^2$$

$$\Sigma_z^2 = \sigma_{z,elec}^2 + \sigma_{z,photon}^2$$

$$\Sigma_{z'}^2 = \sigma_{z',elec}^2 + \sigma_{z',photon}^2$$



Courtesy: Boaz Nash

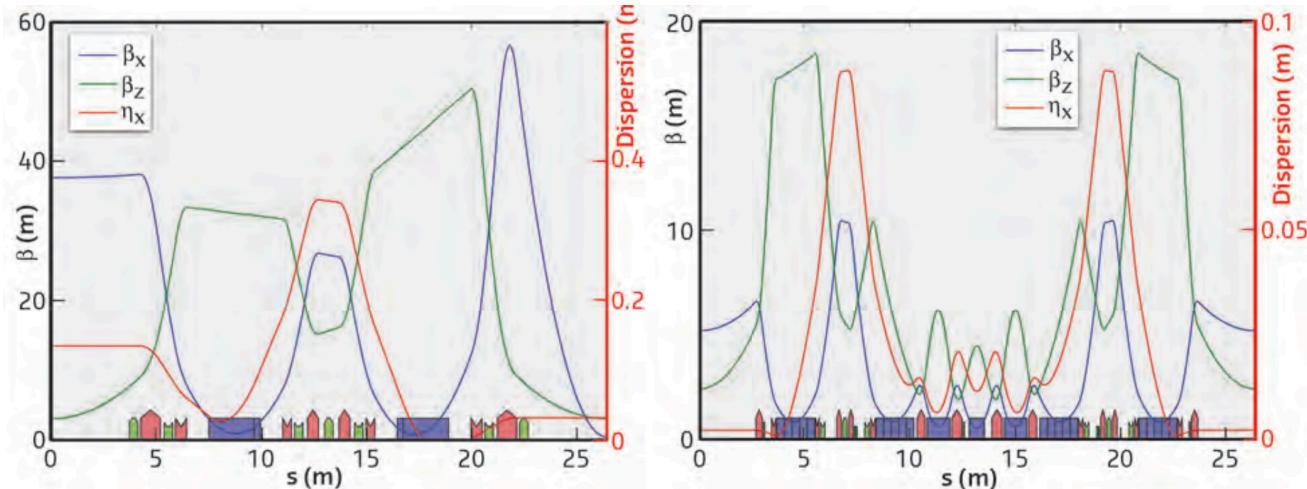
These are at source. A distance D away, beam size become: $\Sigma_{x,0}^2 + \Sigma_{x',0}^2 D^2$

(FOR UNDULATORS, THESE FORMULAS ARE VALID AT THE WAIST, AT THE UNDULATOR RESONANCE, AND SUPPOSING GAUSSIAN EMISSION OF PHOTONS)

ShadowOui performs “numeric convolution” by Monte Carlo sampling of the electron beam [Gaussian] and photon emission [non Gaussian]

EBS vs ESRF electron lattice

	Parameter	S28A	Present high beta	Present low beta	Symbol	Unit
ID source	Horizontal beta at ID centre	5.2	37.6	0.4	β_x	m
	Horizontal dispersion at ID centre	2.0	134	31	D_x	mm
	Vertical beta at ID centre	2.4	3.0	3.0	β_y	m
	Horizontal beam size at ID centre	27.2	387.8	37.4	σ_x	μm
	Vertical beam size at ID centre	3.4	3.5	3.5	σ_y	μm
	Horizontal beam div. at ID centre	5.2	10.3	106.9	σ_x'	μrad
	Vertical beam div. at ID centre	1.4	1.2	1.2	σ_y'	μrad
	Relative source point transverse disp.	0				mm
	Relative source point longitudinal disp.	0				m



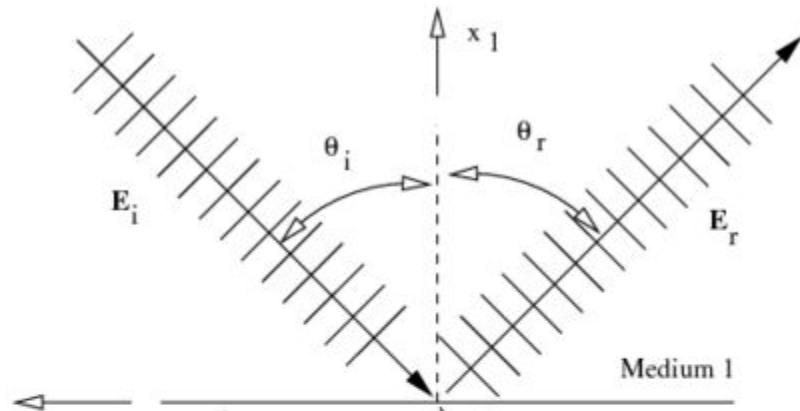
Optical elements

For each optics element SHADOW includes:

- Geometrical model: how the direction of the rays are changed (reflected, refracted or diffracted)
- Physical model: how the ray intensity (in fact electric fields) decreases because of the interaction
 - Structures along the surface => playing with the direction
 - Structures in depth => playing with the reflectivity

Mirrors

Geometrical model

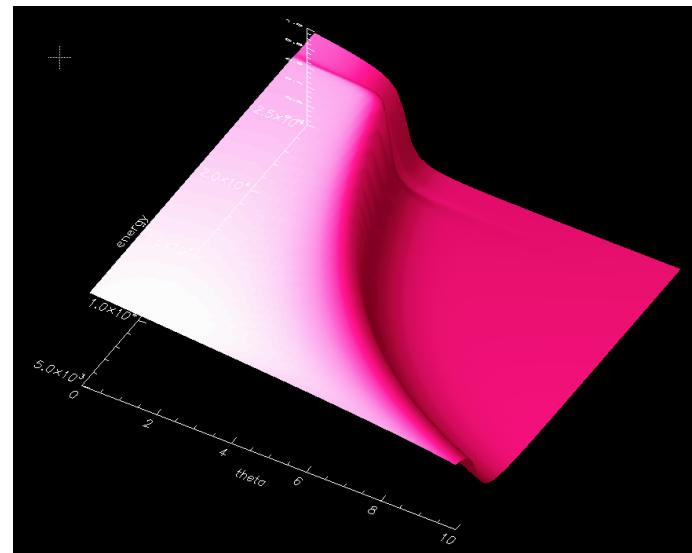


$$\hat{d}_s = 2 \left(\hat{d}_n \cdot \hat{d}_i \right) \hat{d}_n - \hat{d}_i,$$

Physical model

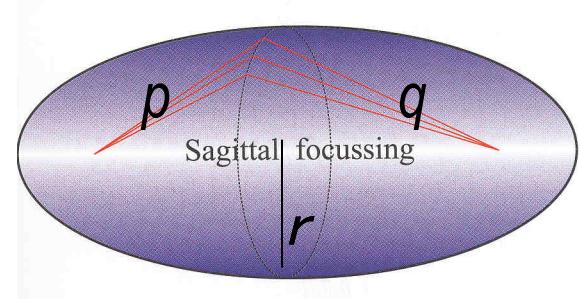
Fresnel equations give the reflectivity as a function of angle and photon energy. As a consequence, one gets the critical angle:

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



Mirror shape

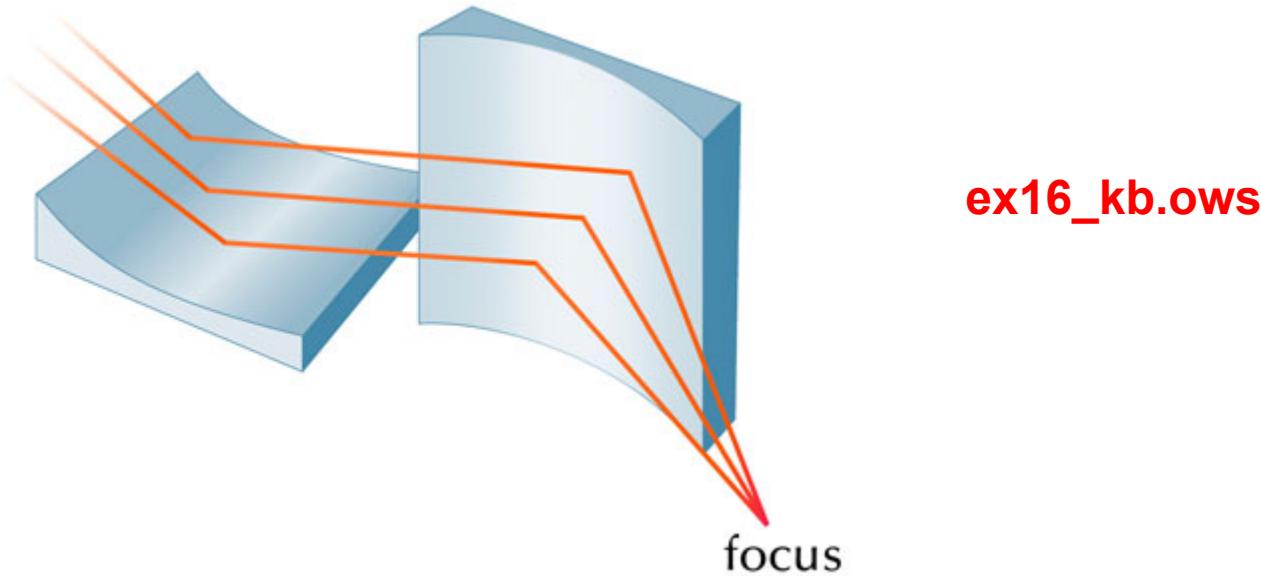
- Point to point focusing (ellipsoid)
- Collimating (paraboloid)
- Focalization in two planes
 - Tangential or Meridional (ellipse or parabola)
 - Sagittal (circle)
- Demagnification: $M=p/q$
- Easier manufacturing:
 - 2D: Ellipsoid => Toroid
 - Only one plane: cylinder Ellipsoid (ellipse)=> cylinder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



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

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

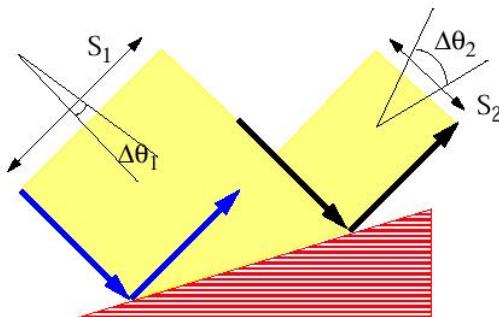
Kirkpatrick-Baez



Crystals

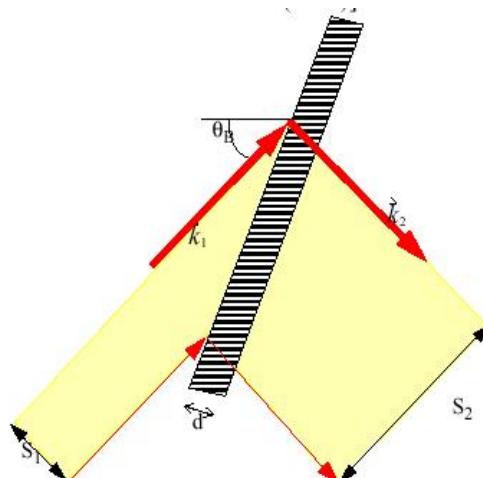
Geometrical model

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](#)

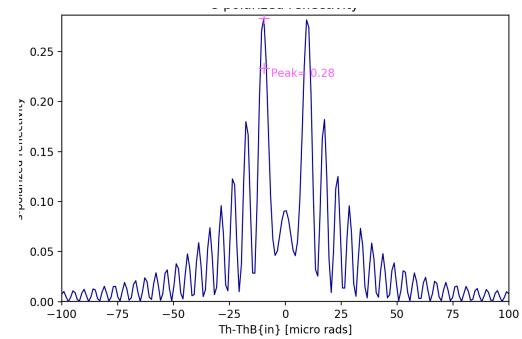
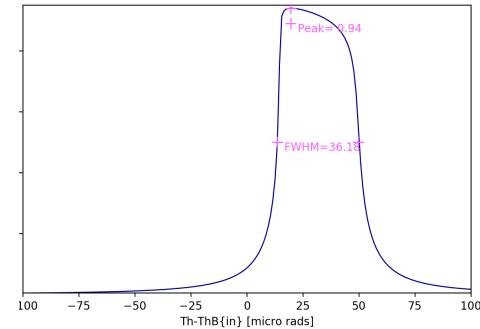


LAUE or transmission

[\(ex23_crystal_lau.ows\)](#)

Physical model

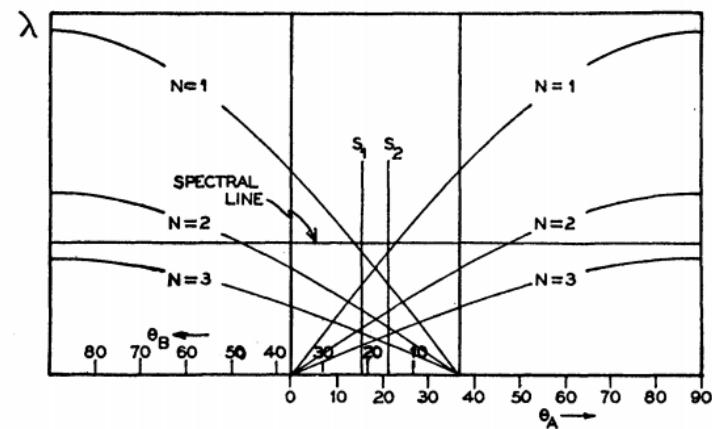
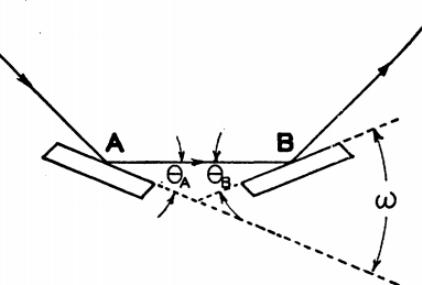
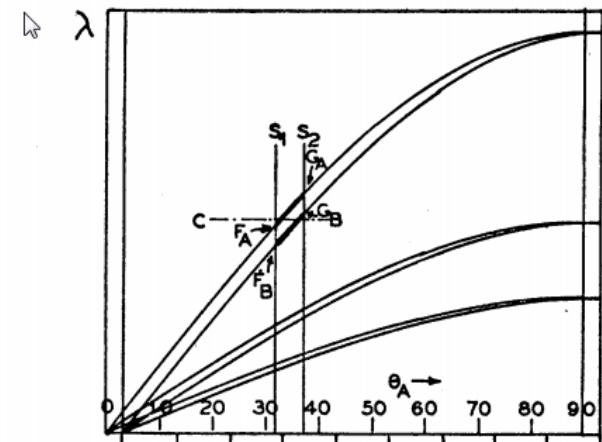
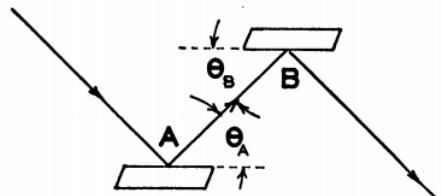
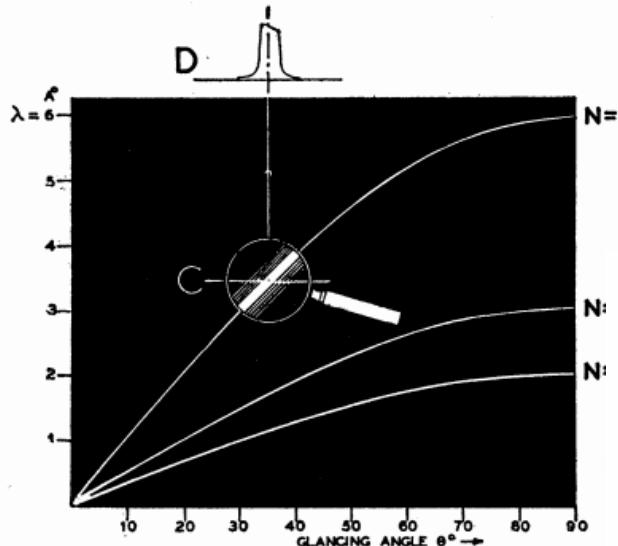
(crystal reflectivity) is given by the Dynamical Theory of Diffraction and gives the “Darwin width”



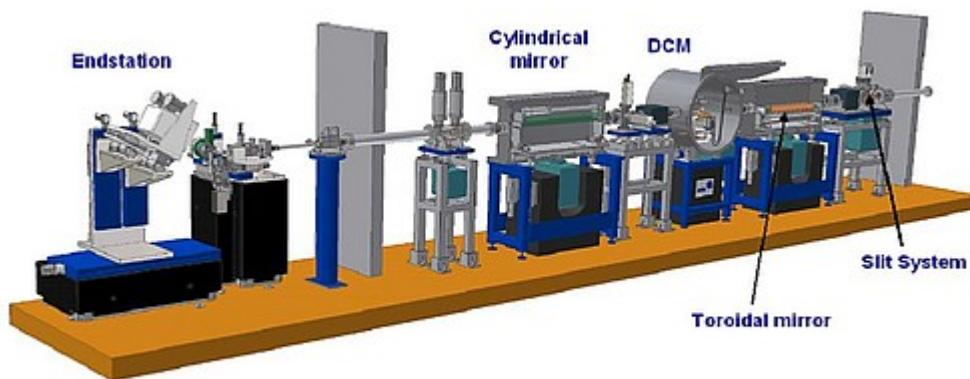
Theory of the Use of More Than Two Successive X-Ray Crystal Reflections to Obtain Increased Resolving Power

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

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



Other



ex19_beamline.ows

LENSE = TWO INTERFACES

Geometrical model

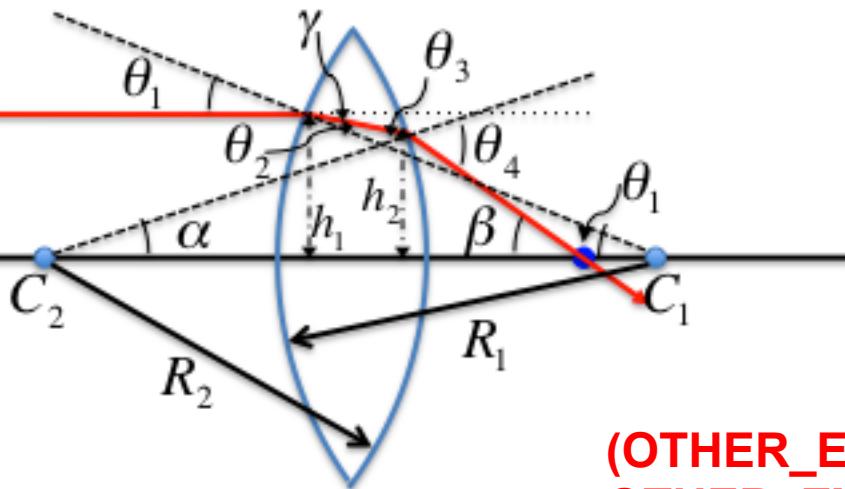
Physical model

Law of Refraction (Snell's Law)

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

absorption in media

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



(OTHER_EXAMPLES/lens_elliptical.ows)
OTHER_EXAMPLES/CRL_Snígirev_1996.ows
ex24_transfocator.ows

CRL = n identical Lenses

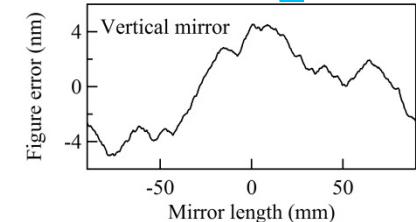
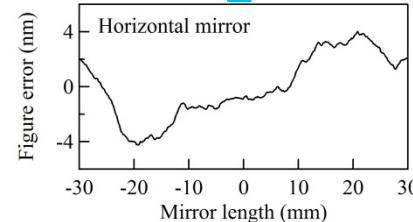
TRANSFOCATOR = m different CRLs

HYBRID METHOD IN SHADOW (X. Shi *et al.*)

Combining ray tracing and wavefront propagation

$$\text{Plane wave} \times \exp\left[-ik\left(\frac{x^2}{2f_x} + \frac{z^2}{2f_z}\right)\right] \times \exp[-i2k \sin \theta_x \cdot \text{Height}(x)] \times \exp[-i2k \sin \theta_z \cdot \text{Height}(z)]$$

Ideal lens with focal lengths of f_x and f_z



Ray tracing of the beamline

$$E(x, z) \rightarrow \text{FFT} \xrightarrow{\mathcal{F}(u, v)} \times \exp\left[-\frac{i2\pi^2}{k}(u^2 + v^2)y\right] \xrightarrow{\mathcal{F}'(u, v)} \text{Inverse FFT} \rightarrow E(x', z')$$

