Computer simulations and ray-tracing for hard X-ray optics

TUTORIALS on XOP and SHADOWVUI (EXERCISES AND ANSWERS)

Manuel Sanchez del Rio, ESRF, BP 220, F-38043 Grenoble Cedex

Spectral characteristics of synchrotron sources and characteristics of optical elements (Exercises to be done with XOP)

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    3. Asymmetric wiggler (id20)
    4. Undulator sources (angular distribution)
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Bibliography

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1. emission characteristics of synchrotron radiations sources: Bending Magnets

You will learn:

- to calculate bending magnet spectra using BM
- the basic use of Xplot

Simulate bending magnet spectra for different sources. Calculate numerical values, and fill them in the table below.

i) Maximum flux in number of photons (considering 1 mrad of horizontal aperture)

ii) Total power emitted by the BM in the full energy range.

Try to remember and check (or guess from numerical values)

iii) How the total power scales with the electrons energy?

iv) What is the power in the energy range from zero to the E_c? and from E_c to infinity?

Facility	E [GeV]	I [mA]	B [T]/R[m]	E_c [eV]	i (Flux)	ii (Total Power [W])
ESRF	6.04	200	0.8/ 25.2			
Elettra	2	300	1.2/ 5.56			
LNLS	1.37	175	1.67/ 2.74			
SLS	2.4	400	1.45 & 5/ 5.52 & 1.6			
APS	7	100	0.6/ 38.9			
NSLS	2.58	500	0.77/ 11.2			
SSRL	3	100	1.22/ 8.20			

Information source:

ESRF: www.esrf.fr

Elettra: http://www.elettra.trieste.it/about/parameters.html

LNLS: http://www.lnls.br/info/info.htm

SLS:)

Others: http://www-als.lbl.gov/als/intersrc/existing.html

Hints:

Use *XOP|Bending Magnet |BM* to create the spectra. Numerical values can be obtained from the resulting *BM|Show|View Results* window and plots can be done using *BM|Show|Plot Results*, which creates a graphical window (Xplot). Power values can be calculated by integrating the power density spectra or read directly from the results window.

Integration of the power spectrum can be done with *Xplot|Calculations|Width/Integral/MinMax* menu. For integrating over a limited range of abscissas, just select the desired interval with *Xplot|Edit|Limits|Set...* and the apply the *Xplot|Calculations|Width/Integral/MinMax* again.

The questions iii) and iv) can be answered without using the computer. Question iv) can be checked by calculating the normalized cdf(power spectrum) using first *Xplot|Calculations|cdf* to calculate cdf(power spectrum) and then normalizing the result with *Xplot|Calculations|Operations with columns*

Answer

Start the BM (using File|MB input parameters>Load from file…) application, enter the correct parameters and use "Show" menu to visualize the results. The ESRF parameters can be loaded in BM using the XOP input files `ex1_bm.xop`.

Facility	E [GeV]	I [mA]	B [T]/R[m]	E_c [eV]	i (Flux)	ii (Total Power [W])
ESRF	6.04	200	0.8/ 25.2	19414	2.72e13	149.9
Elettra	2	300	1.2/ 5.56	3193	1.34e13	12.16
LNLS	1.37	175	1.67/ 2.74	2085	5.41e12	3.17
SLS	2.4	400	1.45 & 5/ 5.52 & 1.6	5555.7& 19158	5.41e12& 2.16e13	33.87& 116.8
APS	7	100	0.6/ 38.9	19557	1.58e13	86.9
NSLS	2.58	500	0.77/ 11.2	3409.4	2.90e13	27.9
SSRL	3	100	1.22/ 8.20	7303.8	6.77e12	13.91

iii) How the total power scales with the electrons energy?
Proportional to E^4 when keeping constant the bending radius R
iv) What is the power in the energy range from zero to the Ec? and from Ec to infinity? P[0,E_c]=P[E_c,∞]=0.5 Total Power

2. emission characteristics of synchrotron radiations sources: Conventional wigglers

You will learn:

- to calculate standard wiggler spectra using Xwiggler and WS.
- understand the pros and cons of each program
- use applications input files

Simulate spectra for different ESRF *conventional* wigglers. Calculate

i)   Maximum flux (for I=200 mA)
ii)   Critical Energy corresponding to maximum deflection (from *Show parameters*)
iii)   Calculate the effective critical energy with Xplot
iv)   Total emitted power (for I=200 mA)

	λ_u[m]	K	N	Max Flux ph/sec/0.1%bw	Ec [eV]	Tot Power at I=200 mA [kW]
Id9	**0.070**	**5.43**	**22**			
Id11	**0.125**	**14.7**	**12**			
Id17	**0.150**	**19.6**	**11**			

Used symbols:

λ_u: magnetic period of the insertion device

N: number of periods

K: deflection parameter

Information source: http://www.esrf.fr/machine/support/ids/Public/Ids/installed_IDs.html
and beamline web pages

Hints: Use the Xop|Sources|wigglers|Xwiggler to create the spectra. Make calculations, for instance, from 100 to 100000 eV with 200 eV step. Save the flux spectrum of id9 in an ASCII file (for comparison with results of undulator model, to be done later).

Use the Xop|Sources|wigglers|Ws for calculating the spectrum of id11. Compare with previous results.

Use Xplot|Calculations|Width/Integral/MinMax to get maxima. The effective critical energy can be calculates using the normalized cdf(flux), as done before.

Answer

use the XOP input files:

```
ex2_xwiggler_id9.xop
ex2_xwiggler_id11.xop and ex2_ws_id11.xop
ex2_xwiggler_id17.xop
```

	λ_u[m]	K	N	Bmax [T]	Max Flux ph/sec/0.1%bw	Ec [eV]	Tot Power at I=200 mA [kW]
Id9	0.070	5.43	22	0.83	1.06e15	20204 web:20000	4.86 web 4.74
Id11	0.125	14.7	12	1.24	1.58e15 at 5.1keV (web 1.4e17??)	30631 (web 29000)	10.415 (web:20)
Id17	0.150	19.6	11	1.5-1.4	2.11e15	34034 (web:33500)	13.9 (web:14.3)

Note that
1) XWIGGLER generates the full emission of the wiggler versus photon energy (i.e., integrated over the full emission angle)
2) WS creates emission either integrated over a given aperture area placed at a given distance, or integrated over given emission angle (set the distance to zero in this case). Note that for comparison with XWIGGLER the slit must be large enough to receive the full emission. However, very large aperture will result in inaccurate calculations because the integral is doing over a mesh with few points in X and Y (max 50×50).

3. emission characteristics of synchrotron radiations sources: Asymmetric wiggler (ESRF-id20)

You will learn:
- to calculate the flux of asymmetric wiggler spectra using Xwiggler
- Use magnetic field from B(y) map or from harmonic decomposition.

Calculate the emission spectrum of an asymmetric wiggler
i) Calculate the maximum flux and the total emitted power XWIGGLER
ii) Calculate B as a function of the harmonics (use Xop|Tools|Xop macro, load and run the file ex3_id20.mac)

	λ_u[m]	K	N	Max Flux[*] ph/sec/0.1%bw	Ec [eV]	Tot Power[*] [kW]
Id20(asym)	0.210	15	8			

Hints: Use Xop|Xwiggler. The magnetic field data for Id20 is available in the files ex3_h.dat or ex3__b.dat (harmonics and magnetic field, respectively).

Answer

Use the XOP input files:
    ex3_xwiggler_id20_b.xop
    ex3_xwiggler_id20_h.xop

	λ_u[m]	K	N	Bmax[T]	Max Flux[*] ph/sec/0.1%bw	Ec [eV]	Tot Power[*] [kW]
Id20(asym)	0.210	15	8	0.9	1.58e15	(19000) 11200 22465	(2.2) 1.597

Notes:
1) With XOP 2.0, the XWIGGLER application for asymmetric wigglers does not work in Windows platforms, only in Linux ones.

4. emission characteristics of synchrotron radiations sources: Undulator sources (angular distribution)

You will learn:
- to calculate the angular distribution of the undulator emission using Xurgent and Xus
- to calculate and visualize the effect of electron beam emittances.

a) Calculate the distribution of flux (at an energy corresponding to the first harmonic, E=166.8 eV) versus emission angle for the yellow book example (no emittance, N=14, E_e=1.3 GeV, λ_u=3.5cm, K=1.87). Use Xurgent and Xus

ii) Calculate the distribution of flux (at an energy corresponding to the first harmonic) versus emission angle for ESRF U46 (E_e =6.04 GeV, N=35, λ_u =46mm, K=2.76) in three cases: i) no emittance, ii) undulator placed in an ESRF high beta section, and iii) low beta. Use Xus (and Xurgent)

	High Beta	Low beta	BM
σ_x [μm]	395	57	126
σ_z [μm]	9.9	10.3	36.9
$\sigma_{x'}$ [μrad]	10.5	88.3	108
$\sigma_{z'}$ [μrad]	3.9	3.8	1.1

Information source: http://www.esrf.fr/machine/support/ids/Public/Sizes/sizes.html

Answer

Use the XOP input files:
```
ex4_xurgent_yellowbook.xop
ex4_xus_yellowbook.xop
ex4_xurgent_hb_u46.xop
ex4_xus_hb_u46.xop
ex4_xurgent_lb_u46.xop
ex4_xus_lb_u46.xop
```
In Xus the results are under Xus|Show|Plot 3D surface|Total intensity

5. emission characteristics of synchrotron radiations sources: Undulator sources (flux and spectral density)

You will learn:

- to calculate the photon flux, spectral density and total power emission of undulators

i) Calculate the flux and spectral power spectra for the three insertion devices of ESRF-id9 (low beta). Use a $3\times3\text{mm}^2$ slit placed at 27 m from the source. Give the maximum flux and total power.

ii) Compare the ESRF-W70 flux with the result obtained with the wiggler model.

	N	K	[mm]	Power [W]	Flux
U20	81	0.27	20	45.5	6.38e13
U46	36	2.76	46	571.8	1.88e14
W70	22	5.43	70	472.0	9.45e13

Hints: Use Xop|Sources|Undulator|Xurgent and/or Xop|Sources|Undulator|Xus. Compare results. Check power results with web data at: http://www.esrf.fr/exp_facilities/ID9/id9.html

Answer

i) Use the files:

```
ex5_xurgent_id9_u20.xop
ex5_xurgent_id9_u46.xop
ex5_xurgent_id9_w70.xop
```

ii) For comparison, integrate over $1\times0.5 \text{ mrad}^2$:
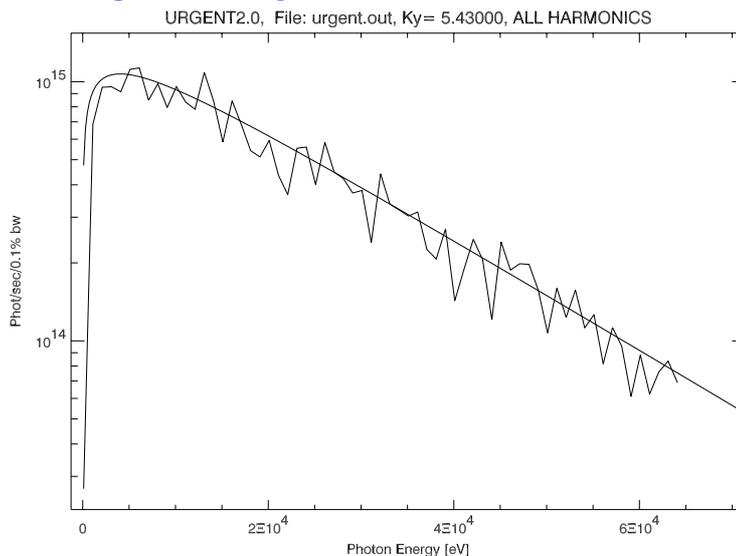
6. Filters and mirrors: effect on source

You will learn:

- to save an Xop source to files to be used with Xpower
- to calculate filter transmission and mirror reflectivity and to see their effects on the source spectrum.
- evaluate absorbed and transmitted power

Calculate how a 500 µm Be window plus a Rh mirror (set at 3 mrad of grazing angle) modify the BM flux calculated in the previous exercise 1. Calculate the absorbed power by these elements. Add other filters (e.g., Al, Mo, etc).

Hints: From the *Xop|BM* window used previously, create the files with the source spectra by using *BM|File|Write files for xop/Optics*. Open the *Xop|Optics|Mirrors&Filteres|XPOWER* application. From the main parameter window, select the source to either *xop/source Flux* or *xop|source Power*. Fill-in the optical elements parameters. The items in the *XPOWER|Show* menu will present the results. Use *Show|Cumulative transmission* to see the sequential effect of the optical elements on the source. Use the *Xplot|Save* button to over plot the spectra after the different elements.

Answer

use the XOP input file `ex6_xpower.xop` Dashed line: source. Dotted line: after Be filter. Continuous line: after Be filter and Rh mirror. See absorbed and transmitted power using Show|Parameters
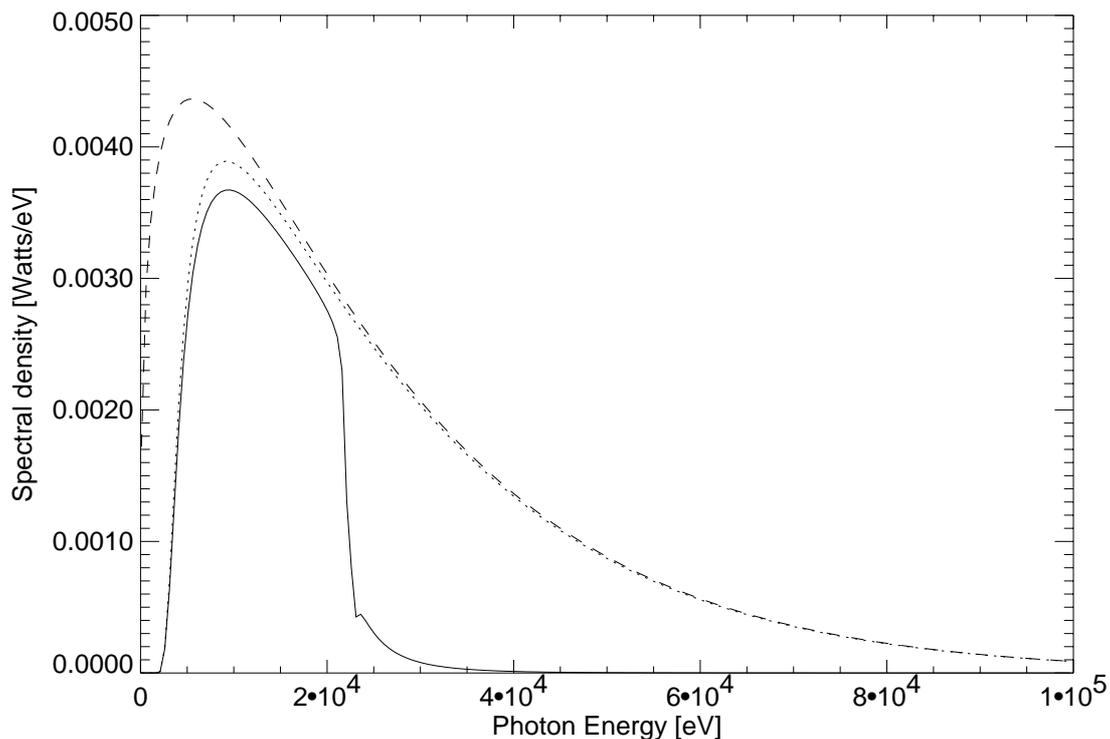
7. Crystal monochromators

You will learn:
- calculate diffraction profiles of perfect crystals
- calculate the response of two crystals (+,-) (curve multiplication)
- calculate rocking curves (convolution)
- calculate harmonic suppression

i) Calculate the diffraction profiles, Bragg angle, width, peak and integrated reflectivity of Si 111 at the energies 5 keV, 8 keV, 12 keV, 50 keV, 80 keV and 120 keV.

ii) For the 8 keV case, calculate the diffracted profile of a double Si111 reflection in (+,-) configuration. Calculate the rocking curve resulting of the rotation of the second crystal respect to the first one.

iii) For a Si111 double crystal monochromator at 8 keV, calculate the angular tilt of the second crystal needed to suppress the third harmonic reflection.

Hints: Use the *Xop|Optics|Crystals|XCrystal* application to create the profiles. The peak, width and integrated reflectivity values can be obtained using *Xplot|Calculations|Width/Integral/MinMax* on each profile. For the double reflection (+,-) one should multiply a given diffraction profile by itself using the *Xplot|Calculations|Operations with columns* item. Use *Xplot|Save Plot* button to over plot the new curve on the original one. The rocking curve is calculated by convoluting the diffraction profile with itself. For doing that, use the *Xplot|Calculations|Convolution and Correlation* entry, and make autoconvolution normalized to the second set.

For the harmonic suppression one should calculate the main Si111 reflection at 8 keV and the third harmonic (Si333 at 24 keV). Check that both cases give the same Bragg angle. Keep two Xplot windows, one for each profile. Estimate the misalignments one must introduce to suppress the Si333 reflection (should be larger than the diffraction profile width). Create a new set of data for the shifted Si333 reflection by changing the angular (abscissas value with *Xplot|Calculations|Operations with sets*. Save the result to a file. Multiply the original Si333 reflection by the shifted one using the *Xplot|Calculations|Operations with sets* of the Xplot window of the original Si333 Xplot window. Repeat the process of shifting with the main reflection Si111 using the same value of angular misalignment. Calculate the new peak, width and integrated reflectivity, and compare with the double non-misaligned reflection (+,-).

Answer

i)

Crystal	E [keV]	θ_B [deg]	W[μrad]	Peak	Integ Int
Si111	5	23.3	61.3	0.86,	60
Si111	8	14.3	36.5	0.94,	40
Si111	12	9.5	23.8	0.97,	28
Si111	50	2.27	5.55	1.00,	6.7
Si111	80	1.42	3.48	1.00,	4.2
Si111	120	0.94	2.31	1.00,	2.9

ii) Continuous line: convolution (rocking curve). Dashed line: single reflection. Dotted line: double reflection
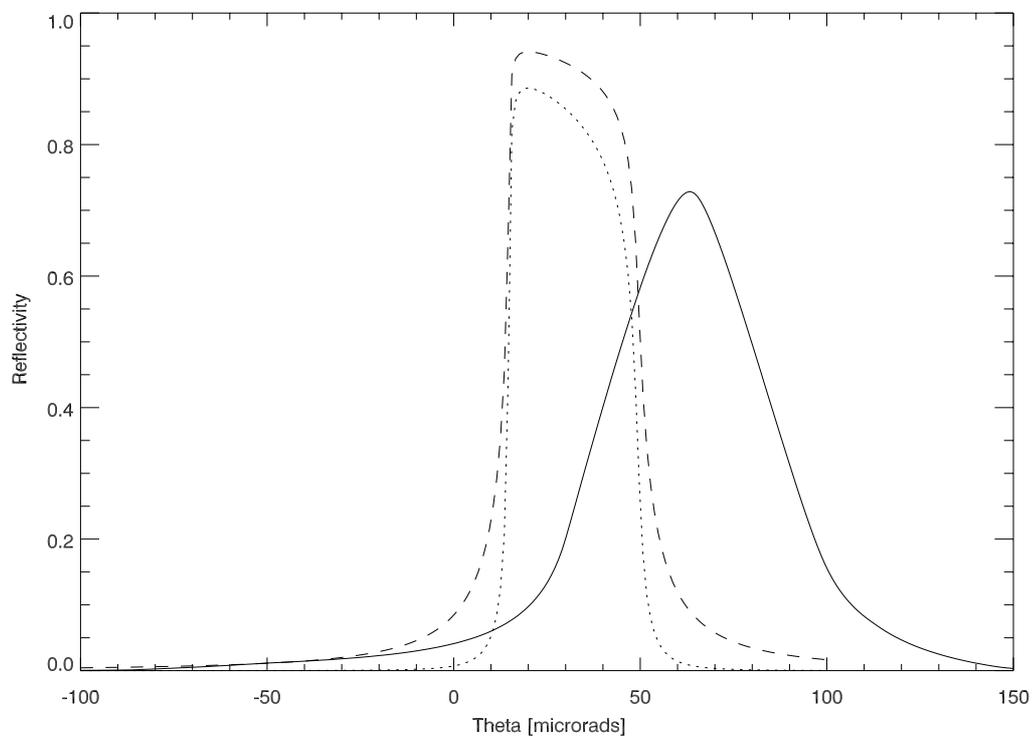
iii)
Si333 single reflection: W=3.1, P=0.99, I=3.45 => Shifting 3.5 μrad
Si333.Si333(shifted): W=3.1, P=0.07, I=0.24
Si111.Si111: W=33.8, P=0.88, I=29.2
Si111.Si111(shifted): W=32.3, P=0.88, I=28.4

8. Bent crystals

You will learn:

- to calculate diffractions profiles of bent crystals
- understand the limitations of the available models
- to see the transition from dynamical to kinematical theory

i) Calculate the deformation of Si111 symmetric Bragg diffraction profile at 12 keV for different values of the bending radius (from 100m to 5cm). For each curve calculate the integrated reflectivity and see the transition from the Dynamic theory value (R>>) to the Kinematical theory value (R<<).

ii) Calculate the diffraction profile in Laue for Si111 at 33 keV and asymmetry angle a=63.78 deg, and curvature radius 13m.

Hints: Use *Xop|Crystals|Crystal_bent* application. Use the "multilamellar" theory for the Bragg reflection and the "Penning&Polder" theory for the Laue system.

Use the files `ex8_xcrystal_bent.xop` and `ex8_xcrystal_bent_bragg.xop` for examples for Laue and Bragg configurations, respectively.

Answer

i)

R[cm]	FWHM[mrad]	Integrated reflectivity
5 (dashed)	92	0.395
25	0.39	0.300
50 (dotted)	0.19	0.22
100	0.11	0.136
2000 (cont)	0.03	0.97

ii)

Crystal_Bent 1.2 {cryst_pp} Si 111 E=33144.0eV, t=0.70mm, R=13.0m, a=63.7deg
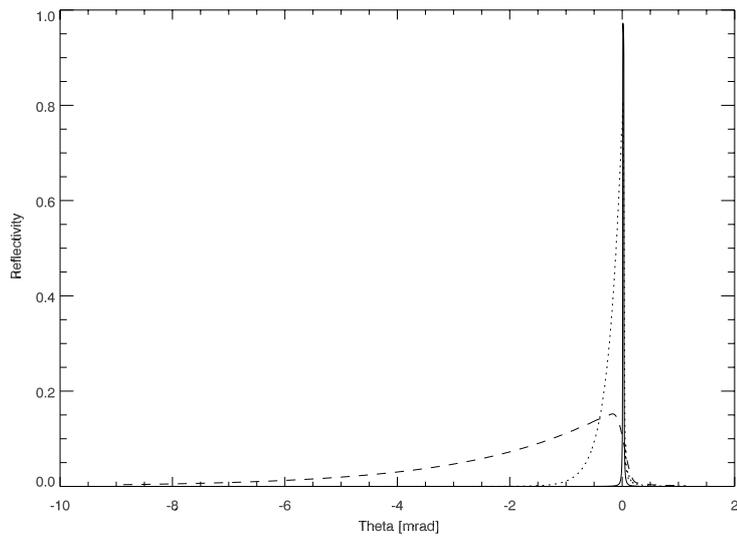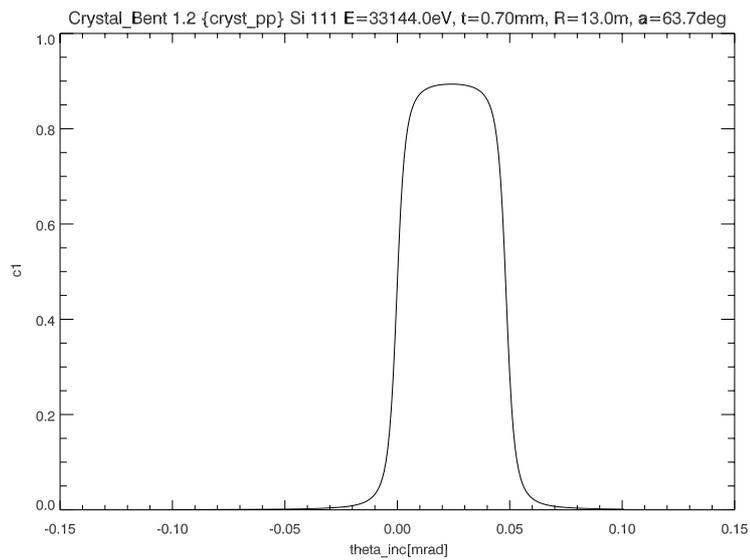
9. Reflectivity curves of multilayers.

You will learn to:
- use Mlayer to calculate reflectivity from simple multilayers
- understand the limitations of Mlayer
- start and use IMD as Xop extension
- understand the basic features of multilayer reflectivity spectra

i) Using MLAYER calculate the reflectivity as a function of grazing angle, from zero to 6 deg, of [W (25 Å)/Si (25 Å)]×50 on Si at an energy of 8050 eV

ii) Using IMD, using no slope errors (if not specified), calculate the following reflectivity spectra at E=8050 eV:
1. [W (25 Å)/Si (25 Å)]×50 on Si
2. [W (10 Å)/Si (40 Å)]×50 on Si
3. [W (5 Å)/Si (45 Å)]×50 on Si
4. [W (25 Å)/Si (25 Å)]×10 on Si
5. [W (25Å)/Si (25 Å)]×50 on Si, roughness σ=5 Å
6. SiO(90 Å) [W (5 Å)/Si (45 Å)]×50 on Si

Comment the results.
Hints: load in IMD the input file ex9_imdWSi.dat which contains an input for the Wsi multilayer

Answer

i) Use the file ex9_mlayer.xop
ii) Start with the file ex9_imdWSi.dat.

The following features can be observed:
1) A plateau corresponding to the total reflection zone.
2) Outside the plateau, the background decreases with q^{-4}. Changes in this background are due to the roughness in the interfaces and experimental background.
3) Satellite maxima. The angular spacing depends on the bilayer periodicity d. Their angular separation is determined by the Bragg law. If the spectrum extends over many peaks, it is possible to observe absences of some peaks, which are related to Γ. Peaks at $Γ^{-1}$ are absent.
4) Kiessig fringes, which period depends on the total multilayer thickness (i.e., number of bilayers).
5) If a top or capping layer exists (usually an oxide layer) it creates side maxima close to the satellites.
6) The satellite width is proportional to 1/N, N being limited by the absorption of the stack. Although the theoretical width is the same for all satellites, in experimental measurements one usually sees an increase of the satellite width as the satellite order increases.
7) The effect of increasing N is also to increase peak intensity in satellites. This is limited by the roughness and stack absorption.
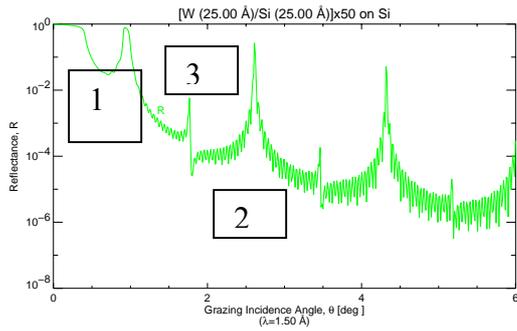
[W (25.00 Å)/Si (25.00 Å)]x50 on Si

Reflectance, R

Grazing Incidence Angle, θ [deg]
(λ=1.50 Å)

1

3

2

[W/Si] multilayer, N=50, d=50.00 Å, Γ=0.500
W layer (1), z=25.00 Å
Si layer (2), z=25.00 Å
Si substrate

[W (10.00 Å)/Si (40.00 Å)]x50 on Si

Reflectance, R

Grazing Incidence Angle, θ [deg]
(λ=1.50 Å)
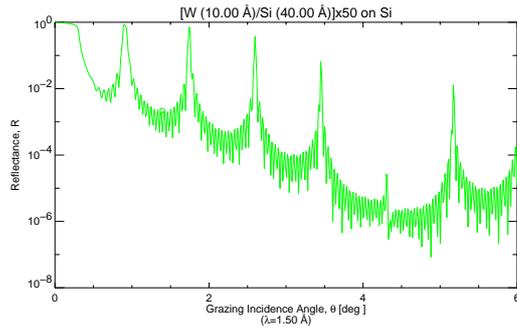
[W/Si] multilayer, N=50, d=50.00 Å, Γ=0.200
W layer (1), z=10.00 Å
Si layer (2), z=40.00 Å
Si substrate

[W (5.00 Å)/Si (45.00 Å)]x50 on Si

Reflectance, R

Grazing Incidence Angle, θ [deg]
(λ=1.50 Å)

3

3

3
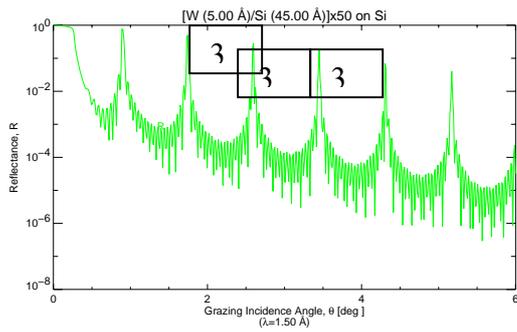
[W/Si] multilayer, N=50, d=50.00 Å, Γ=0.100
W layer (1), z=5.00 Å
Si layer (2), z=45.00 Å
Si substrate

[W (25.00 Å)/Si (25.00 Å)]x10 on Si

Reflectance, R

Grazing Incidence Angle, θ [deg]
(λ=1.50 Å)

4
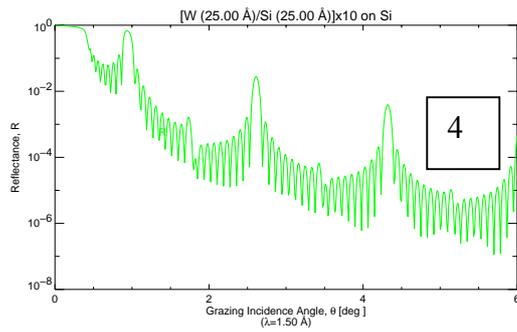
[W/Si] multilayer, N=10, d=50.00 Å, Γ=0.500
W layer (1), z=25.00 Å
Si layer (2), z=25.00 Å
Si substrate

[W (25.00 Å)/Si (25.00 Å)]x50 on Si

Reflectance, R

Grazing Incidence Angle, θ [deg]
(λ=1.50 Å)
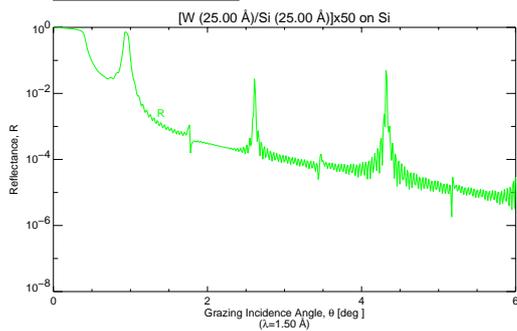
[W/Si] multilayer, N=50, d=50.00 Å, Γ=0.500
W layer (1), z=25.00 Å, σ(Si/W)=5.00 Å (step)
Si layer (2), z=25.00 Å, σ=5.00 Å (step)
Si substrate, σ=5.00 Å (step)

SiO (90.00 Å)/[W (25.00 Å)/Si (25.00 Å)]x50 on Si

Reflectance, R

Grazing Incidence Angle, θ [deg]
(λ=1.50 Å)

1

3

5

4

2
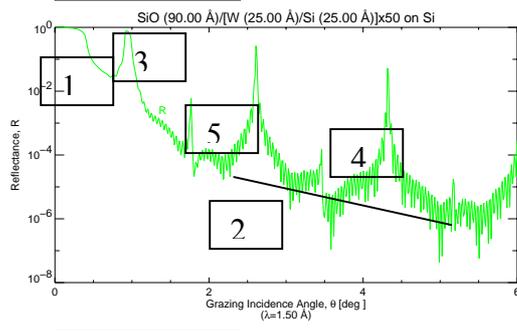
SiO layer (1), z=90.00 Å
[W/Si] multilayer, N=50, d=50.00 Å, Γ=0.500
W layer (2), z=25.00 Å
Si layer (3), z=25.00 Å
Si substrate

15

10.   Quick tour to other XOP applications

Open and run the following applications:

- DABAX main interface and applications
- XXCOM
- MAMON
- CRL

11. Learning reference frames in SHADOW using a geometrical source.

You will:

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

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 the following macro, that reads the source file `begin.dat`, 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 rewrites the source file `begin.dat` with the modified source. Visualize the new result.

```
a=ReadSh('begin.dat')
x = GetShCol(a,1)
z = GetShCol(a,3)
f = GetShCol(a,10)
bad1 = Where(x LE 0)
bad2 = Where(z LE 0)
f[bad1]=-100
f[bad2]=-1100
a.ray[9,*]=f
putrays,a,'begin.dat'
```

iii) Create a mirror optical element, with incident angle 45 degrees, 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 ex11a.ws and ex11b.ws, for zero and 90 deg mirror orientation angle, respectively.

Answer
Pay attention to make plots using "Rays: Good Only" and "Cartesian Axes: Yes"
Source (x,z) plane



17
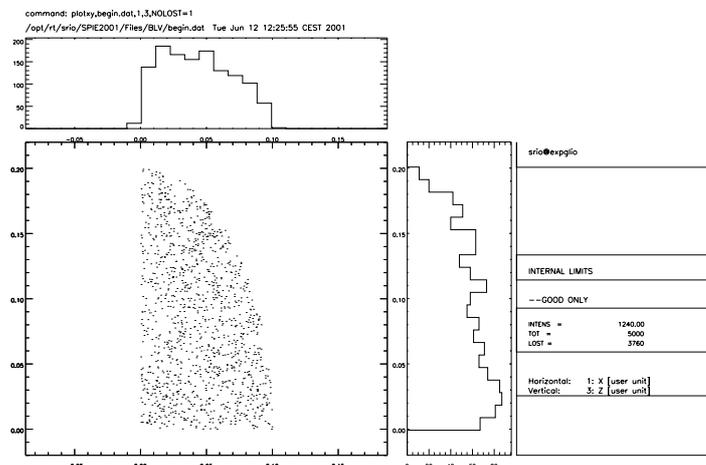
a) Mirror orientation angle = 0
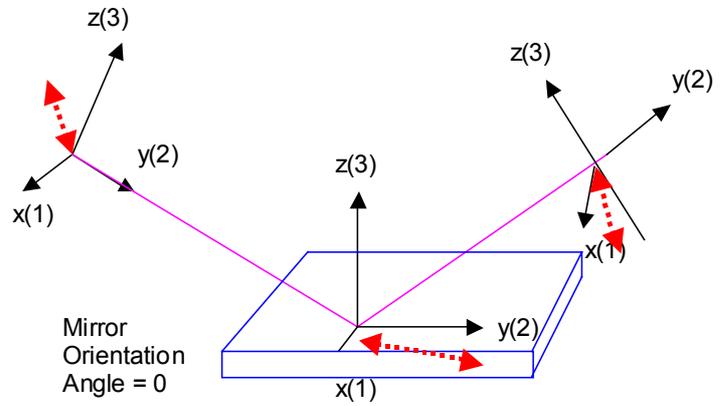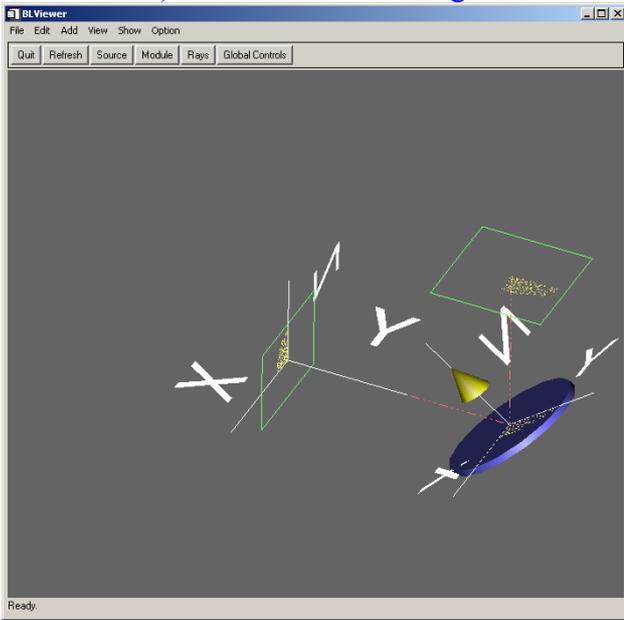
Left: footprint (Y,X) plane. Right: image (X,Z) plane

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b) Mirror orientation angle = 90 deg
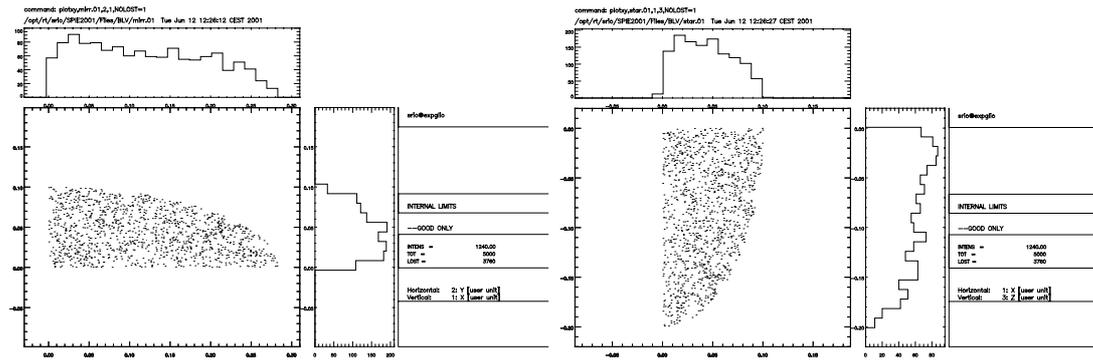
Mirror Orientation
Angle = 90 deg
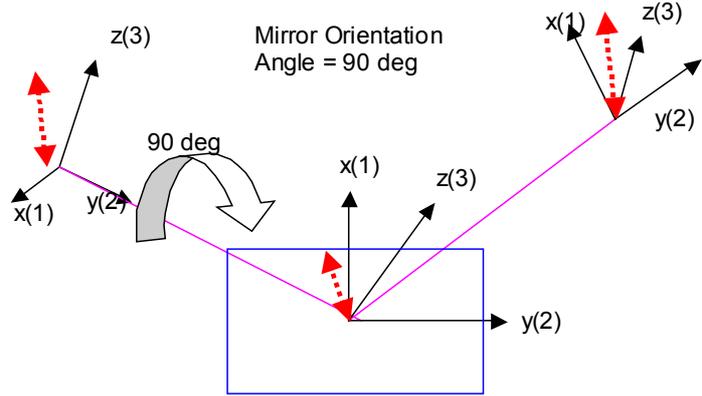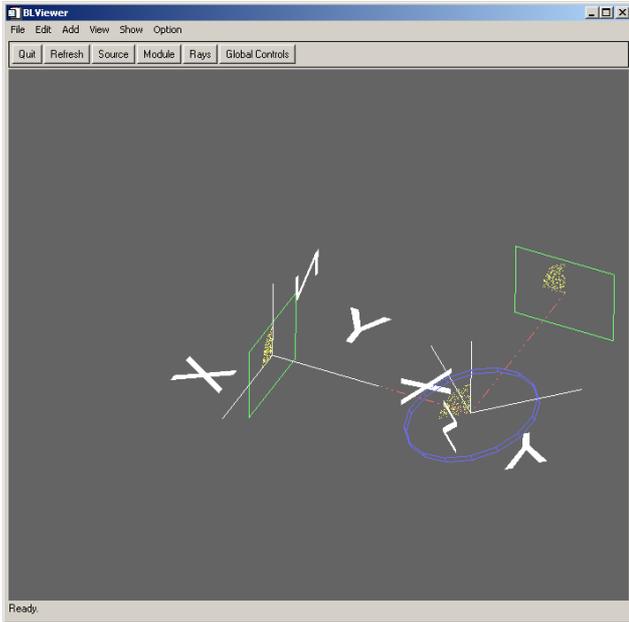
Left: footprint (Y,X) plane. Right: image (Z,X) plane:
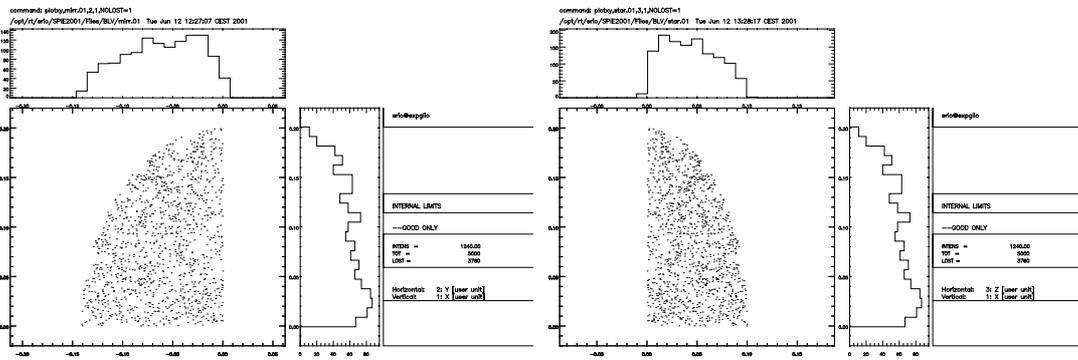
12.   Synchrotron sources: Bending magnets.

You will learn to
- simulate bending magnets

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'), top view (y,x) and phase space (z,z'). Make histograms of intensity (total, σ-polarized and π-polarized) as a function of the vertical divergence. Plot also the degree of circular polarization (S3 component of the Stokes vector). Plot the total intensity at 18 keV versus vertical divergence and compare with the result at 8 keV. Verify that the radiation is more collimated.

ii) Simulate the same source but on a limited vertical divergence (e.g., +/- 50 µrad).

Hints: you may load the workspace `ex12.ws`, where this system is defined, for full vertical emission.

Answer

i)

Use Plotxy with file `begin.dat` for plotting the cross section (x,z), the divergence space (x',z'), top view (y,x) and phase space (z,z')
histograms of intensity (total, σ-polarized and π-polarized, from top to bottom, respectively) at 8 keV, versus vertical divergence in rads.
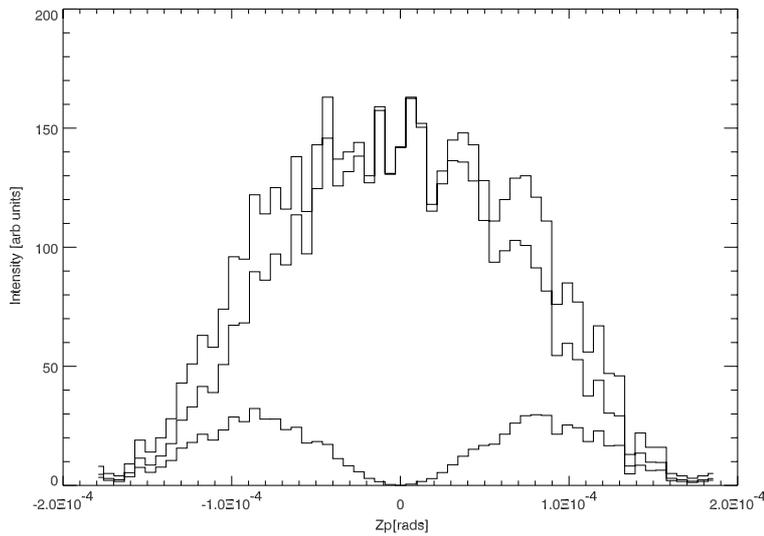
Histograms of total intensity at 8 keV and 18 keV (the histogram of 18 keV has been shifted vertically for clarity) and circular polarization for 8 keV, versus vertical divergence in rads.
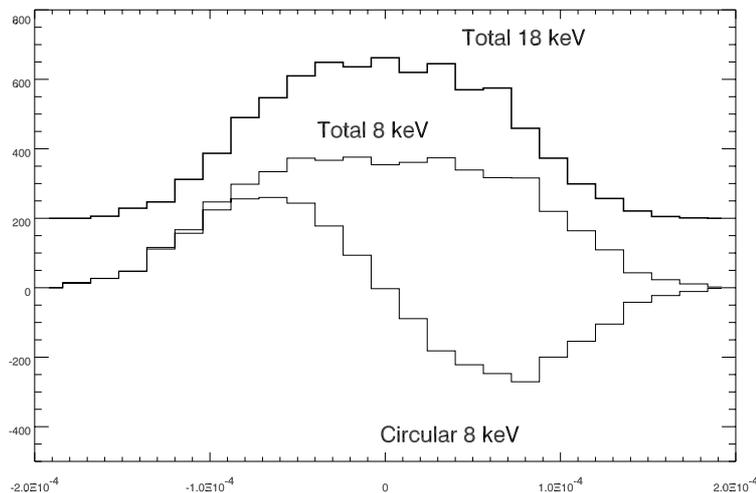
ii)

13. Insertion devices

You will learn to
- Simulate wigglers and undulators

a) Simulate the standard 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).
Hint: you may use the workspace file `ex13a.ws`

b) Simulate the ESRF U46 undulator at the energy corresponding to the third harmonic. Play with the maximum aperture angle to create many rings.
   i)   No emittance, max aperture angle 0.15 mrad
   ii)   No emittance, max aperture angle 0.015 mrad
   iii)   The same with emittances.
Hint: you may use the workspace file `ex13b.ws` which implements the case using emittances and max aperture angle of 0.015 mrad.

Answer

a)

E [keV]	x'[mrad]	z'[mrad]
10	3.1	0.20

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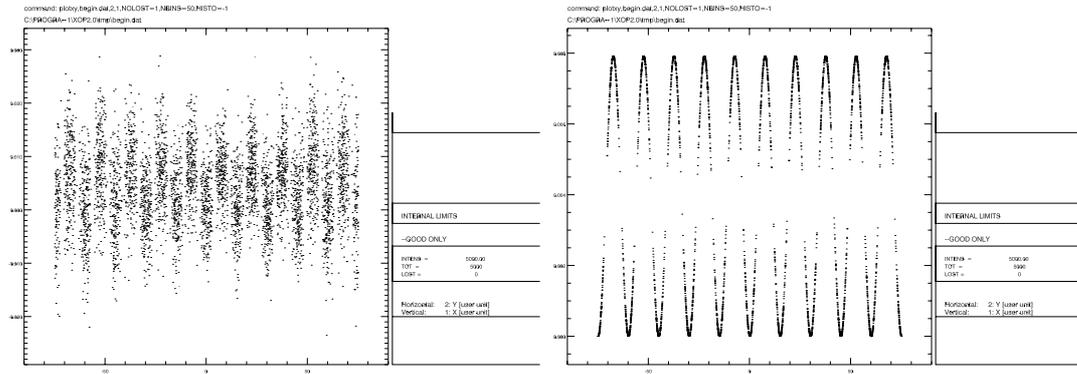
b)

Plot of the divergence space (X',Z') for the undulator with (left) and without (right) emittances using a maximum angular acceptance of 0.15 mrad.
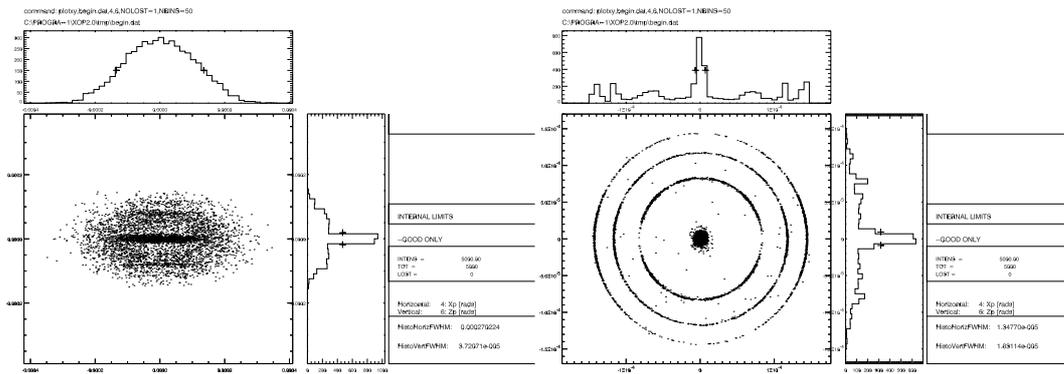
14.   Beam propagation (phase space (z,z') ellipses)

You will learn to
- Define screens and slits associated to optical elements

a) Using the already created bending magnet source (, add an optical element with several screens at 0 (source position), 50, 75 and 100 cm from the source. See the tilt of the (z,z') diagram.

b) Define an aperture (20 μm×20 μm) in the first screen and see its effect in screens #2 and #3.

Hints: Use the *Modify oe...* button to define the oe parameters (these parameters are not important at this moment). Use the *Screen Manager...* button in the oe window to create and define the screens/slits. Then Run shadow using the button "Run Shadow/trace". Visualize the screens using the PlotXY facility and loading the files `screen.0101` for the first screen, `screen.0102` for the second, etc.
You may use the workspace files `ex14a.ws` and `ex14b.ws`. They also contain a macro for visualizing the four screen planes in a single screen.

Answer
a)
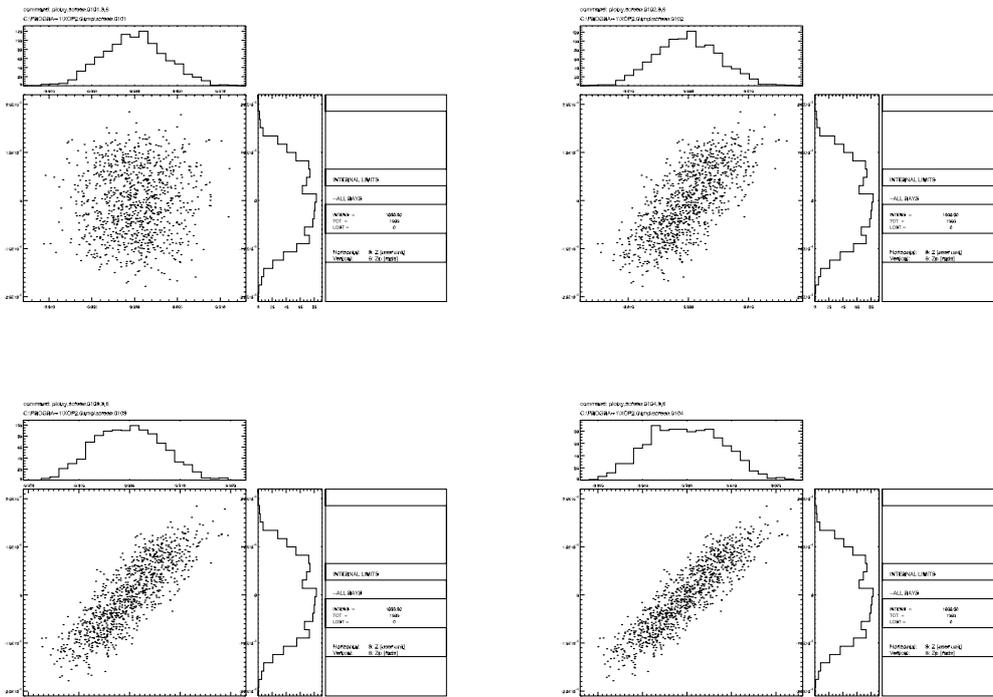
b)
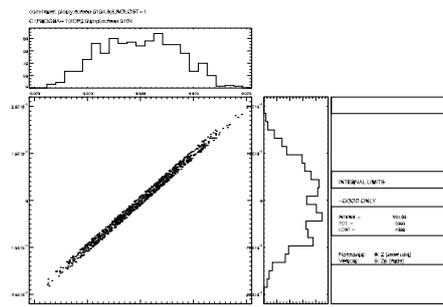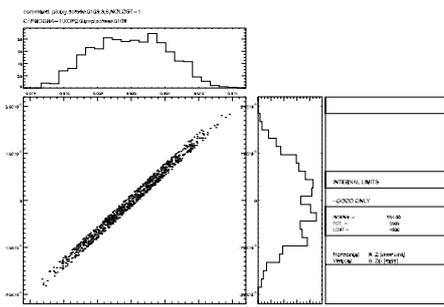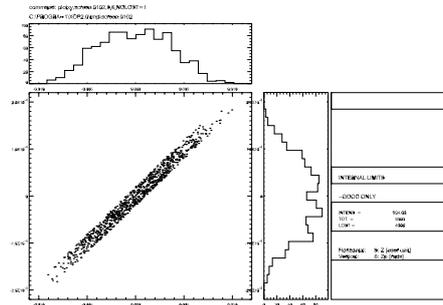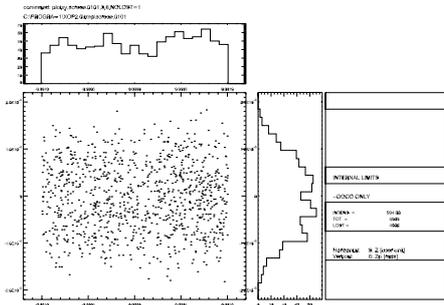
15. Focusing with grazing incidence mirrors: effect of aberrations.

You will learn to
- Use a geometrical source to simplify the simulation of an undulator
- 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.

Create a geometrical source with Gaussian shape (σ_x=57 μm, σ_z=10.4 μm) and Gaussian divergence ($\sigma_{x'}$=88.5 μrad and $\sigma_{z'}$=7.2 μrad) to simulate the emission of an ESRF 1.65 m undulator at 10 keV in a Low beta section (these numbers are taken from the web).

a) 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) for a grazing angle of 0.12 degrees. Study the effect of the spherical aberrations and its influence depending on the magnification factor.
See also the dependence on mirror dimensions and incident angle.

b) Enter the effect of mirror reflectivity. Consider a Rh (ρ=12.4 g/cm^3) coating and a source with energy distribution in 5-45 keV (box-distribution). Visualize the results using both scattered plot and contour curves (including reflectivity). Plot also the intensity versus energy.

Hints. Use the oe menu to enter the mirror values. *The angles [in deg] are INCIDENT angle and not GRAZING angle.* Shadow can calculate the surface parameters (curvature radii, ellipse axes, etc). by selecting in the screen under the "Figure..." the "internal/calculated" entry. After running Shadow, calculate the spot sizes using either InfoSh or from the histogram widths. The resulting mirror parameters can be seen using the "MirInfo" button. You may also use the workspace files ex15a.ws and ex15b.ws which implement a toroidal mirror for magnification 1/3, considering and not considering, respectively, mirror reflectivity. For including reflectivity, the preprocessor PreRefl must be used before running SHADOW to create the reflectivity file, called here reflec.dat.

Answer
a) toroidal (bottom left); M=1/30 ellipsoidal (bottom right)
The aberrations effect increases if
  i)   one goes to more grazing angle
  ii)   one reduces the magnification factor (i.e., mode demagnification of the source)
  iii) 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 "limits check" entry in the screen
under "Figure", and plot the rays using rays: "good only"
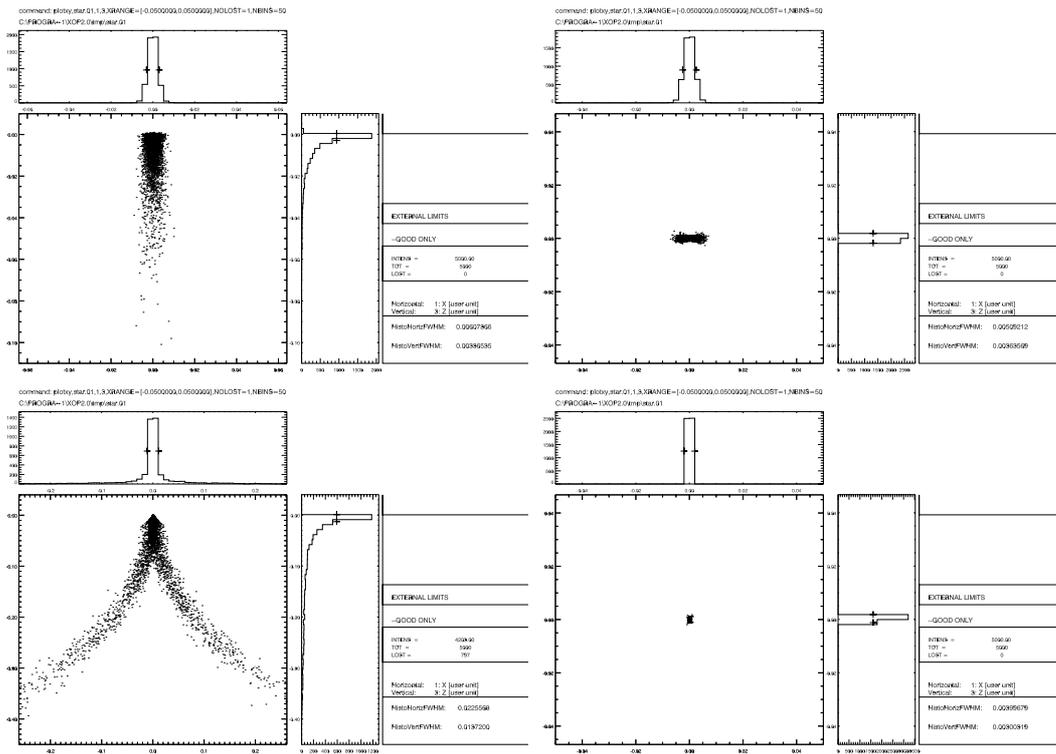
b) Spot (left); I(E) plot (right). Note that the left plot is not longer a scattered plot
(showing rays) but a contour curve plot where the contours are calculated using rays
weighted with their intensity.
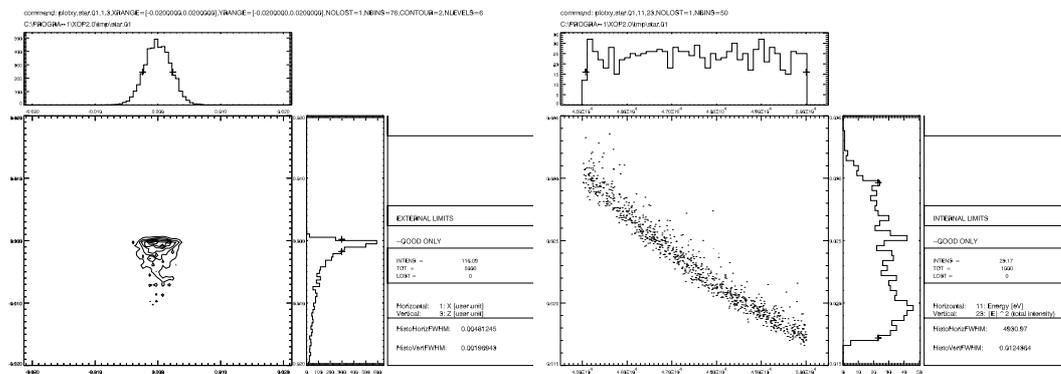
16.   Kirkpatrick-Baez system

You will learn to
- define an optical system with two mirrors
- define a cylindrical mirror with circular or elliptical section
- tell SHADOW to calculate automatically the mirror parameters in the case that focal planes not coincident with continuations planes
- exercise with the mirror orientation angle.
- define mirror dimensions

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.

Hint: you may use the workspace file `ex16a.ws`, which contains this case with cylindrical mirrors, and automatic (internal) calculation of the mirror parameters given the distances of the focal planes. The workspace file `ex16b.ws` contains the same system, but the mirror parameters (i.e., radii) are external parameters.

Answer

Spot with cylindrical mirrors in the plane (Z,X), 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 resulting mirror parameters are (check them using `MirInfo`) R(M1)=739455.7 cm and R(M2)=691710.4 cm.
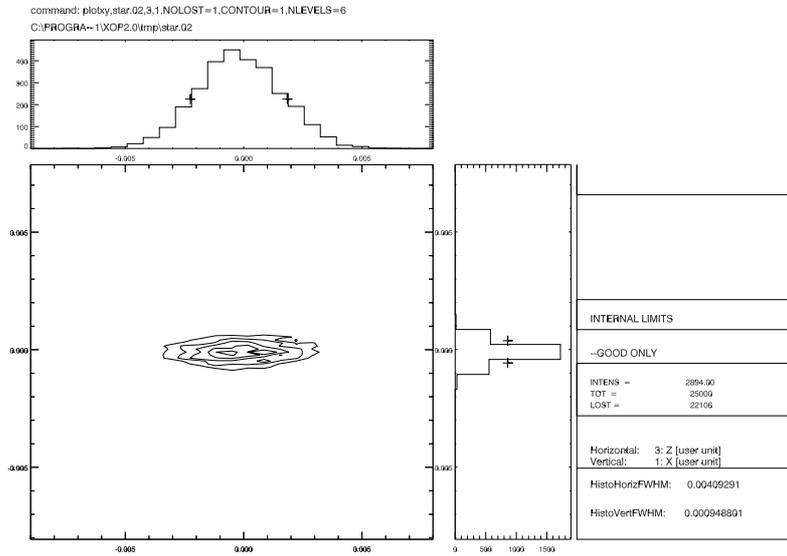
17.   Double crystal monochromator.

You will learn to
- 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)

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

a) 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.

b) 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.

Hint: you may use the workspace file `ex17a.ws` for (+,-) and `ex17b.ws` for (+,+). Notice that the workspace file does not contain the file with the reflectivity for the crystal, so you will need to run the `bragg` preprocessor. 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 (i.e., file `star.01`) is:

C:\PROGRA~1\XOP2.0\tmp\star.01 Sun Mar 04 21:07:13 2001
FWHM of the histogram is : 6.27051
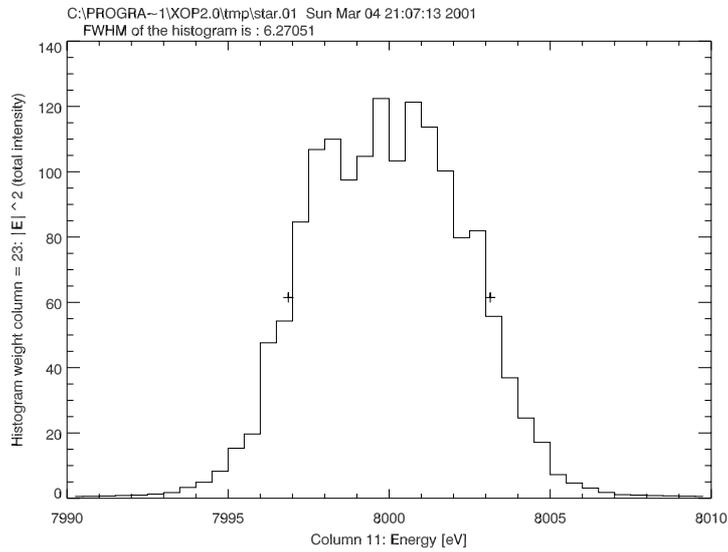
b) Left: resolution function for (+,-) (non-dispersive configuration). Here the mirror orientation angles are 0 and 180 deg for the first and second crystals, respectively. Right: resolution function for (+,+) (dispersive configuration). The mirror orientation angle is 0 for both crystals.

C:\PROGRA~1\XOP2.0\tmp\star.02 Sun Mar 04 21:09:36 2001
FWHM of the histogram is : 6.12256

C:\PROGRA~1\XOP2.0\tmp\star.02 Sun Mar 04 21:10:11 2001
FWHM of the histogram is : 0.986816
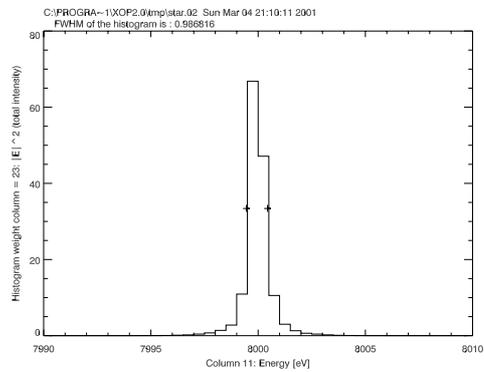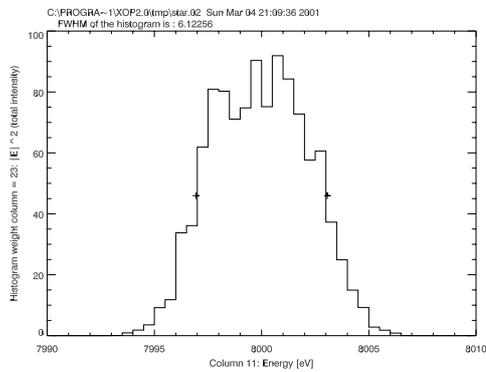
18. Sagittal focusing

You will learn to
- define a cylindrical mirror for sagittal focusing
- define "externally" the optical element radius of curvature
- optimize the focal spot

a) Using the (+,-) system defined in the last exercise, 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.

Use `ShadowVUI|Results|ray_prop` to find the position of the best focus. Calculate its size.

b) 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: Use the program ShadowVUI|Utils|Optical|Tang and sag radii (rcil) to calculate the curvature radius: Rs(8keV,M=1/3)=371 cm. You may use the workspace files `ex18.ws` corresponding to M=1/3.

Answer

a) Focusing system: Spot width=0.031 cm, I/I_0=1090/25000, ΔE=6 eV

Non-focusing system: Spot width=12.0 cm, I/I_0=1090/25000, ΔE=5.8 eV

Best focus at about 0.7 cm downstream the focal position. The spot size does not change appreciably.

b) p=30m, q=1m, R_s=47.8 cm, Spot width=0.012 cm, I/I_0=168/25000, ΔE=5.8 eV
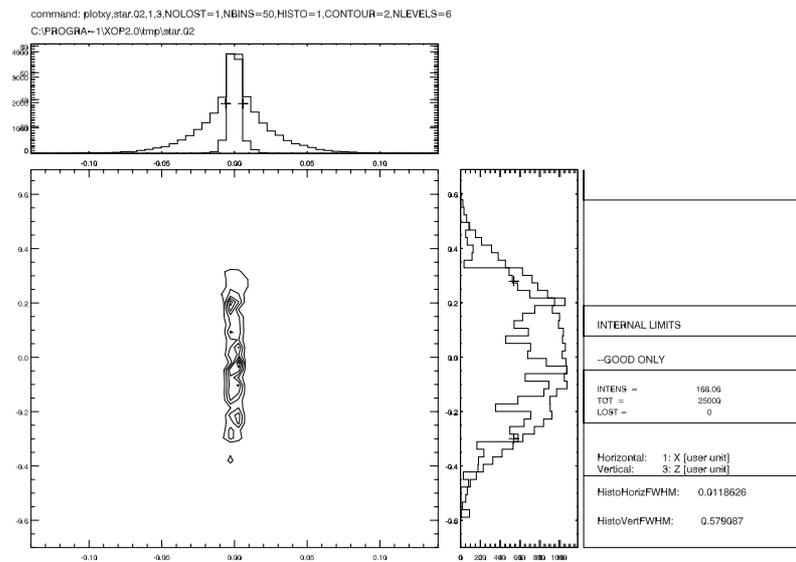
The study of the variation of the intensity as a function of the magnifications needs to run shadow for many points of M. It can be done manually or with a macro. The result should show an optimum magnification of M=1/3 for large divergence values. Its effect can be seen in the following figure (M. Sanchez del Rio "Ray tracing simulations for crystal optics" SPIE proceedings, vol. 3448, 230-245, 1998)
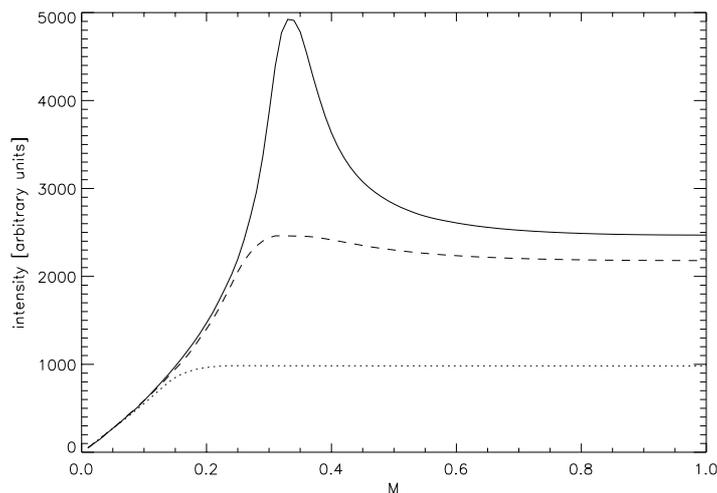
Intensity (in arbitrary units) versus magnification factor M for a point and monochromatic (E= 20 keV) source placed at 30 m from the sagittaly bent crystals. Three beam divergences are considered: 1 mrad (dotted), 2.5 mrad (dashed) and 5 mrad (continuous). We clearly observe the maximum of the transmission at M=0.33 when focusing the 5 mrad beam, as predicted by the theory

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19.   Simulation of a complete beamline.

You will learn to:
- Combine several optical elements
- Obtain final results for a beamline in terms of flux, resolution and spot size.

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

Calculate:
i)   Beam geometry at the sample position
ii)   Energy resolution
iii)   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 5×10^{13} ph/sec/0.1%bw

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

Hint: you may use the workspace file ex19.ws

Answer

ΔE_{source}=4 eV (optimized source bandwidth); ΔE=1.3eV; I/I_0=1420/5000

Transmitivity in one eV=T=(I/ΔE) /(I_0/ΔE_{source})(1420/1.3)/(5000/4)

Number of photons at the source in one eV bandwidth =N= 5 10^{12}

Total number of photons = N×T×ΔE

Intensity distribution in the (X,Z) plane at the image position (note the different vertical and horizontal scales)

command: plotxy,star.04,1,3,NOLOST=1,HISTO=1,CONTOUR=2,NLEVELS=6

/opt/rt/srio/SPIE2001/Files/BLV/star.04 Wed Jun 13 15:53:46 CEST 2001

srio@expglio

INTERNAL LIMITS

--GOOD ONLY

INTENS =	1419.23
TOT =	5000
LOST =	0

Horizontal:	1: X [user unit]	
Vertical:	3: Z [user unit]	
HistoHorizFWHM:		0.00470276
HistoVertFWHM:		0.000663026

35
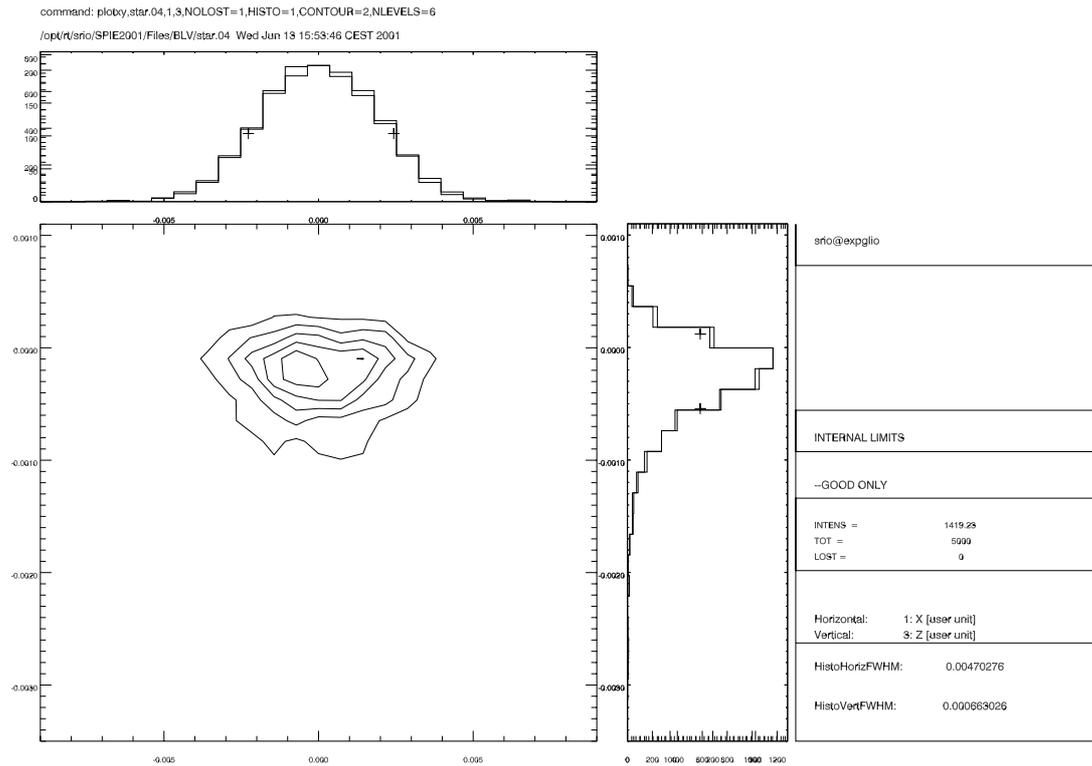
20.　　　　Slope errors.

You will learn to:
- Use `waviness_gen` 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

a) Load the Kirkpatrick-Baez system of exercise 16. Set mirror surface to be elliptical. Check that mirror dimensions are 40×4 cm^2 . Calculate spot sizes without slope errors.

b) use the program `waviness_gen` to create maps of slope errors:
- i) Run from a DOS shell `waviness_gen < wav_test1.inp` to create a slope of 0.5 arcsec and visualize the resulting surface using `presurface,'wav_test1.dat'` from a macro window.
- ii) Do the same with `wav_test2.dat` to obtain a rippled surface.
- iii) Use now the file `wav1.inp`. What are the slope error values?
- iv) 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. Call the result `wav1opt.inp`. Create another file wav2opt.inp with the same inputs but changed the seed. Then visualize the resulting surfaces and run SHADOW's `presurface` for both surfaces (use for that a macro and type there `xsh_run,'presurface'`). Take as inputs `wav1opt.dat` and `wav1opt2.dat` and call the resulting files `wav1opt.sha` and `wav2opt.sha`, respectively.
- v) in SHADOWVUI oe menu, select modified surface: surface error…, and use then external spline with the corresponding *.sha file, one different file for each mirror to avoid coupled unphysical effects. Calculate then the spot size.

Hints: use the workspace `ex20a.ws` for part a. Run `ex20b.ws` for part b.

Answer
a) 8×40 μm²
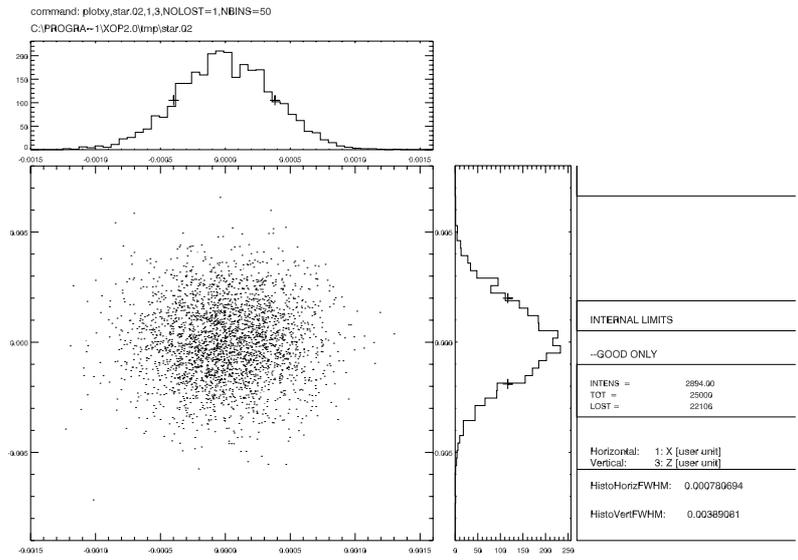
b)
### i) and ii)
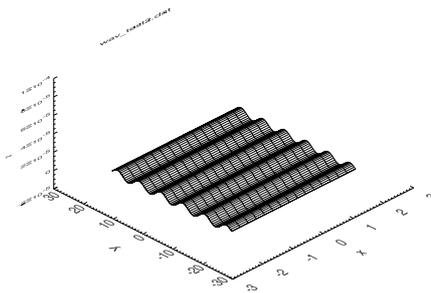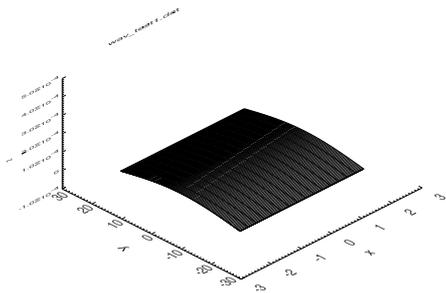
iii) 0.28 arcsec (Y) × 0.73 arcsec (X)
iv)

v) $88 \times 98\ \mu m^2$

command: plotxy,star.02,1,3,NOLOST=1,NBINS=50
C:\PROGRA~1\XOP2.0\tmp\star.02

INTERNAL LIMITS

--GOOD ONLY

INTENS =   2894.90
TOT =   25000
LOST =   22106

Horizontal: 1: X [user unit]
Vertical: 3: Z [user unit]

HistoHorizFWHM: 0.00877800

HistoVertFWHM: 0.00976495
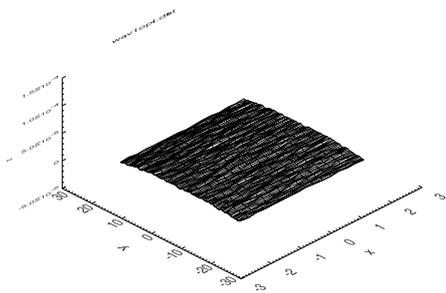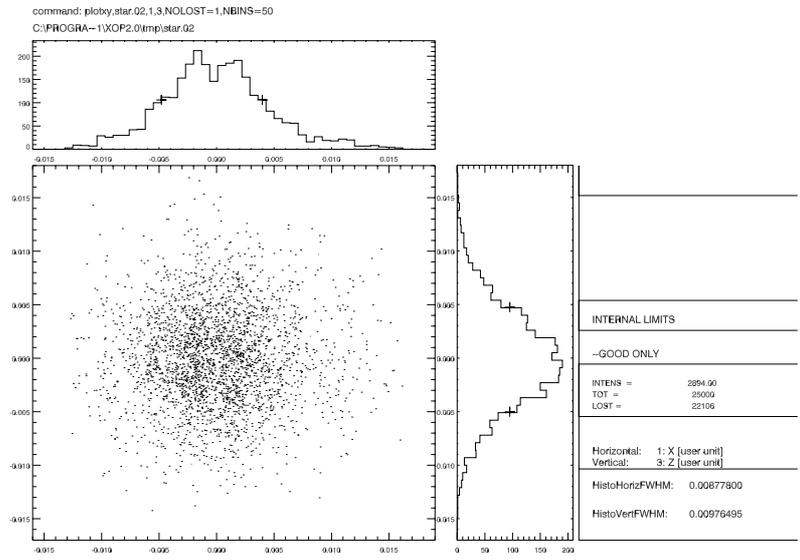
## 21.	Thermal bump.

You will learn to:
- use a macro to create a file sampling a thermal bump
- use `presurface` to inject it in SHADOW
- see the effect of the bump in energy resolution.

Load the `ex21.ws` workspace. Create the source. Run the macro to create a Gaussian bump. Run SHADOW's `presurface` with `bump.dat` to create y. Run the system (a single Si111 crystal) without and with thermal bump. See the changes in the energy resolution.

Answer

With bump:

Without bump

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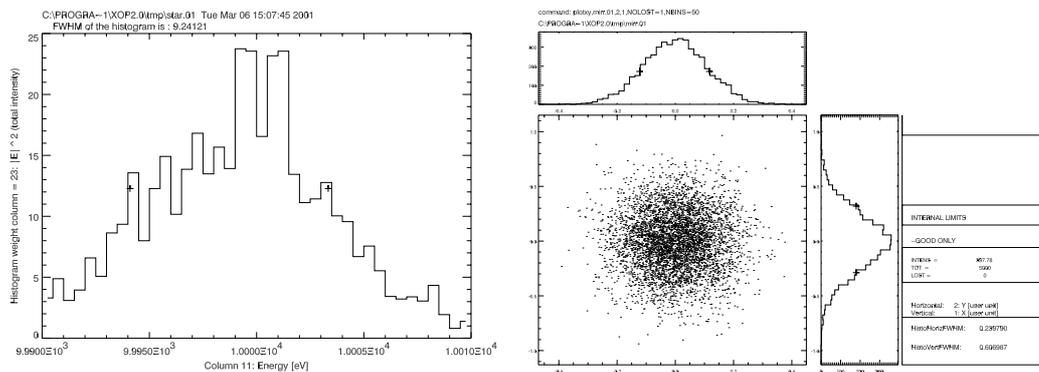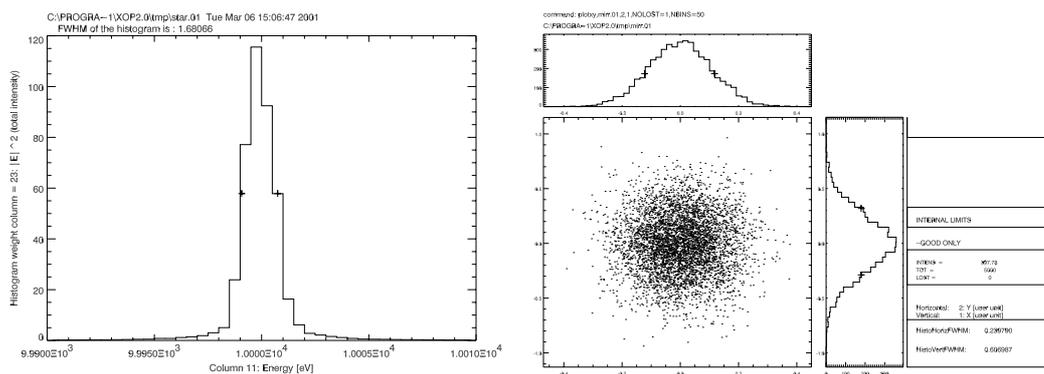
22. Curved crystal monochromators: Rowland and off-Rowland configurations

You will learn to:

- 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

a) Using the same Gaussian source as in exercise 21, verify the focusing conditions for a symmetrical Si111 Bragg crystal at 10 keV, with p=30m. Calculate ΔE. Calculate ΔE for R_t=5000 cm and R_t=2500 cm. Explain the differences.

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

Answer

a)

For the focusing conditions, we have R_t=15171 cm (use `ex22a.ws`)

For R_t=5000 we then have ΔE=1.36 eV (use `ex22b.ws`)

For R_t=2500 cm we then have ΔE=2,3 eV (use `ex22c.ws`)

b) Use the file `ex22d.ws`.

R_t=10622 cm, q=1185 cm; $.\Delta E$=0.85 eV; spot size = 0.77×0.033 cm^2.

command: plotxy,star.01,1,3,NOLOST=1,NBINS=50,HISTO=1,CONTOUR=2,NLEVELS=6
C:\PROGRA~1\XOP2.0\tmp\star.01

INTERNAL LIMITS

--GOOD ONLY

INTENS = 848.61
TOT = 5000
LOST = 0

Horizontal: 1: X [user unit]
Vertical: 3: Z [user unit]

HistoHorizFWHM: 0.728438

HistoVertFWHM: 0.0313131
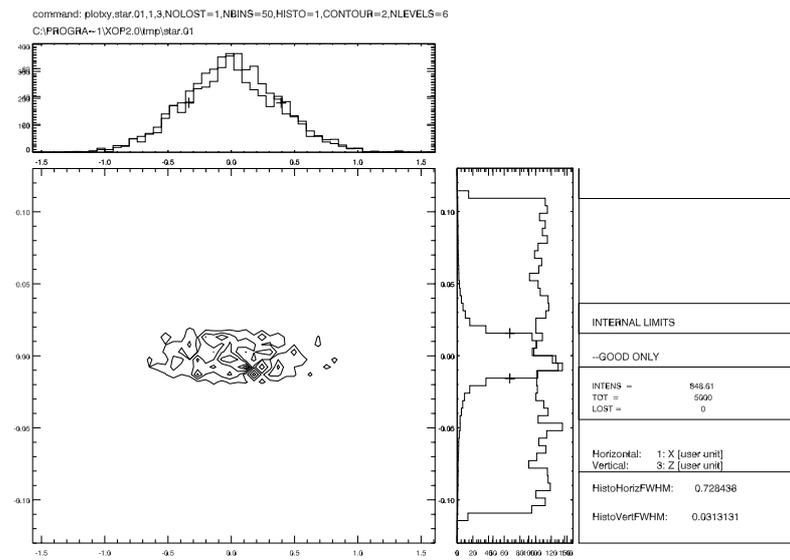
23.   Crystals in Laue geometry

You will learn to:
- Set Laue crystals in SHADOW
- See the transformation in the phase space
- Apply a macro to copy intensity from one file to another.

Implement the system in file ex23.ws, consisting in an asymmetric Laue diamond (111) crystal (a=3.55 Å) and a symmetric Bragg germanium (220) crystal (a=5.66 Å) in non-dispersive configuration. Notice that the diamond crystal has two associated screens, one before and another after it. Run the system, and then the macro that copies the electric vectors (i.e., intensities) from screen 2 to screen 1. Make histograms for these two screens and verify the changes in width for the z and z' coordinates. Relate these changes to the Liouville theorem.
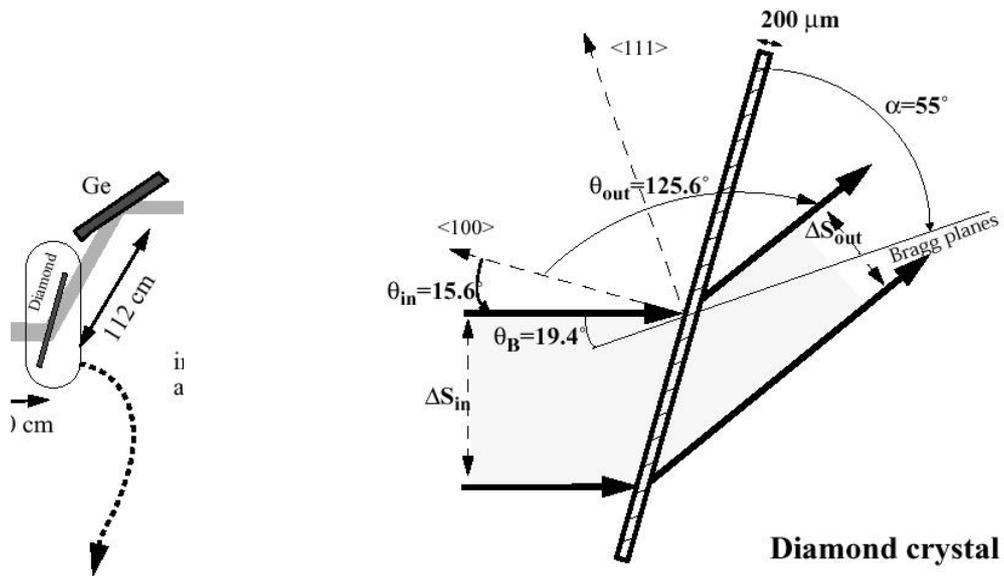
Answer
Phase space (Z,Z') before the crystal

command: plotxy,screen.0101mod,3,6,NOLOST=1,NBINS=50,HISTO=2,CONTOUR=2,NLEVELS=6
C:\PROGRA~1\XOP2.0\tmp\screen.0101mod

INTERNAL LIMITS

--GOOD ONLY

INTENS =   351.93
TOT =   5000
LOST =   0

Horizontal: 3: Z [user unit]
Vertical: 6: Zp [rads]

HistoHorizFWHM: 0.109498

HistoVertFWHM: 2.41566e-005
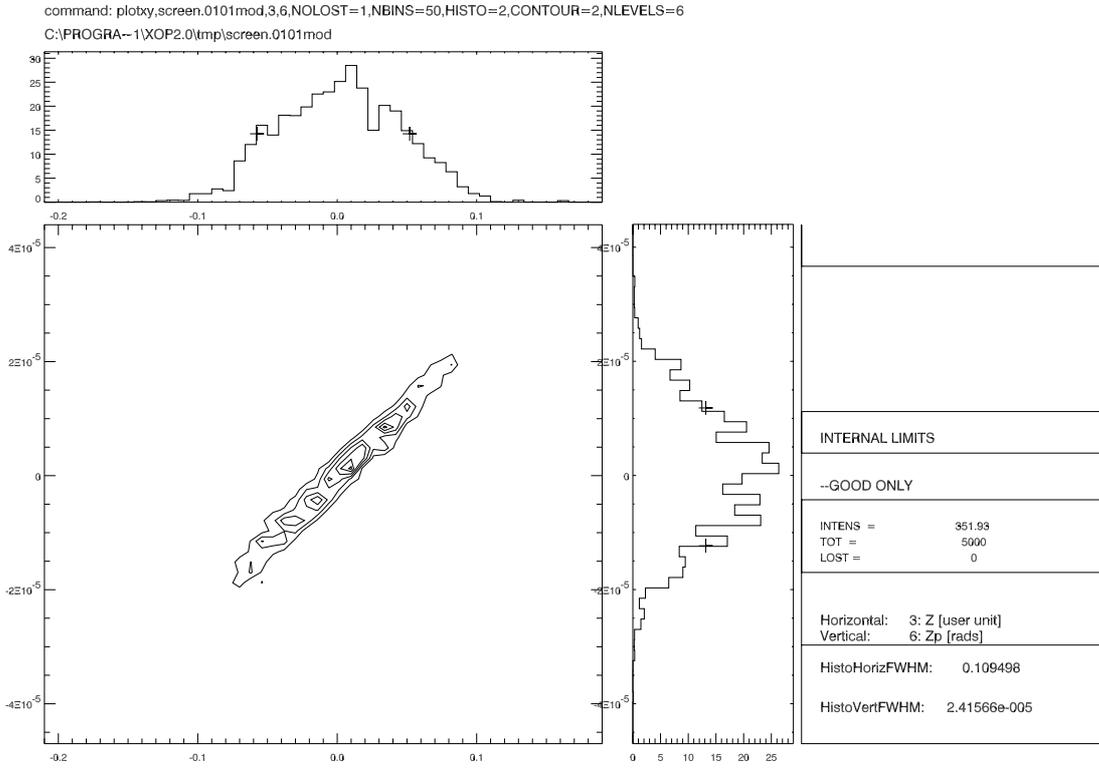
Phase space (Z,Z') after the crystal

command: plotxy,screen.0102,3,6,NOLOST=1,NBINS=50,HISTO=2,CONTOUR=2,NLEVELS=6
C:\PROGRA~1\XOP2.0\tmp\screen.0102

INTERNAL LIMITS

--GOOD ONLY

INTENS =   1819.33
TOT =   25000
LOST =   6

Horizontal: 3: Z [user unit]
Vertical: 6: Zp [rads]

HistoHorizFWHM: 0.0623501

HistoVertFWHM: 4.77073e-005

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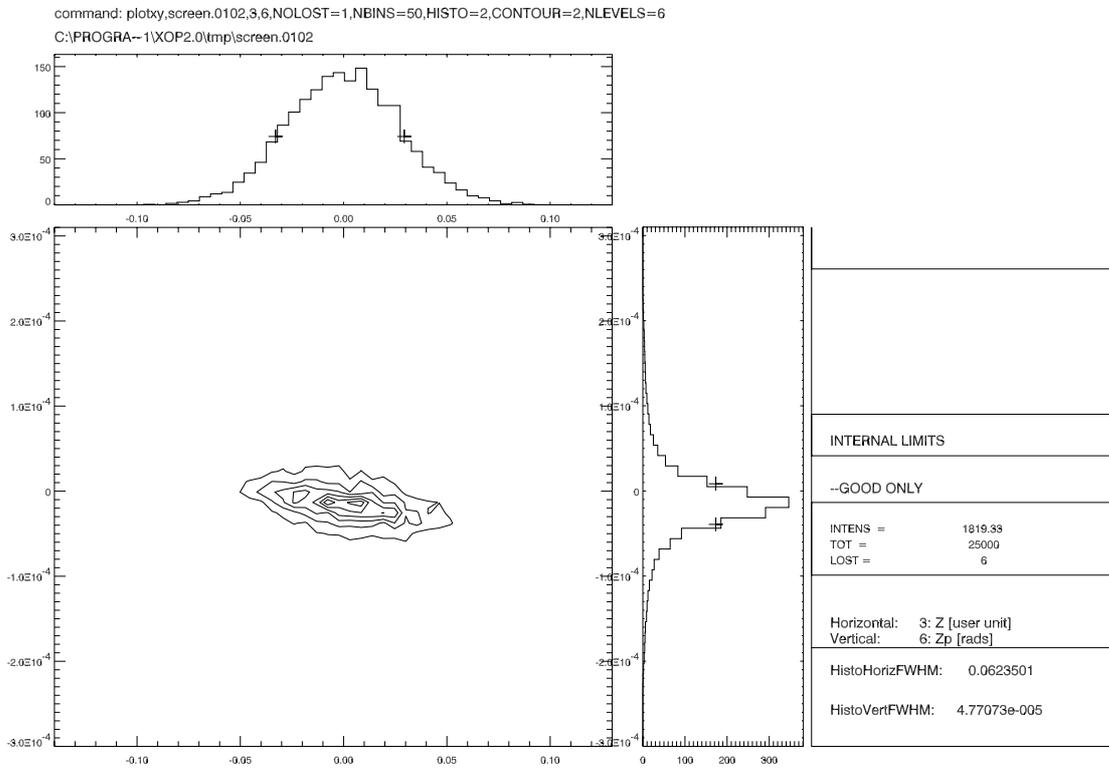
24.   Macros: loops, grid-patterns, ad-hoc ray-tracing and post-processing

Study the example SHADOWVUI workspaces in
`C:\progra~1\xop2.0\extensions\shadowvui\workspaces`:

- `Ellipses_in_phase_s.ws` An example of grid source and presentation of its results using a macro
- `ESRF_bm5.ws`: shows how to run the source and the system from a macro
- `Loop.ws`: shows how to run shadow in a loop, and how to accumulate results.
- `Grid_pattern.ws`: shows how to trace grids with SHADOW using macros

Appendix - The very basics of SHADOW

SHADOW introduction

SHADOW is a ray-tracing program specially optimized for the design of the synchrotron radiation beamline optics. It has been developed by F. Cerrina et al. at the University of Wisconsin.

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 (or 12) variables or *column*s. 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 to scale 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.)

SHADOW files

The binary files containing the rays at different points are:
- `begin.dat` binary file containing the beam at the source position
- `mirr.xx` binary file containing the beam on each o.e. (i.e. `mirr.02` is the beam on the second o.e)
- `star.xx` binary files with the beam at the image created by each o.e. The image of a given o.e. is the source for the following o.e.
- `screen.xxyy` SHADOW can (optionally) create the image file in a different points of the beamline, or screens. Screens are associated to a given o.e., and can allow to define apertures (slits or beam stoppers) and absorbers (filters). `xx` refers to the o.e. and `yy` refers to the screen order (i.e. `screen.0204` means the fourth slit associated to the 2nd o.e.)

The files containing the list of variables used as input/output for SHADOW are:
- `start.xx` an ASCII file with the list of variables for the source or optical elements (start.00 for the source, start.01 for the first o.e, start.02 for the second, and so on)
- `end.xx` the same as `start.xx` but with few parameters recalculated after the run

SHADOW frame

The coordinate system of SHADOW is (schematic,):

z(3)

Source
(`begin.dat`)

Image (`star.xx`) or
screen (`screen.xxyy`)

y(2)

z(3)

y(2)

z(3)

x(1)

x(1)

y(2)

x(1)

Optical element
(`mirr.xx`)

x(1)
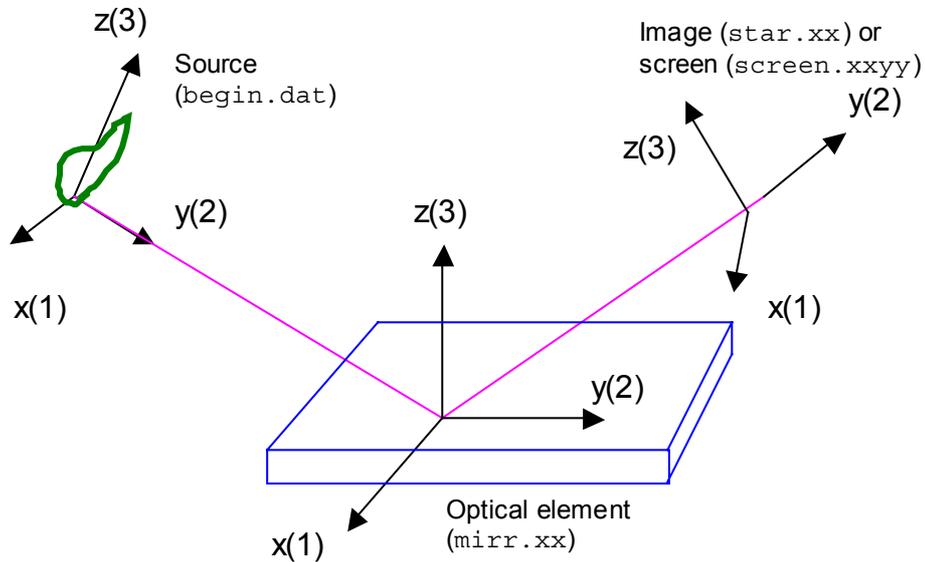
Note that:
- The `y(2)` coordinate is along the beam direction
- The frame is rotated if one o.e. is rotated
- The position, orientation, etc. of any o.e. is always referred to the previous one

Effect of o.e. orientation in SHADOW frame
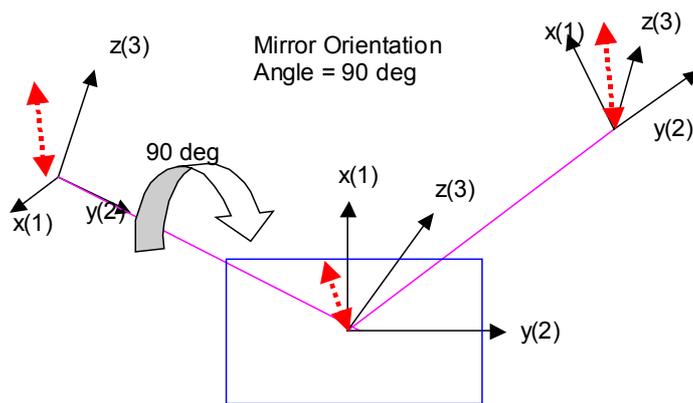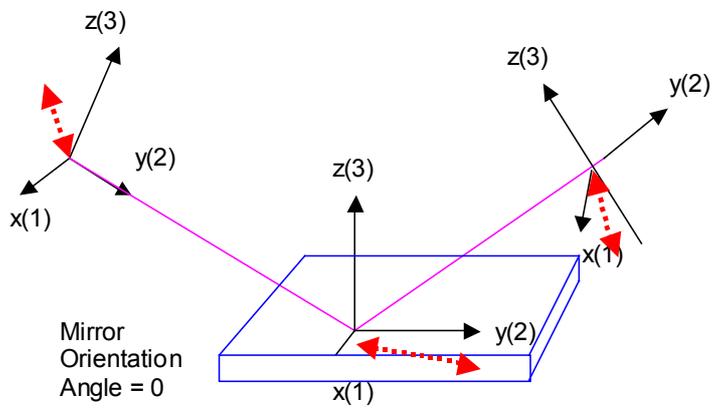
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- J.G. Chen, C. Welnak and F. Cerrina "SHADOW: s synchrotron radiation and X-ray optics simulation tool" Nucl. Instrum. and Meth. A347 (1994) 344-347
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