HERCULES 2019

Simulating beamline optics by ray-tracing using ShadowOui

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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

https://oasys-kit.github.io/

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

Beamline Experiment Chain

Storage Ring (e^- optics) → Radiation devices (e^- -> g) → Beamline (g optics) → Sample (g−matter interactions)

OrAnge SYnchrotron Suite

OASYS

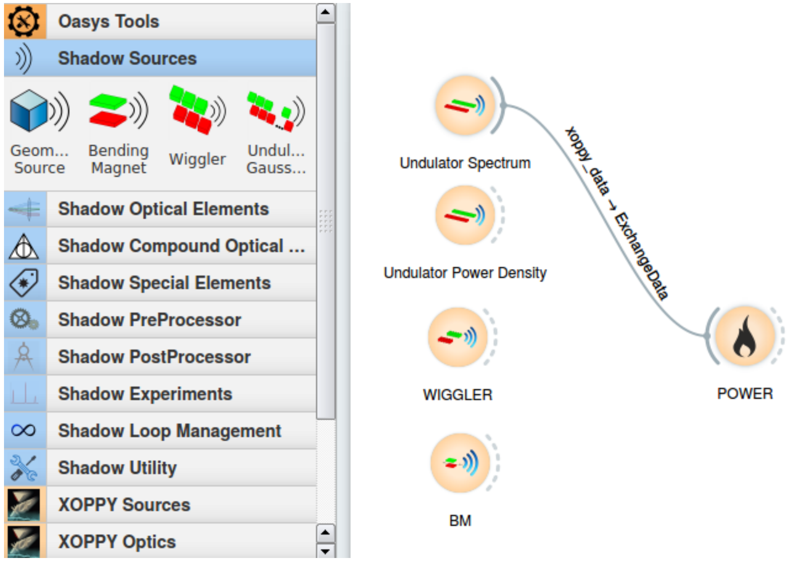
Powered by orange

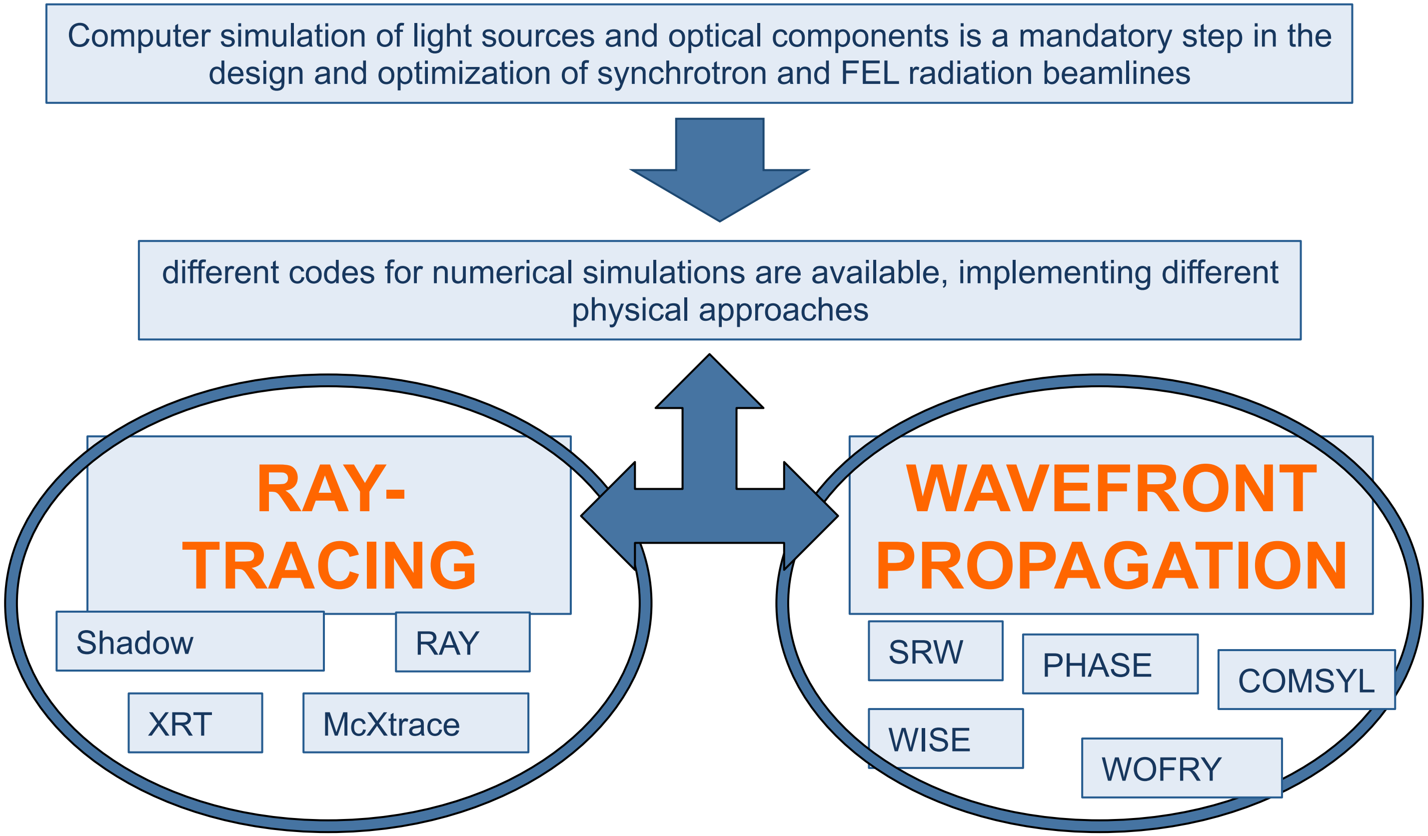
Suite of Add-ons

Shadow | XOP | crystal | X-ray server | WISE | WOFRY | COMSYL

Source emission (XOPPY)

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

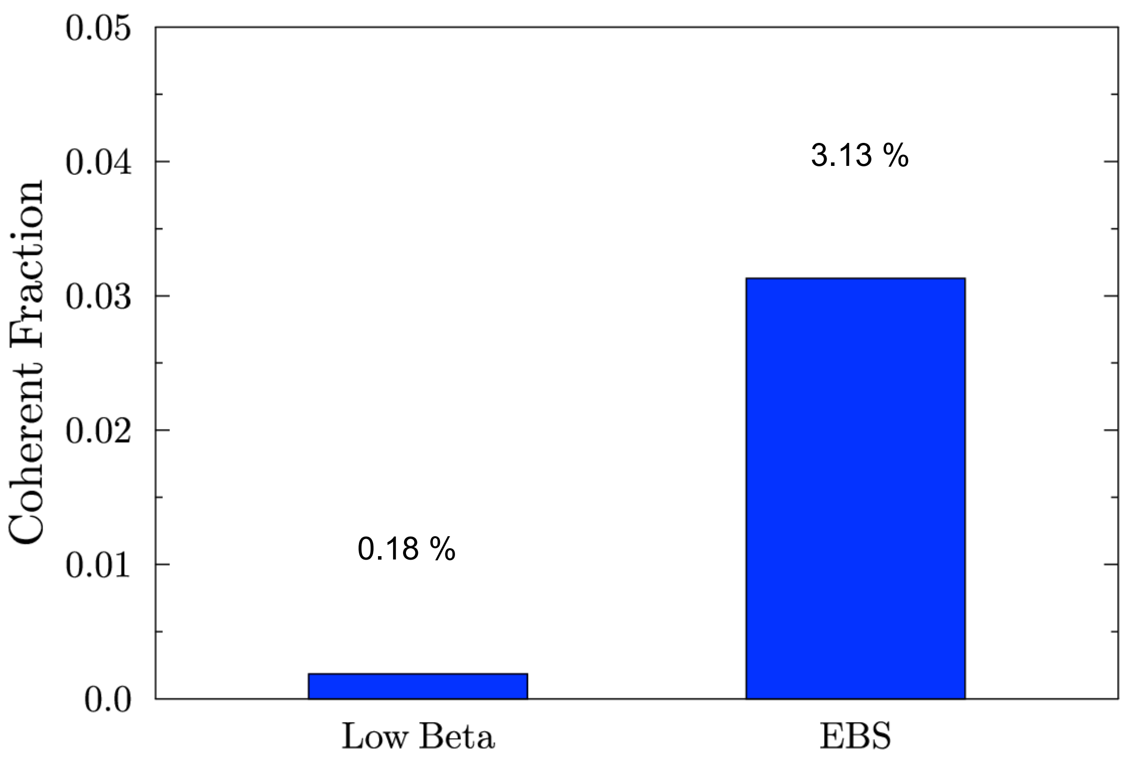



Computer simulation of light sources and optical components is a mandatory step in the design and optimization of synchrotron and FEL radiation beamlines
different codes for numerical simulations are available, implementing different physical approaches
RAY-TRACING
Shadow
RAY
XRT
McXtrace
WAVEFRONT PROPAGATION
SRW
PHASE
COMSYL
WISE
WOFRY

AT HIGH ENERGIES, WE ARE FAR FROM DIFFRACTION-LIMIT (=FULLY COHERENCE)

U17 2m @ 17 keV (K=0.4842) L=2m Coherent Fraction

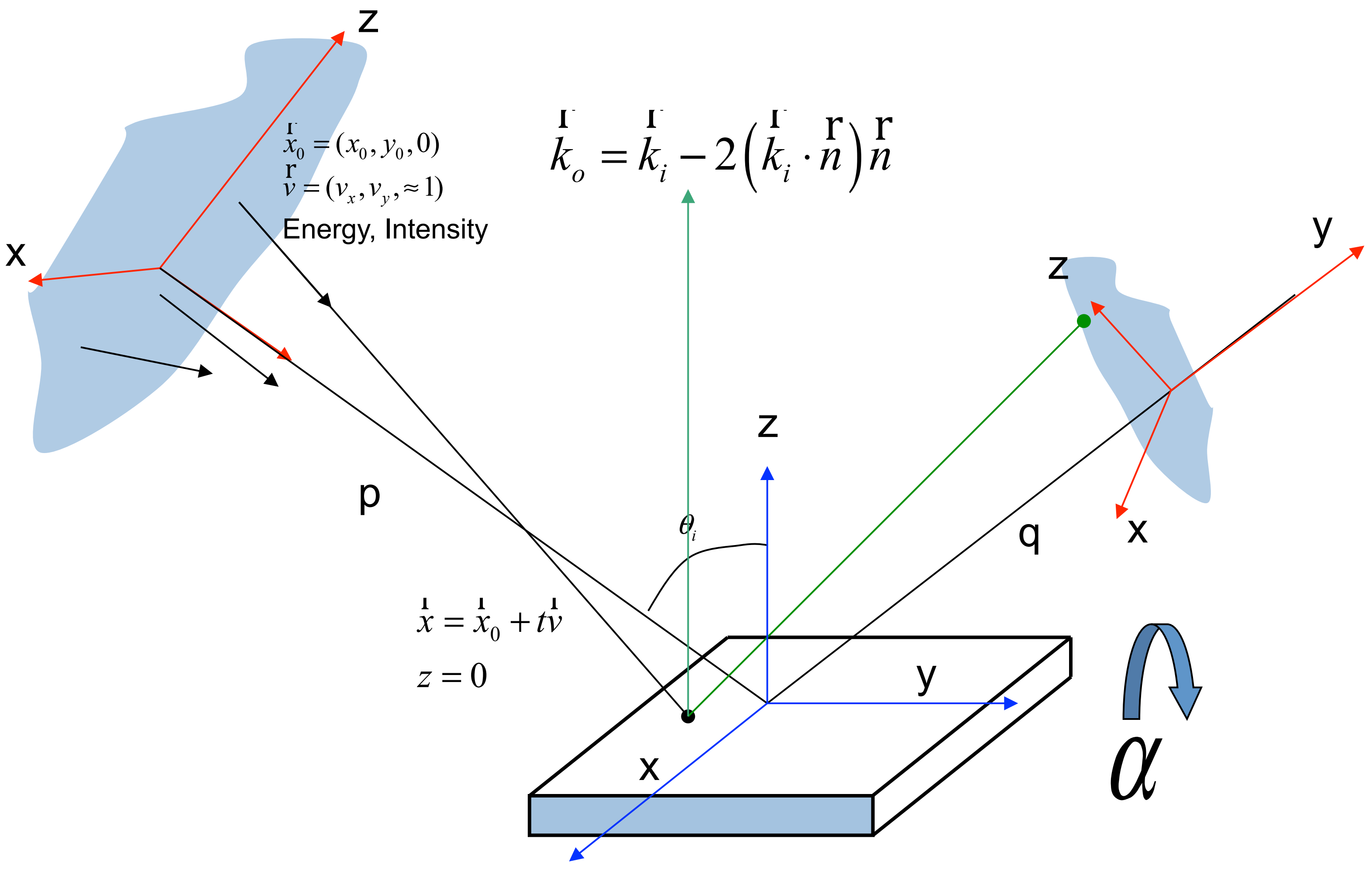
THEREFORE, ANY BEAMLINE SIMULATION MUST START WITH RAY TRACING (INCOHERENT BEAMS)



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_RNICE8/start_oasys.sh`

Trace (the beamline)



Compute e⁻ beam sizes

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

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):

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

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

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

ShadowOui asks for s and e at waist (plus distance from waist to center of device) ex13_insertiondevices.ows

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

below resonance

on resonance

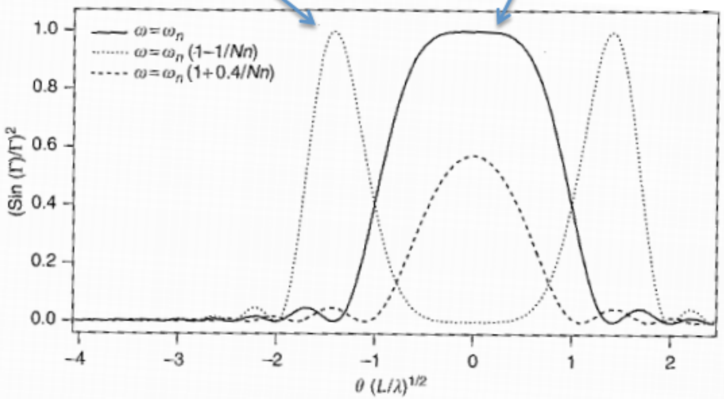


Figure 3.3 Graph of $(\sin(\Gamma)/\Gamma)^2$ as a function of the angle $\theta = \sqrt{\theta_x^2+\theta_z^2}$ for three different frequencies. ω_n is an abbreviation for $n\omega_1\,(0,0)$.

78 *P. Elleaume*

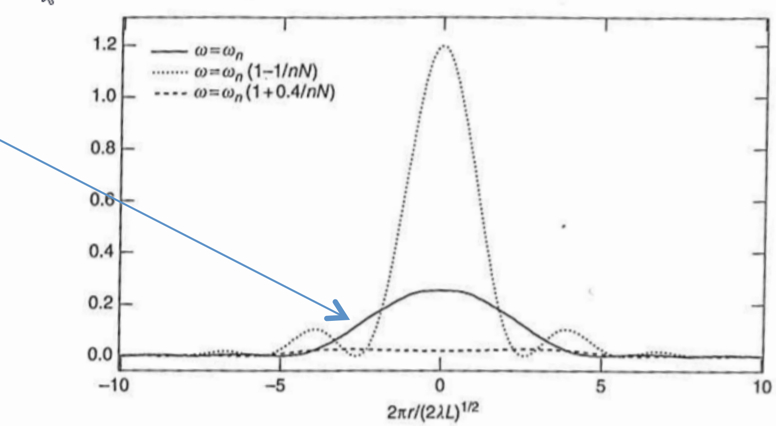


Figure 3.4 Spectral flux per unit surface in the middle of the undulator for three frequencies close to the on-axis resonant frequency $\omega_n = n\omega_1(0,0)$.

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

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

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

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

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

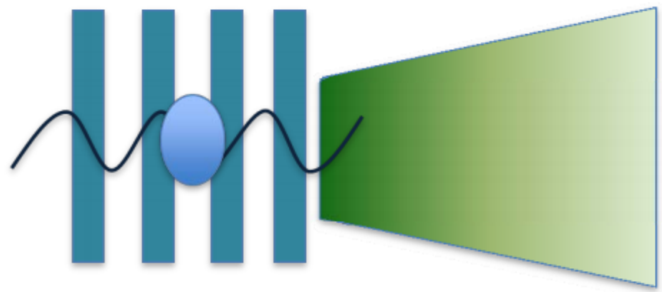
Photon beam size and divergence is determined by a combination of electron beam and single electron emission

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

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

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

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



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 SUPOSSING GAUSSIAN EMISSION OF PHOTONS)

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

Optical elements

For each optics element SHADOW includes:

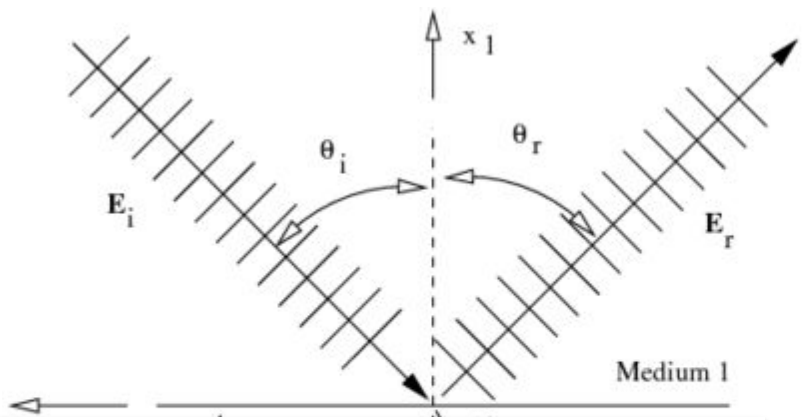
- Geometrical model: how the direction of the rays are changed (reflected, refracted or diffracted)
- Physical model: how the ray intensity (in fact electric fields) decreases because of the interaction

•Structures along the surface =>playing with the direction

•Structures in depth => playing with the reflectivity ex15_aberration.ows

Mirrors

Geometrical model

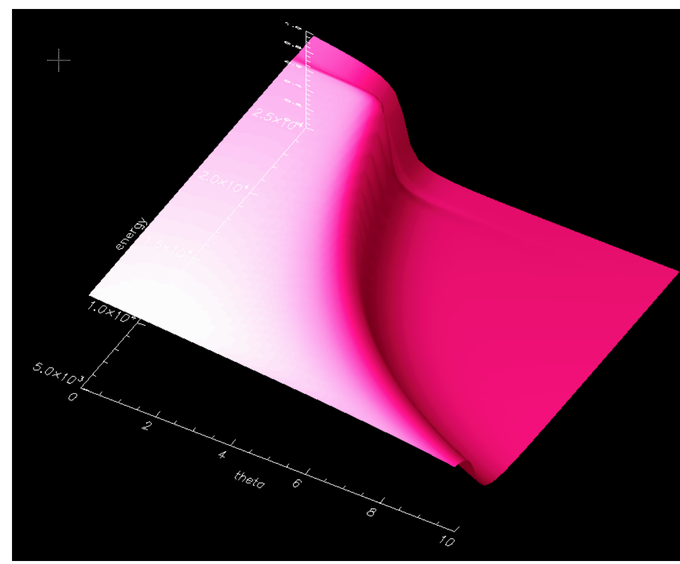


$$\hat{\mathbf{d}}_s = 2\left(\hat{\mathbf{d}}_n \cdot \hat{\mathbf{d}}_i\right)\hat{\mathbf{d}}_n - \hat{\mathbf{d}}_i,$$

Physical model

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

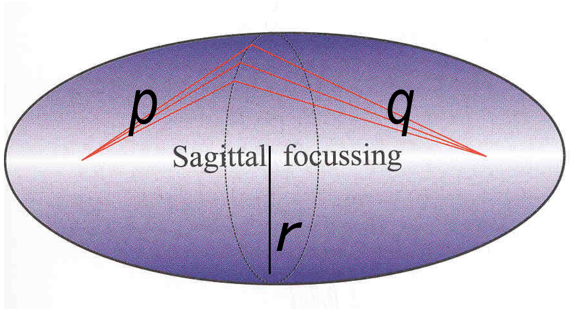
$$1=\left(\frac{n_1}{n_2}\right)^2\cos^2\theta_c \quad\Leftrightarrow\quad \sin\theta_c=\sqrt{2\delta-\delta^2}\approx\sqrt{2\delta}$$



ex15_aberration.ows

Mirror shape

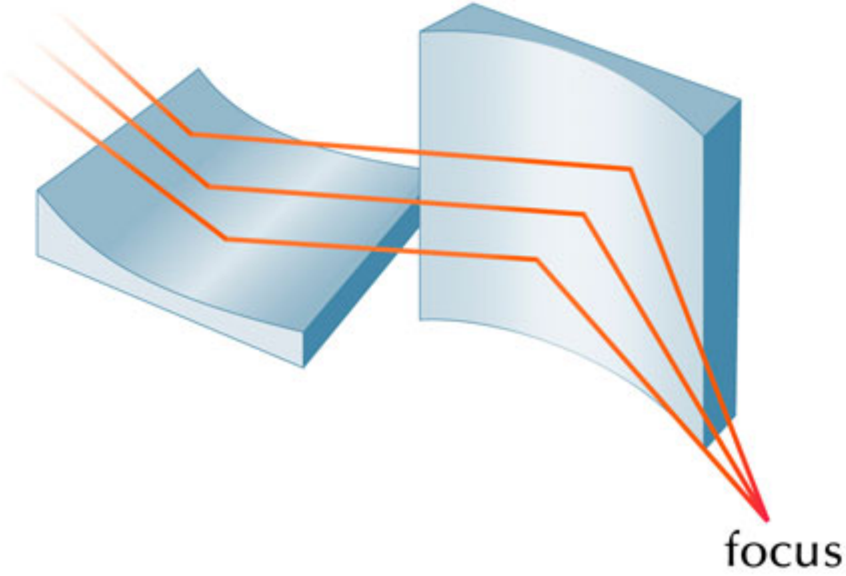
- Point to point focusing (ellipsoid)
- Collimating (paraboloid)
- Focalization in two planes
  - Tangential or Meridional (ellipse or parabola)
  - Sagittal (circle)
- Demagnification: M=p/q
- Easier manufactiring:
  - 2D: Ellipsoid => Toroid
  - Only one plane: cylinder Ellipsoid (ellipse)=> cylinder (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



ex16_kb.ows

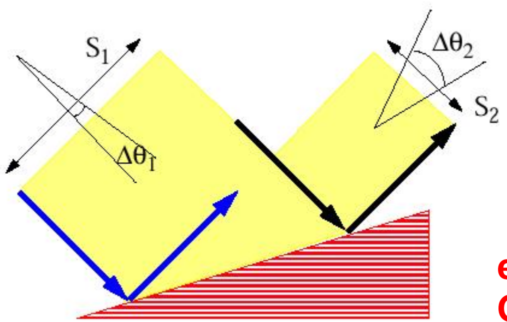
Crystals

Geometrical model

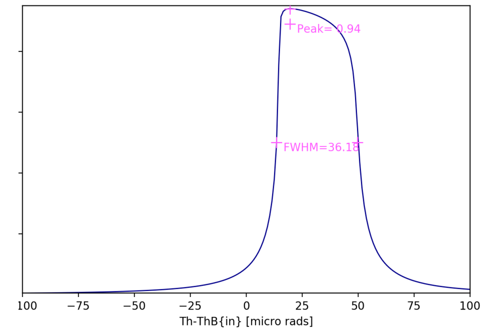
like a grating originated by the truncation of the Bragg planes with the crystal surface. Crystals are dispersive elements, except for the most used case of Bragg-Symmetric reflection.

Physical model

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



BRAGG or reflection



ex17_sagittalfocusing.ows
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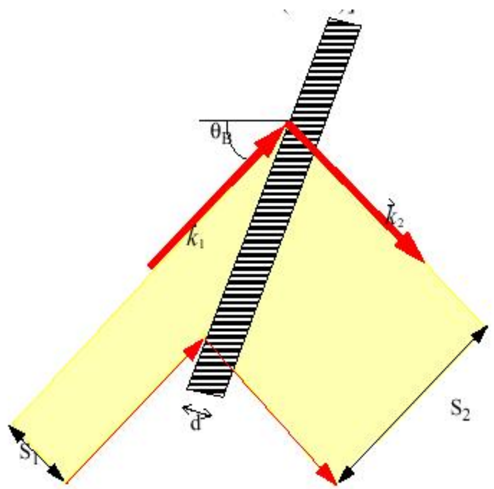
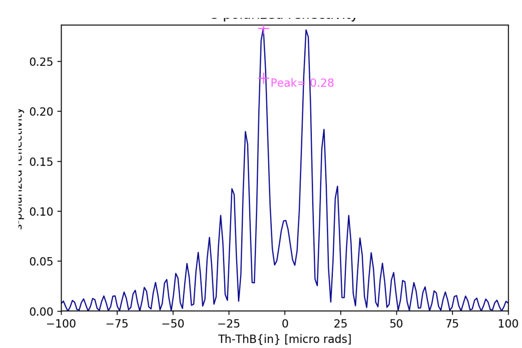
OTHER_EXAMPLES/crystal_asymmetric_backscattering.ows



LAUE or transmission

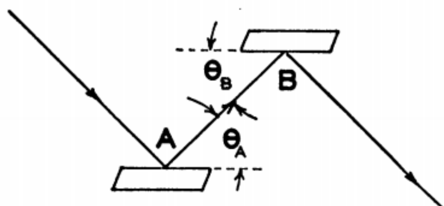


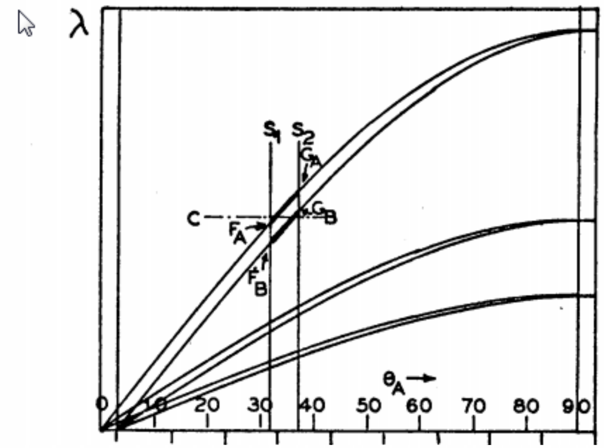
(ex23_crystal_laue.ows)

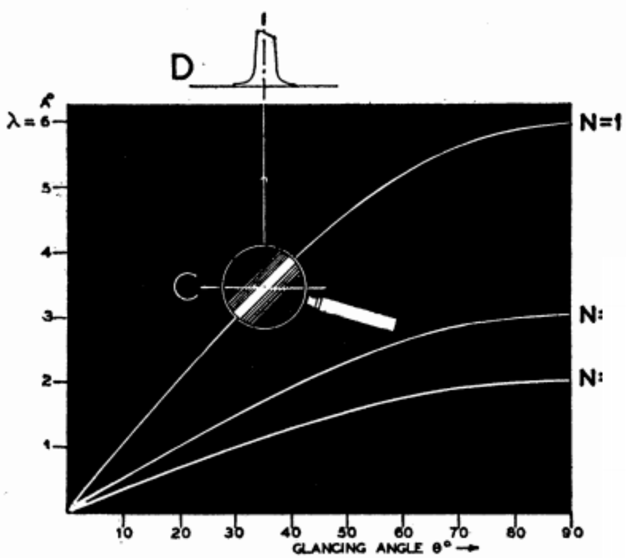
Theory of the Use of More Than Two Successive X-Ray Crystal Reflections to Obtain Increased Resolving Power

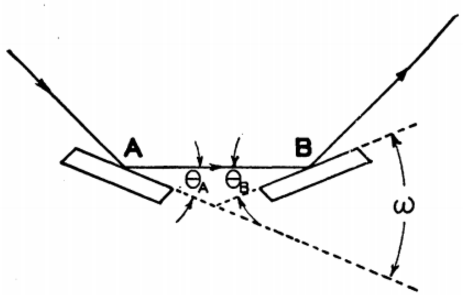
J W. M. DuMond Phys. Rev. **52**, 872 – (1937)

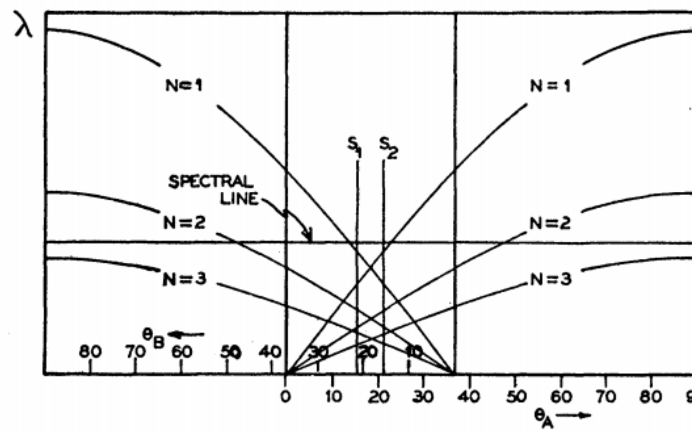
http://dx.doi.org/10.1103/PhysRev.52.872



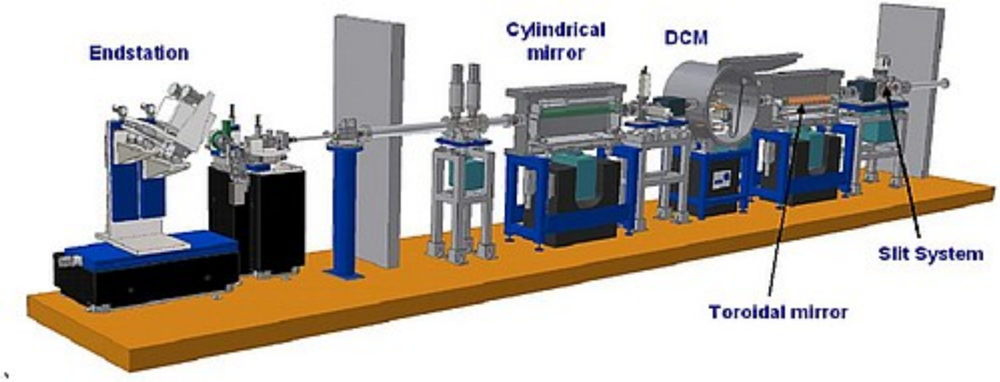








Other



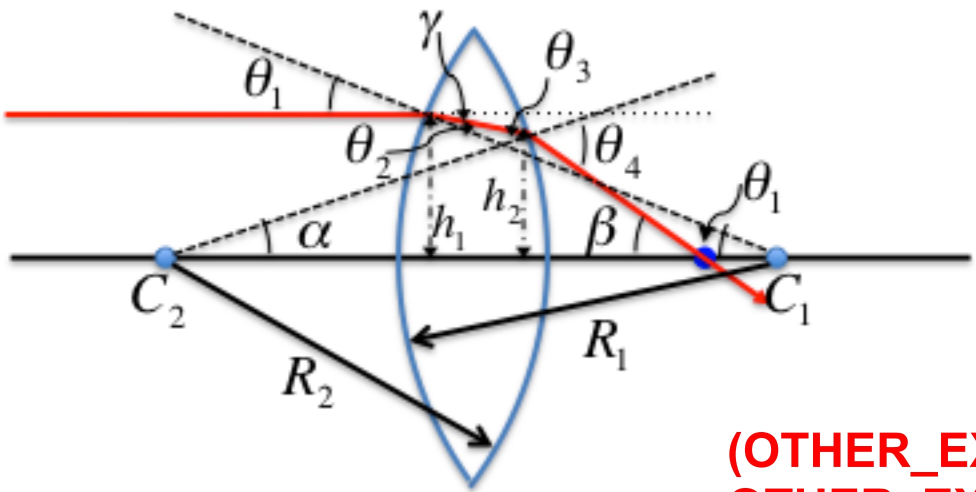
ex19_beamline.ows

LENSE = TWO INTERFACES

Geometrical model

Law of Refraction (Snell's Law)

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



Physical model

absorption in media

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

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

CRL = *n* identical Lenses

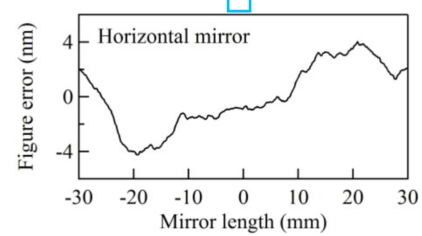
TRANSFOCATOR = *m* different CRLs

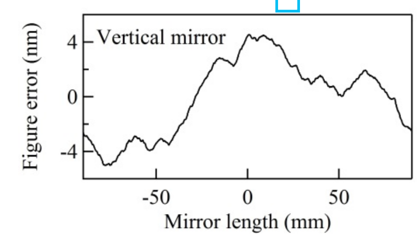
HYBRID METHOD IN SHADOW (X. Shi *et al.*)

Combining ray tracing and wavefront propagation

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

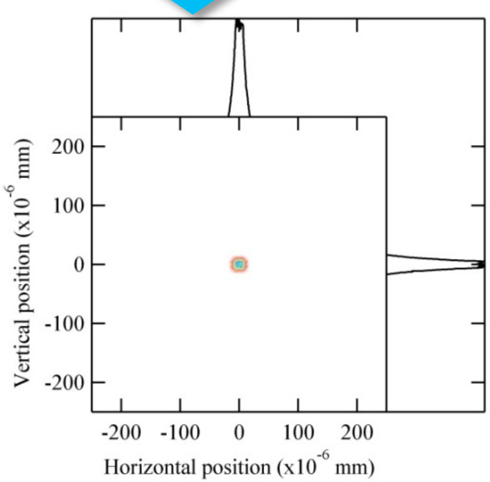
Ideal lens with focal lengths of f_x and f_z





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

Ray tracing of the beamline



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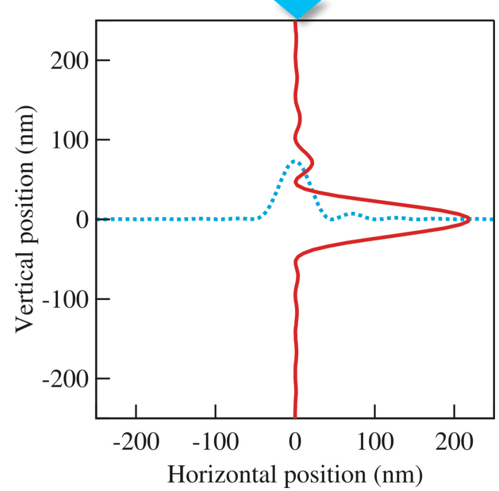

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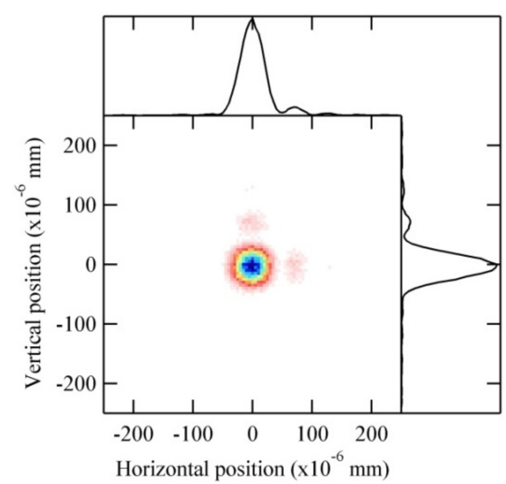
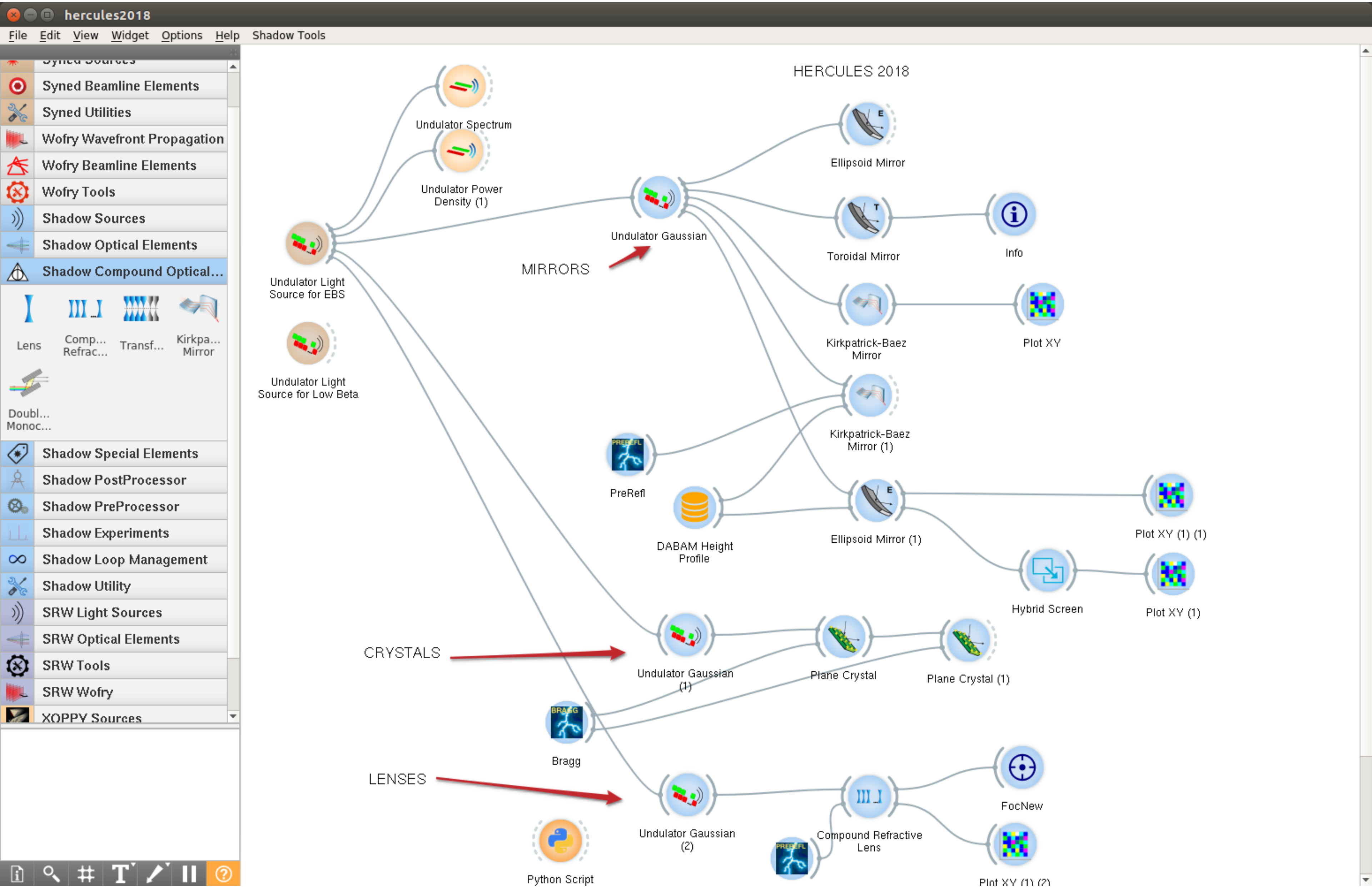


X. Shi, R. Reininger, M. Sanchez del Rio, L. Assoufid " J. Synchrotron Rad. (2014) 21, doi:10.1107/S160057751400650X

X. Shi, M. Sanchez del Rio and Ruben Reininger Proc. SPIE 9209, 920911 (2014); doi:10.1117/12.2061984

X. Shi, R. Reininger, M. Sánchez del Río, J. Qian and L. Assoufid Proc. SPIE 9209, 920909 (2014); doi:10.1117/12.2061950


hercules2018
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Synced Beamline Elements
Syned Utilities
Wofry Wavefront Propagation
Wofry Beamline Elements
Wofry Tools
Shadow Sources
Shadow Optical Elements
Shadow Compound Optical...
Lens
Comp... Refrac...
Transf...
Kirkpa... Mirror
Doubl... Monoc...
Shadow Special Elements
Shadow PostProcessor
Shadow PreProcessor
Shadow Experiments
Shadow Loop Management
Shadow Utility
SRW Light Sources
SRW Optical Elements
SRW Tools
SRW Wofry
XOPPY Sources
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Undulator Spectrum
Undulator Power Density (1)
Undulator Light Source for EBS
Undulator Light Source for Low Beta
Undulator Gaussian
MIRRORS
Ellipsoid Mirror
Toroidal Mirror
Info
Kirkpatrick-Baez Mirror
Plot XY
Kirkpatrick-Baez Mirror (1)
PreRefl
DABAM Height Profile
Ellipsoid Mirror (1)
Plot XY (1) (1)
Hybrid Screen
Plot XY (1)
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Plane Crystal
Plane Crystal (1)
Bragg
LENSES
Undulator Gaussian (2)
Compound Refractive Lens
FocNew
Python Script
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