Tutorials on computer simulations for X-ray optics

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Contents

1 Learning reference frames in SHADOW using a geometrical source

You will:

- learn to define geometrical sources
- understand the use of a python script for modifying an existing source
- understand reference frames

Questions:

i) Create a collimated (i.e., zero divergence) geometric source with elliptical shape with vertical semi axis twice the horizontal semi axis (e.g., 0.2 cm and 0.1 cm in Z and X, respectively). Visualize it

ii) Apply a python script that received the source and keeps only the rays with positive values of X and Z (i.e., sets the flag as "lost" for rays with negative values of X and Z), and resend the beam. Visualize the new result after this modification of the beam.

iii) Create a mirror optical element, with incident angle 45 deg, and p=q=1m. Trace the system in two cases, with Mirror orientation angle 0 and 90 degrees. Verify the results with the pictures shown before.

Hints: you may load the workspace ex11_referenceframe.ows.

Answer

Pay attention to make plots using "Rays: Good Only" and same aspect ratio (click the blue octagon in)

Source (x,z) plane before and after applying the script that select only "positive" rays

Figure 1:

Source (x,z) plane before and after applying the script that select only “positive” rays

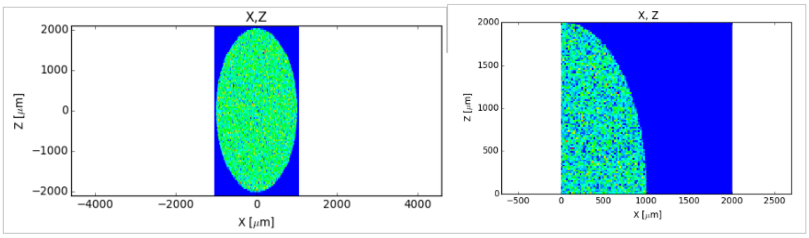
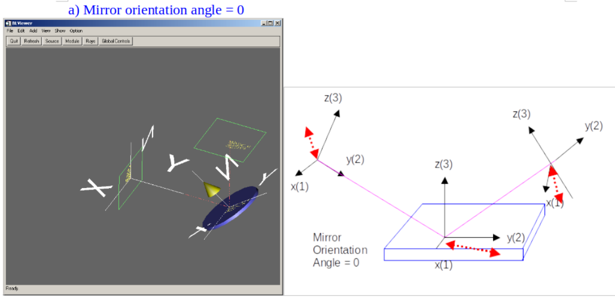


Figure 2:

a) Mirror orientation angle = 0



Left: footprint (Y,X) plane. Right: image (X,Z) plane

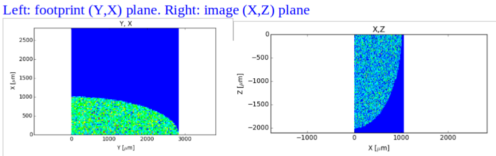
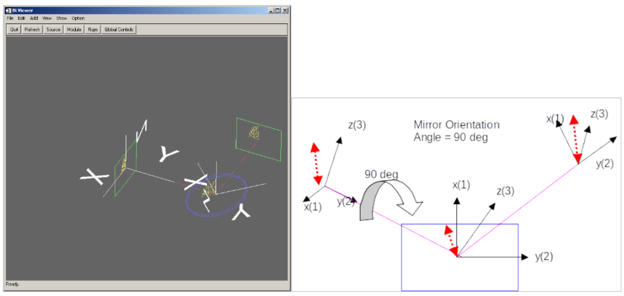
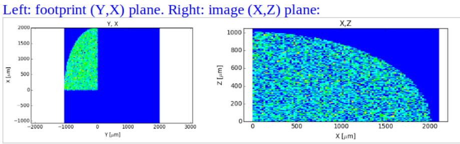


Figure 3:

b) Mirror orientation angle = 90 deg



Left: footprint (Y,X) plane. Right: image (X,Z) plane:



2 Synchrotron sources: Bending magnets

You will:

- simulate bending magnets

Questions:

i) Simulate the source for the ESRF bending magnet (full emission) at a fixed energy (e.g.,. 8 keV). Use one mrad of horizontal divergence. Visualize the cross section (x,z), the divergence space (x',z'), the phase spaces (x,x') and (z,z'). Visualize the top view (y,x). Make histograms of intensity (total, s-polarized and p-polarized) as a function of the vertical divergence. Plot also the degree of circular polarization (S3 component of the Stokes vector).

ii) Change the source energy to 18 keV and compare the plot f intensity versus vertical divergence with the result at 8 keV. Verify that the radiation is more collimated. Simulate the same source but on a limited vertical divergence (e.g., +/- 50 μrad).

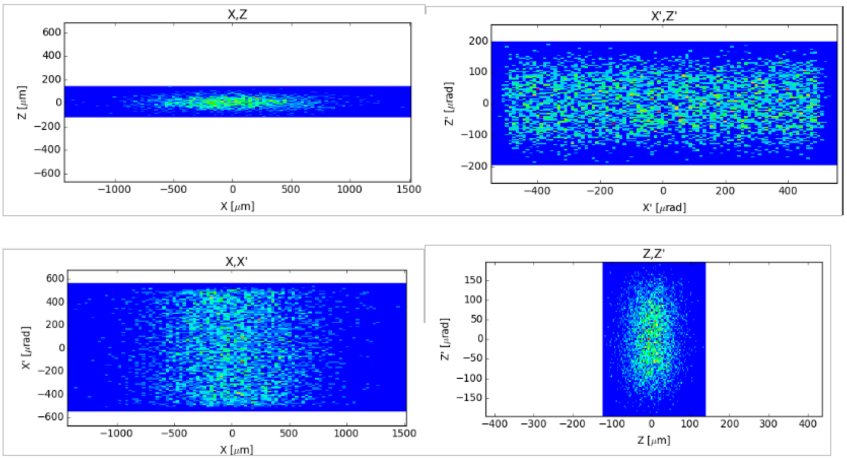
Hints: you may load the workspace ex12_bendingmagnet.ows, where this system is defined, for full vertical emission.

Notes: By default one can use Calculation Mode = Precomputed, and select an "infinite" Max vertical half-divergence (we set to 1 rad which contains everything that is radiated). Shadow will calculate rays following the full emission. In case that one wants to work very far from the critical energy (like for infrared beamlines), one should use "Exact Calculation". In this case, the Max vertical half-divergence should be larger than the natural full divergence but not much larger. For example, in this case one can set 0.001: 1 mrad is still much larger than the full vertical emission (200 mrad).

Answer

Open the "Bending Magnet" widget, click "Run Shadow/Source" and display in the right panel using "Detailed Plot" the cross section (x,z), the divergence space (x',z'), and phase spaces (x,x'), (z,z'):

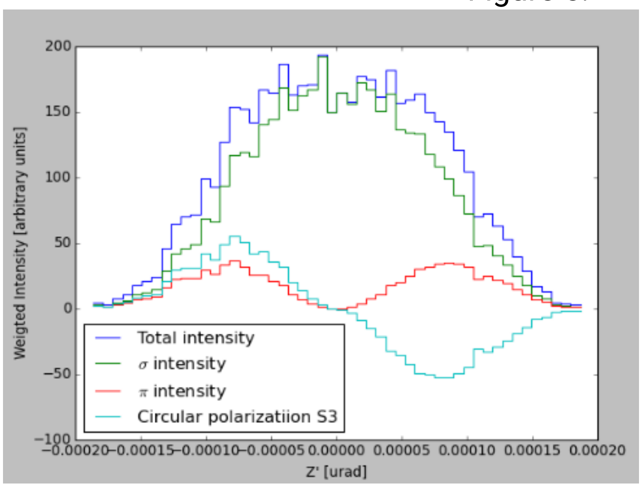
Figure 4:



Another way is to plug a "Plot XY" widget and select the wanted coordinates for the plot. This can also be used to display the "top view" (y,x).

Plug the "Histogram" widget to display histograms of intensity weighted by 23:Total Intensity, 24:s-polarized, 24: p-polarized, S3-Stokes or circular polarization). Although it is not possible to combine histograms in a single plot, it is always possible to prepare a simple script that performs customized plots, like the one included in the workspace that produces:

Figure 5:



3 Synchrotron sources: Insertion devices

You will:

- Simulate wigglers and undulators

Questions:

i) Simulate the old wiggler for the ESRF ID17 (medical beamline) the energy interval 10000±10 eV . Calculate the total horizontal divergence (width of the x' histogram) and visualize a top view of the emission (y,x) with finite emittance and source size, and without emittances (i.e., setting emittances and sigma's to zero).

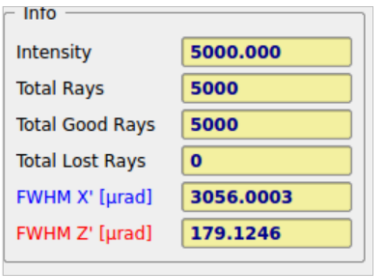
ii) Simulate the ESRF U46 undulator with gap tunned to have its third harmonic at 7833.5 eV. Use Gaussian approximation and understand the parameters.

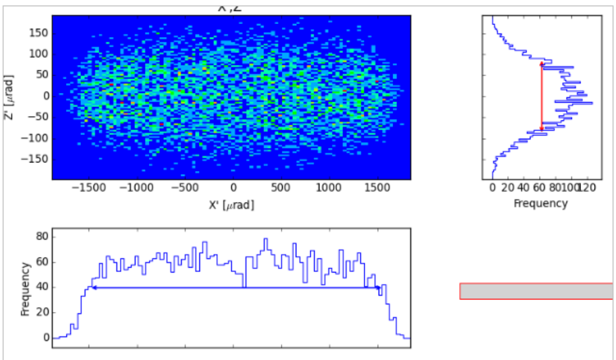
Hints: you may use the workspace file ex13_insertiondevices.ows

Answer a)

E [keV]	x'[μrad]	z'[μrad]
10	3056	179

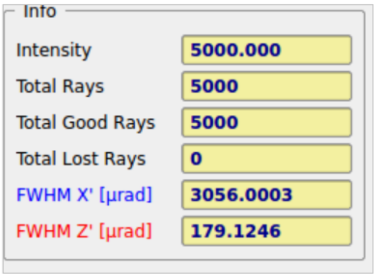
Figure 6:

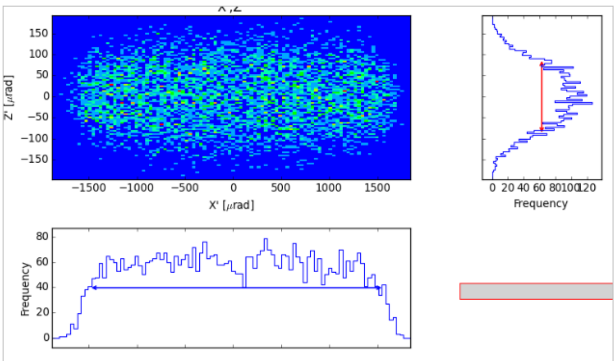




Plot of X versus Y for the wiggler with (left) and without (right) emittances:

Figure 7:





b) Use the “Undulator Gaussian” widget and input the corresponding parameters for the electron beam and photon energy. This application will create a source using the Shadow Geometrical source with divergences and sizes corresponding to the photon beam. These values or the photon beam (S,S’) comes from a convolution (sum in quadrature) of the values for the electron beam (se se’) with the values corresponding to the photon emission of a single electron beam (sg, sg’) and wavelength l=1.58274326 A (7833.5 eV), and undulator length L=1.65 m .

The formulas used are (Onuki Elleaume: Undulators, Wigglers and their applications, CRC press, 2002):

$$\sigma_\gamma = 2.74 \frac{1}{4\pi}\sqrt{L\lambda} \qquad \sigma_\gamma' = 0.69\sqrt{\lambda/L}$$

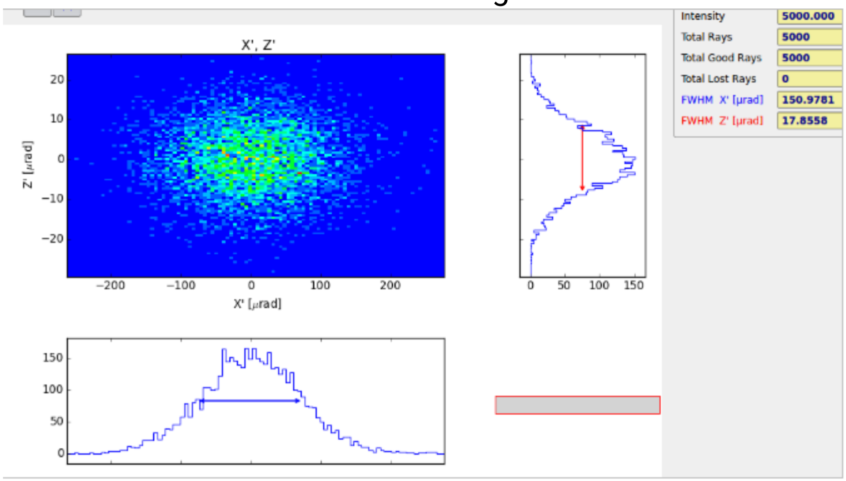
In our case:

	σ_e	σ_e'	σ_y	σ_y'	Σ	Σ'
X	57 μm	68.4 μrad	3.52μm	6.758μrad	57.11μm	68.73μrad
Y	10.3μm	3.78μrad	3.52μm	6.758μrad	10.887μm	7.74μrad

These values can be checked in the “Source Info” available using the “Info” widget.

Plot of the divergence space (X’,Z’) for the undulator.

Figure 8:



4 Beam propagation (phase space (z,z’) ellipses)

You will:

- Define screens and slits associated to optical elements
- Learn about the phase space changes when the beam propagates
- “Optimize the source” in the sense shadow will only store rays that enter in a defined aperture

Questions:

i) Using the created bending magnet source (example 12) add several screens at 0 (source position), 50, 75 and 100 cm from the source. See the tilt of the (z,z’) diagram.

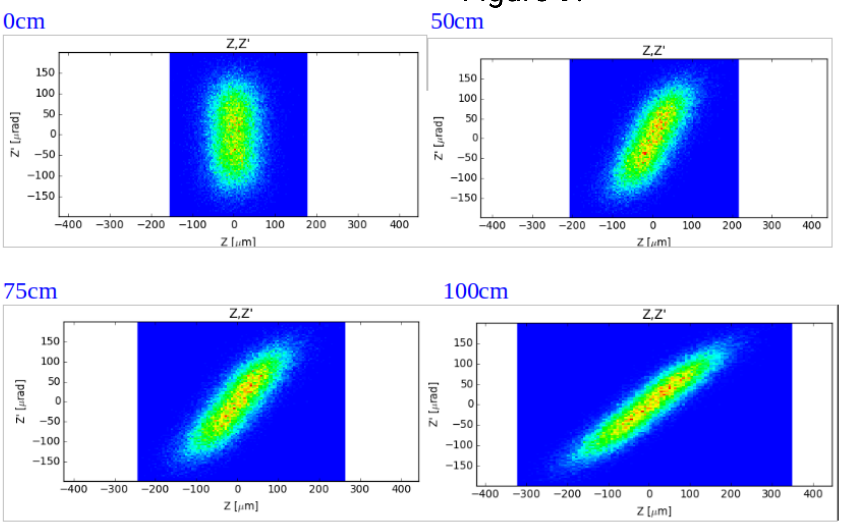
ii) Define an aperture (20 m×20 m) in the first screen and see its effect in screens 2 and 3.

Hints: You may use the workspace files ex14a_beampropagation.ows. It also, contains the system with slit, but using an optimised source in order to avoid losing most of the rays at the slit.

Answer

a)

Figure 9:

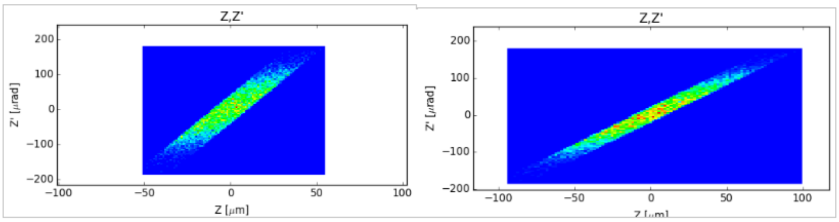


Note that instead of defining the different screens, one can directly plug a “Plot XY” to the source and widget and use “Position of the image” = Retraced and play with the distances.

b)

Figure 10:

75cm 100cm



5 Focusing with grazing incidence mirrors: effect of aberrations

You will:

- Use different mirror shapes in SHADOW
- Experience with the automatic calculation of the mirror parameters.
- Include mirror reflectivity by using the "prerefl" preprocessor
- Visualize results using contour curves.

Questions:

Create a geometrical source with Gaussian shape (sx=57 um, sz=10.4 um) and Gaussian divergence (sx'=88.5 urad and sz'=7.2 urad) to simulate the emission of an ESRF 1.65 m undulator at 10 keV in a Low beta section.

i) Study the case of different mirror shapes (spherical, toroidal and ellipsoidal) for focusing the source with distances (p,q)=(30m,10m) (magnification 1/3) and (30m,1m) (magnification 1/30). Set the grazing angle to 2 mrad. Study the effect of the spherical aberrations and its influence depending on the magnification factor. Study the dependence on mirror dimensions and incident angle.

ii) Enter the effect of mirror reflectivity. Consider a Rh (density=12.4 g/cm3) coating and a source with energy distribution in 5-45 keV (box-distribution). Visualize the results. Plot also the intensity versus energy.

Hints: For the different mirrors, Shadow can calculate the surface parameters (curvature radii, ellipse axes, etc). by selecting the parameters in Basic Settings $\rightarrow$ Surface Shape -> Type = "internal/calculated" . The resulting mirror parameters can be seen using the "MirInfo" tab from the "Info" widget. For including reflectivity, the preprocessor PreRefl must be used. The workspace file ex15a_aberrations.ows contains this exercise.

Notes: kkk

Answer

The aberrations effect increases if

- one goes to more grazing angle

- one reduces the magnification factor (i.e., mode demagnification of the source)
- one uses larger mirrors. Small mirrors reduce aberration because cut rays which arrive far from the mirror center. Obviously, this effect reduces also the intensity. For analysing that, use the Basic Settings->Dimensions->Limits Check entry.

Figure 11: M=1/3 Toroidal: 43 mm x 26 mm FWHM, Ellipsoidal 40 mm x 9 mm

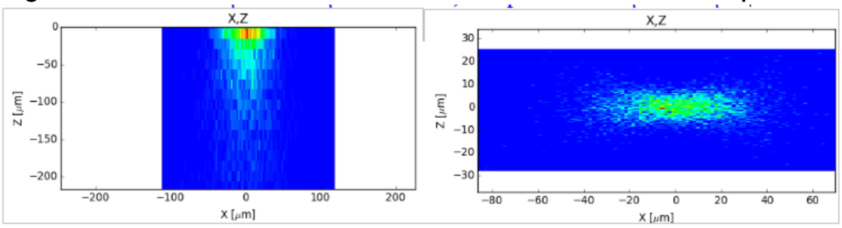
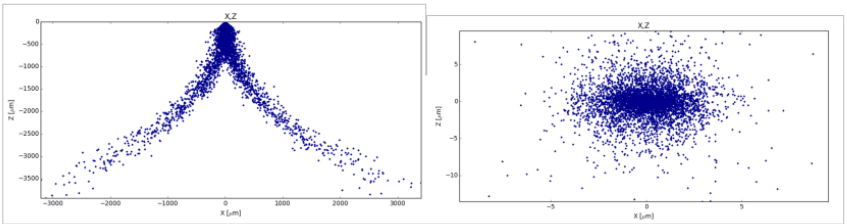
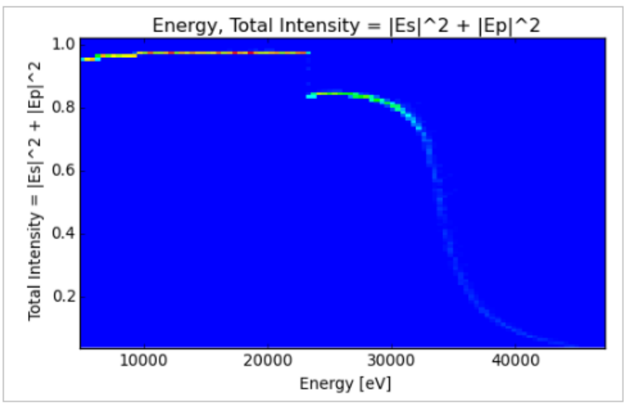


Figure 12: M=1/30 Toroidal: ? um x 39 um FWHM, Ellipsoidal 2.4 um x 1.6 um. Note that a graph type "preview" has bee used to better observe the aberration tails produced by the toroidal mirror.



b)

Figure 13: I(E) plot.



6 Kirkpatrick-Baez system

You will:

- define an optical system with two mirrors either of circular or elliptical section
- tell SHADOW to calculate automatically the mirror parameters in the case that focal planes are not coincident with continuations planes
- learn the impact of the “mirror orientation angle”
- define mirror dimensions

Questions:

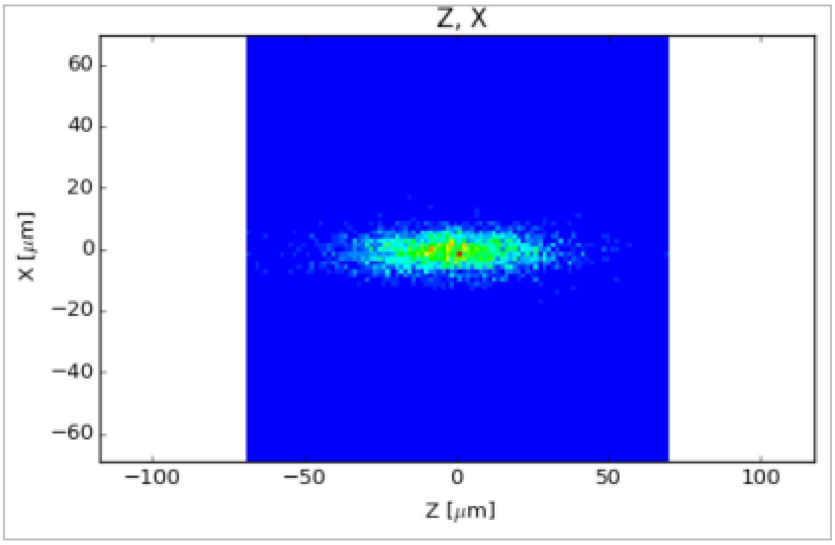
Study the case of the previous exercise (M=1/30) with a Kirkpatrick-Baez system with cylindrical (and later with elliptical) mirrors of length=40 cm and width=4 cm. Distance source-M1=29.5m; Distance M1-M2=1m; Distance M2-spot=9.5m. Use 25000 rays. Do not include the mirror reflectivity.

Hints: Hint: you may use the workspace file ex16a_kb.ows.

Answer

First branch corresponds to the KB with circular (cylindrical) mirrors. Note that the image plane displays (X vs Z) in the “Plot XY” widget, corresponding to the horizontal (Z) and vertical (X) directions. Note that these directions are swapped respect to the source because the mirror orientation angle for the second mirror is 90 degrees. The mirror parameters are input externally R(M1)=739455.7 cm and R(M2)=691710.4 cm. The Resulting spot is 36 mm x 8.3 mm. The second branch corresponds to the KB with elliptical mirrors, where the ellipse parameters are calculated internally. (check them using MirInfo) The Resulting spot is 31 mm x 7 mm. A third branch uses the widget for the compound element “Kirkpatrick-Baez Mirror” which reproduces the elliptical KB setup in a simpler way. This branch also implements a trick useful in some cases: if one wants to reverse the axes to come back to X in horizontal and Z in vertical is possible to use an “Empty Element” with incident angle zero, output angle 180 deg and mirror orientation angle 90 deg.

Figure 14:



7 Double crystal monochromator

You will:

- create crystal reflectivity data using the “bragg” preprocessor
- use the “autotunning” facility to align the crystal
- calculate the energy resolution for a crystal and a combination of systems
- optimise the source bandwidth
- play with the mirror orientation angle. Relate its values to the crystal dispersion ((+,-) and (+,+) crystal combination)

Questions:

Create a bending magnet source (starting from exercise 12) at 8000$\pm$25 eV with 3 mrad horizontal divergence. Verify its energy dependence and horizontal and vertical divergence values.

i) Implement a flat Si 111 crystal at 30 m from the source. Verify the energy dependence and calculate resolution. Redefine the source energy bandwidth to optimize the calculation in order to obtain the energy dependence with the highest signal.

ii) Add a second crystal 10 cm downstream from the first one in (+,-) and (+,+) configurations (play with the mirror orientation angle). Explain the obtained differences in energy resolution.

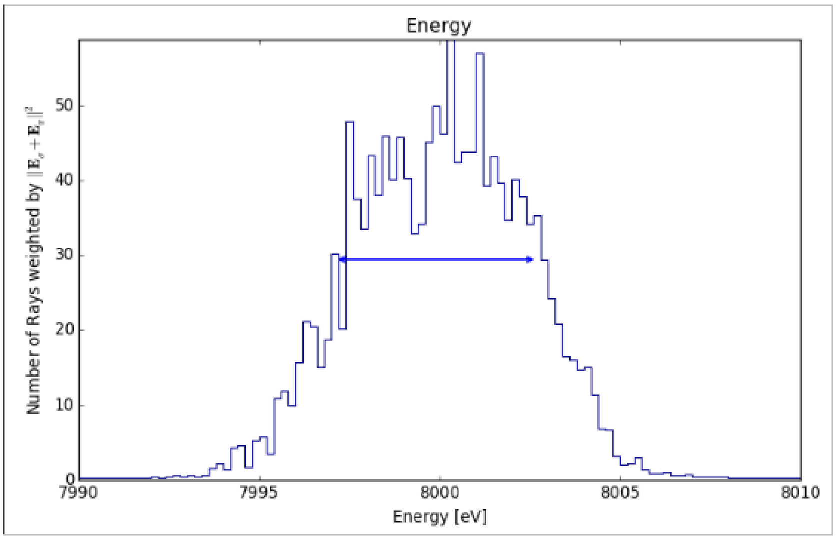
Hints: you may use the workspace file ex17_crystalmono.ows containing three branches:

1. (+,-)
2. (+,+)
3. the double crystal monochromator compound element (same as (+,-).

Use the Bragg preprocessor to create the reflectivity data for a Si 111 crystal. You can create the output file for a large range of energy (e.g., from 5000 to 15000 eV). Pay attention to the file name when you run bragg, because it also appears in the o.e. crystal menus. In this case, the file is called si5_15.111.

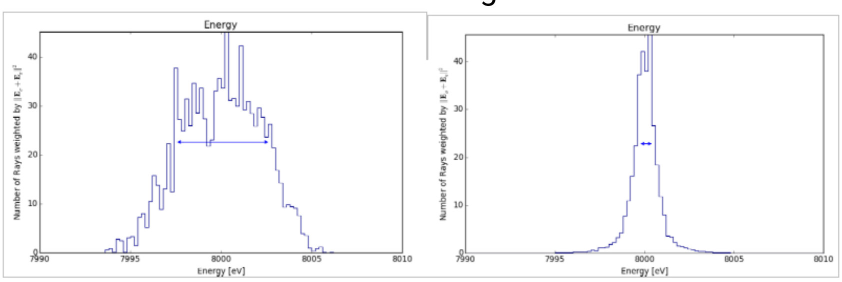
Answer a) The optimized energy range selected is 8000±10 eV. The histogram of the energy (including reflectivity) after the first crystal has FWHM 5.6eV:

Figure 15:



Left: resolution function for (+,-) (non-dispersive configuration). Here the mirror orientation angles are 0 and 180 deg for the first and second crystals, respectively. Note that the width (5.2 eV) is very similar to a single crystal in a), but with a slightly lower intensity due to the absorption of the second crystal. Right: resolution function for (+,+) (dispersive configuration). The mirror orientation angle is 0 for both crystals. Here one can see the effect of the dispersive setup, the final energy resolution depends only on the crystal Darwin width and does not depend on the beam divergence.

Figure 16:



8 Sagittal focusing

You will:

- define a cylindrical mirror for sagittal focusing
- define “externally” the optical element radius of curvature
- optimize the focal spot

Questions:

i) Using the (+,-) system defined in the last exercise at photon energy 20 keV, bend sagittally the second crystal to focus in the horizontal plane at the sample position, placed 1000 cm downstream from the monochromator (monochromator at 3000 cm from the source). Calculate horizontal spot size.

ii) Study the effect of the ratio between the distances mono-sample and source-mono in the transmitted intensity. Study the case of M=1/30. See the effects in energy resolution and system transmitivity. Explain these differences. Verify that ratio 1/3 is the optimum.

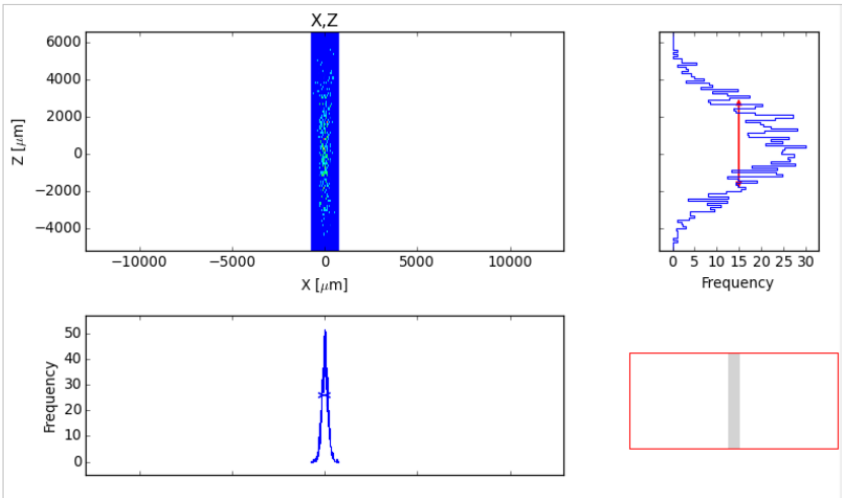
Hints: You may use the workspace files ex18a_sagittalfocusing.ows also contains a python script that scans the magnification. One can see that the intensity peaks at about 1/3. A script is included to calculate the curvature radius: Rs (20 keV, M=1/3)=148.3 cm.

Answer

a) Focusing system: Spot width H=334 mm, I/I0=1090/25000, DE=18 eV Non-focusing system: Spot width H=189mm, I/I0=1094/25000, DE=18 eV Best focus very close to the focal position. The spot size does not change appreciably.

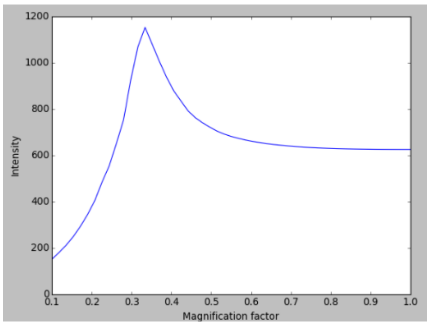
b) p=30m, q=1m, Rs=47.8 cm, Spot width=0.012 cm, I/I0=168/25000, DE=5.8 eV

Figure 17:



The study of the variation of the intensity as a function of the magnifications needs to run shadow for many points of M. It can be done with a macro. The result should show an optimum magnification of M=1/3 for large divergence values. The python script will show this effect (5 mrad).

Figure 18:



Intensity (in arbitrary units) versus magnification factor M for a point and monochromatic (E= 20 keV) source placed at 30 m from the sagittaly bent crystals. The beam divergences is 5 mrad (can be changed in the macro). We clearly observe the maximum of the transmission at M=0.33, as predicted by the theory.

9 Simulation of a complete beamline

You will:

- Combine several optical elements
- Obtain final results for a beamline in terms of flux, resolution and spot size

Questions:

Define the following elements in SHADOW: Geometrical Gaussian source at 10000±10 keV (box distribution) (like in exercise 15 b, but changing the energy interval) M1: Cylindrically collimating mirror in the vertical plane at 25 m. Grazing angle 0.12 degrees. Rh coating (density=12.4 g/cc). Infinite dimensions. MONO: Double crystal monochromator, Si 111, with second crystal sagittally bent (focusing the source into the sample position in the horizontal plane), at 30 m from the source (Rs=296.6 cm) M2: Re-focusing mirror at 35m from the source, focusing at the sample position. Same angle as M1 Sample at 40 m

i) Calculate:

- Beam geometry at the sample position
- Energy resolution
- Transmitivity of the whole beamline. Number of photons at the sample position supposing that at the source we have, at 10 keV, a flux of 5 1013 ph/sec/0.1%bw

ii) How are these results modified using a focusing first mirror and a flat second mirror?

Hints: you may use the workspace file ex19_beamline.ows

Answer

DEsource=4 eV (optimized source bandwidth); DE=1.3eV; I/I0=1406/5000

Transmitivity in one eV=T=(I/DE /(I0/DEsource)=(1406/1.3)/(5000/4)

Number of photons at the source in one eV bandwidth =N= 5 e12

Total number of photons = N×T×DE

Figure 19: Intensity distribution in the (X,Z) plane at the image position

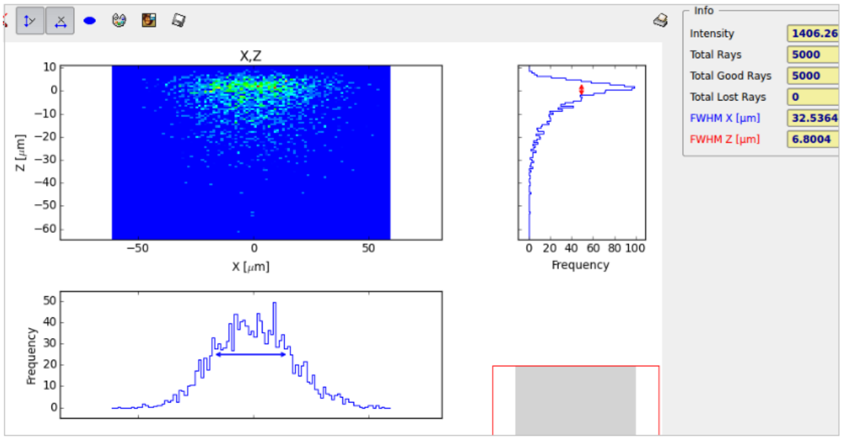
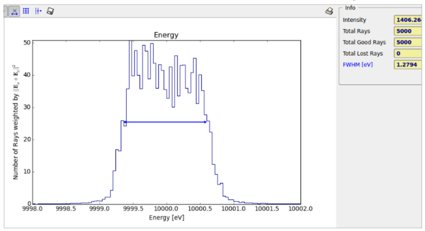


Figure 20: Energy distribution:



10 Slope errors

You will:

- Use Waviness preprocessor to create a file sampling slope errors
- Use presurface to inject it in SHADOW
- See the important effect of slope errors in the focal size

Questions:

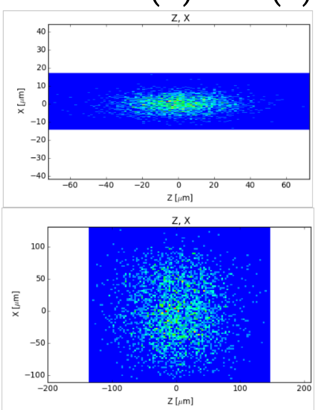
i) Load the Kirkpatrick-Baez system of exercise 6. Set mirror surface to be elliptical. Check that mirror dimensions are 40×4 cm2. Calculate spot sizes without slope errors.

ii) use the preprocessor widget Waviness to create maps of slope errors. For adjusting the slope errors to the wanted values, modify the value of the initial Y slope error in order to get a value close to the desired tangential slope error of 0.5 arcsec rms. Then modify the number of points in X in order to adjust the sagittal slope error to 1 arcsec rms. In the oe "Advanced setting" tab, select "Modified surface" subtab and check the file name containing the errors. This is automatically populated if one connects the Waviness with the Mirror widgets. One can also have a quick preview from there.

Hints: use the workspace ex20_slopeerrors.ows

Answer

Figure 21: Top: No slope errors: 7.5 (V) × 40 (H) um2. Bottom: with Slope errors: 111 (H) × 89 (V) um2



11 Thermal deformations

You will:

- use a python script to create a file sampling a thermal bump
- see the effect of the bump in energy resolution

Questions:

Load the ex21_thermalbump.ows workspace. Run the script to create a Gaussian bump bump.dat Run the system (a single Si111 crystal) without and with thermal bump. See the changes in the energy resolution.

Hints:

Notes:

Answer

Figure 22: No bump: 1.4 eV, H: 8.5 mm, V: 0.59 m

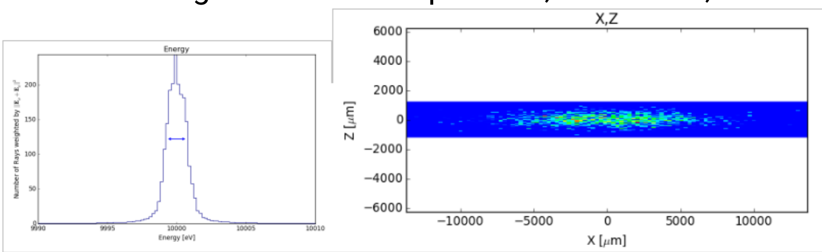
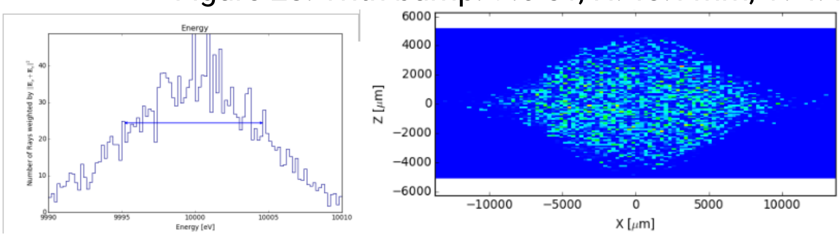


Figure 23: With bump: 9.6 eV, H: 10.1 mm, V: 4.4 m



12 Curved crystal monochromators: Rowland and off-Rowland configurations

You will:

- understand the effect of crystal radius in energy resolution and focusing conditions
- calculate the focusing conditions in and out Rowland configuration
- understand the importance of using contour curves with PlotXY simulate an asymmetric crystal

Questions:

i) Using the same Gaussian source as in exercise 11, verify the focusing conditions for a symmetrical Si111 Bragg crystal at 10 keV, with p=30m. Calculate DE. Calculate DE for Rt=5000 cm and Rt=2500 cm. Explain the differences.

ii) Calculate the Rowland conditions for 10 keV, Si111, p=30m and asymmetry angle α=5 deg. Calculate energy resolution and spot size.

Hints: use ex22_rowland.ows

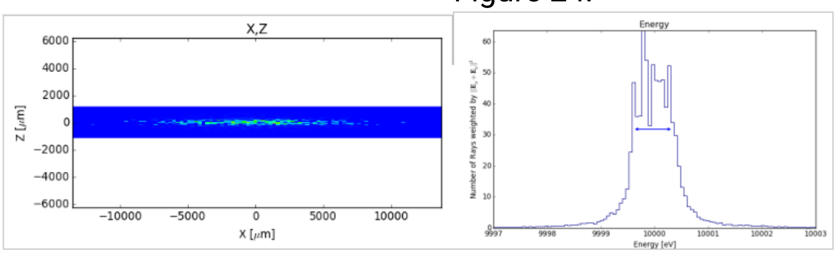
Answer

a) For the focusing conditions (first branch), we have Rt=15171 cm (see results in Info widget) and DE=1.32 eV

For Rt=5000 cm (second branch) we then have DE=1.38 eV For Rt=2500 cm (third branch) we then have DE=3.9 eV

b) Using the script to calculate Rowland conditions, we get Rt=10623.284 cm, q=1184.8 cm; We get DE=0.72 eV; spot size = 7.1 mm × 276 mm.

Figure 24:



13 Transfocators

You will:

- Run a transfocator
- Find the position of the best focus
- Study the changes due to the source energy (chromatic aberrations)

Questions:

i) Implement a monochromatoc Gaussian source of 48.2 (H) x 9.5 (V) m RMS size and 100 (H) x 4.3 (V) rad RMS divergence. Create the same source for two different energies (E1=35200 eV and E2=35700 eV). Implement a transfocator consisting of two CRLs, 2D-focusing (in both H and V), the first made in Be (16 lenses of radius 200 m, separated 50m), and the second in Al (21 lenses of radius 200 m, separated 50m). The focal distances are p=3150 cm and q=1000 cm. This setup is discussen in http://dx.doi.org/10.1117/12.893343

ii) Compare the results using plotxy. Study the beam evolution close to the focal plane using focnew and ray_prop: you will find a small astigmatism, i.e., the H and V foci are at slightly different position (you will find that the astigmatism disappears when using a point source, so it is the result of the final dimensions of the source). Change the energy of the source from 35200 eV to 35700 eV and see the effect in focal position and intensity.

Hints: ex24_transfocator.ows

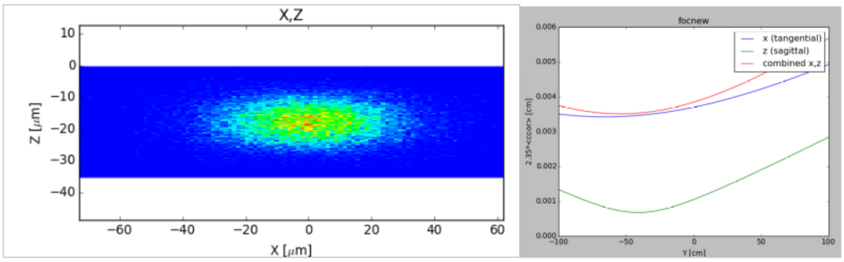
Notes: kkk

Answer

For E=35200 eV we find a focus of 34 x 10 um (FWHM) with I= 11528, best H focus at about -40 cm (you can use focnew or ray_prop implemented in two scripts).

- Sagittal focus at : -65.4294
- Tangential focus at : -40.9559
- Circle of least confusion : -54.2916

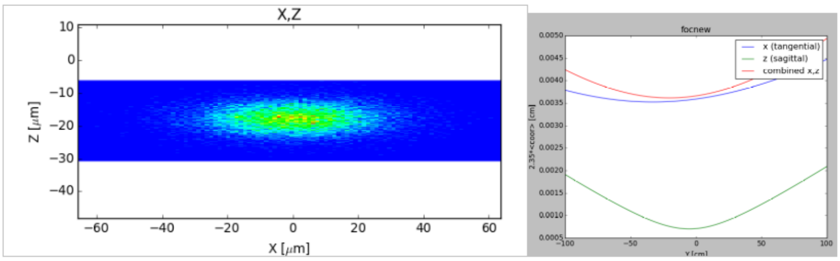
Figure 25:



For E=35700 eV we find a focus of 34 x 6.1 um (FWHM) with I= 11734

- Sagittal focus at : -32.9289
- Tangential focus at : -5.03177
- Circle of least confusion : -20.3752

Figure 26:



A The very basics of SHADOW

SHADOW is a ray-tracing program specially optimized for the design of the synchrotron radiation beamline optics.

SHADOW generates and traces a beam along the optical system. The beam is a collection of rays in a given point of the beamline which are stored in a disk file. The optical system is a collection of optical elements (o.e.) (mirrors, multilayers, slits, screens, etc.) placed in a sequential order.

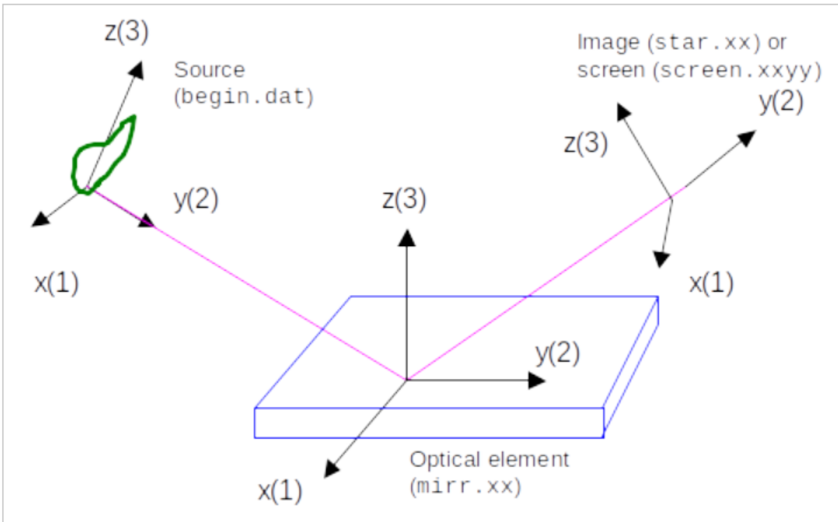
Each ray is an array of 18 variables or columns. Each variable of column has an special physical meaning. The first six defines the geometry: spatial coordinates (Col. 1,2,3 or x, y and z, respectively) and the direction of the ray (cols. 4,5,6, or x',y' and z', respectively). The rest of the columns defines the history of the ray traversing the optical system (electric vector for s-polarization (cols. 7,8,9) and p-polarization (cols. 16-18), flag for lost ray (10), wavelength (11) etc.).

The source is the beam at the starting point. It is generated by SHADOW by sampling the spatial, angular, energy and other qualities of the synchrotron radiations sources (i.e., bending magnets, wigglers and undulators) into a finite number of rays, using a Monte Carlo method. At the source position the intensity of each ray (or better, its probability of observation) is set to 1. This intensity will decrease along the beamline because of the interaction of the ray with the optical elements. The source generated by SHADOW samples linearly the real source, which allows scaling the intensity with the number of photons.

SHADOW traces the source sequentially thought each individual optical element of the optical system. SHADOW solves the intercept of each ray at a given o.e., calculates the output direction and the decrease in intensity. This decrease is calculated for each ray using a physical model (i.e. Fresnel equations for mirrors, Dynamical Theory of the Diffraction for perfect crystals, etc.)

B SHADOW frame

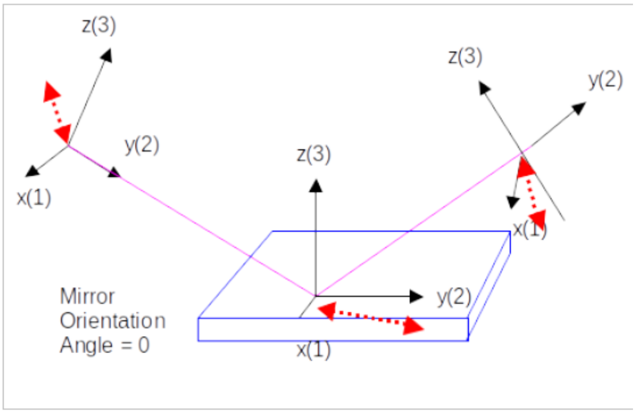
The coordinate system of SHADOW is (schematic):

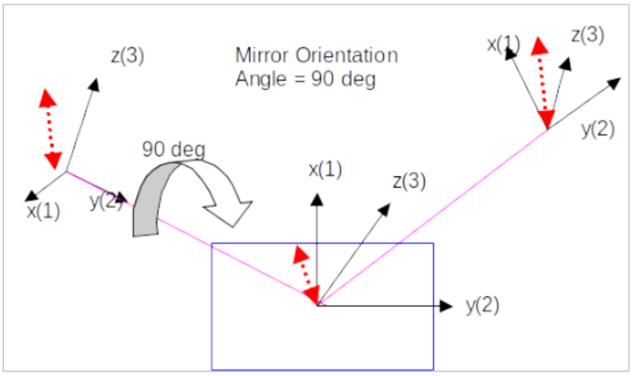


Note that:

- The y(2) coordinate is along the beam direction
- The frame is rotated if one o.e. is rotated
- The position, orientation, etc. of any o.e. is always referred to the previous one

C Effect of o.e. orientation in SHADOW frame





D Script programming (python): survival guide

Before anything, in python:

»> import Shadow

There are only three main objects in Shadow python: a container for the variables needed to create a source (the same variables as in the file start.00), a container for the variables necessary to define an optical element (the same as in the files start.01, start.02, etc.), and a container for the beam (same information as in the binary files begin.dat, star.xx and screen.xxyy)).

Initialize them as:

```
src = Shadow.Source()
oe1 = Shadow.OE()
oe2 = Shadow.OE()
beam = Shadow.Beam()
```

Listing 1:

In the case we want to read variables from existing files do:

```
src.load("start.00")
oe1.load("start.01")
oe2.load("start.02")
```

Listing 2:

For applying to the beam the source:

```
beam.genSource(src)
```

For tracing the two optical elements:

```
beam.traceOE(oe1)
```

```
beam.traceOE(oe2)
```

Access SHADOW beam

The rays are in a numpy array:

»> print(beam.rays) [[0.00039945 0. 0.00034409 ..., 0. 0. 0.]

[-0.00109609 0. 0.00174768 ..., 0. 0. 0.]

[-0.0013806 0. -0.00160363 ..., 0. 0. 0.] ...,

[-0.0005546 0. -0.00137695 ..., 0. 0. 0.]

[0.00045102 0. -0.00234013 ..., 0. 0. 0.]

[-0.00062769 0. 0.00102393 ..., 0. 0. 0.]]

Write binary file:

```
beam.write('star.02')
```

Visualizing results

Shadow.ShadowTools.plotxy(beam,1,3) Shadow.ShadowTools.histo1(beam,1)

Using Scripts in ShadowOui

It is possible to connect a “Python Script” widget to a source or optical element and extract and modify the information there. This is very useful for making things that are not implemented as widgets. The SHADOW objects are inside a large object that the “Python Script” widget receives as in_object and resends as out_object. For example:

```
beam = in_object._beam
```

print((in_object.history[1]._shadow_oe_end._oe.FILE_SCR$_E$*XT*))